# A Greenhouse-Gas Information System Monitoring and Validating Emissions Reporting and Mitigation



Jet Propulsion Laboratory, California Institute of Technology

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*"Trust, but verify."*<sup>1</sup>

Cover page graphic: Harman G. Smith [Raytheon/JPL/Caltech], May 10, 2011

<sup>&</sup>lt;sup>1</sup> A Russian proverb famously and frequently used by U.S. President Ronald Reagan when discussing U.S. relations with the Soviet Union that, partly, motivated the present study.

# A Greenhouse-Gas Information System Monitoring and Validating Emissions Reporting and Mitigation

A report prepared for the DOE Office of Science

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# **Executive Summary**

Current GHG-mitigating regimes, whether internationally agreed or self-imposed, rely on the aggregation of self-reported data, with limited checks for consistency and accuracy, for monitoring. As nations commit to more stringent GHG emissions-mitigation actions and as economic rewards or penalties are attached to emission levels, self-reported data will require independent confirmation that they are accurate and reliable, if they are to provide the basis for critical choices and actions that may be required.

Supporting emissions-mitigation efforts and agreements, as well as monitoring energy- and fossil-fuel intensive national and global activities would be best achieved by a process of

- 1. monitoring of emissions and emission-mitigation actions, based, in part, on,
- 2. (self-) *reporting* of pertinent bottom-up inventory data,
- 3. *verification* that reported data derive from and are consistent with agreed-upon processes and procedures, and
- 4. *validation* that reported emissions and emissions-mitigation action data are correct, based on independent measurements (top-down) derived from a suite of sensors in space, air, land, and, possibly, sea, used to deduce and attribute anthropogenic emissions.

These data would be assessed and used to deduce and attribute measured GHG concentrations to anthropogenic emissions, attributed geographically and, to the extent possible, by economic sector. The validation element is needed to provide independent assurance that emissions are in accord with reported values, and should be considered as an important addition to the accepted MRV process, leading to a MRV&V process.

This study and report focus on attributes of a greenhouse-gas information system (GHGIS) needed to support MRV&V needs. These needs set the function of such a system apart from scientific/research monitoring of GHGs and carbon-cycle systems, and include (not exclusively): the need for a GHGIS that is *operational*, as required for decision-support; the need for a *system that meets specifications derived from imposed requirements*; the need for rigorous *calibration, verification*, and *validation* (CV&V) standards, processes, and records for all measurement and modeling/data-inversion data; the need to develop and adopt an uncertainty-quantification (UQ) regimen for all measurement and modeling data; and the requirement that GHGIS products can be subjected to third-party questioning and scientific scrutiny.

This report examines and assesses presently available capabilities that could contribute to a future GHGIS. These capabilities include sensors and measurement technologies; data analysis and data uncertainty quantification (UQ) practices and methods; and model-based data-inversion practices, methods, and their associated UQ. The report further examines the need for traceable calibration, verification, and validation processes and attached metadata; differences between present science-/research-oriented needs and those that would be required for an operational GHGIS; the development, operation, and maintenance of a GHGIS missions-operations center (GMOC); and the complex systems engineering and integration that would be required to develop, operate, and evolve a future GHGIS.

Present monitoring systems would be heavily relied on in any GHGIS implementation at the outset and would likely continue to provide valuable future contributions to GHGIS. However, present monitoring systems were developed to serve science/research purposes. This study concludes that *no component or capability presently available is at the level of technological maturity and readiness required for implementation in an operational GHGIS today*. However, purpose-designed and -built components could be developed and implemented in support of a future GHGIS.

The study concludes that it is possible to develop and provide a *capability-driven prototype* GHGIS, as part of a Phase-1 effort, within three years from project-funding start, that would make use of and integrate existing sensing and system capabilities. As part of a Phase-2 effort, a *requirements-driven, operational* GHGIS could be developed, within ten years from project-funding start. That schedule is driven by the development and long lead-times for some system components. The two efforts would be focused on different deliverables but could commence concurrently, to save time, if that was deemed desirable. We note that, developing and supporting an *operational* GHGIS will require a new approach and management, sustained funding and other support, as well as technical advances and development of purpose-built components that meet the requisite specifications.

A functioning GHGIS will provide the basis for reasoned choices on how best to respond to rising GHG levels, especially when proposed U.S. actions are compared with or conditioned on the actions of other nations. GHGIS will also allow for the independent assessment of the claims of others so that the United States can participate fairly and equitably in any process aimed at reducing GHG emissions.

The envisaged GHGIS will yield a host of benefits that extend beyond those of its primary intent. From a fundamental-research perspective, GHGIS will also provide an unprecedented wealth of Earth-science information. In addition, it will provide monitoring with new sources and methods that will yield country-level, regional, and sectoral information of value in a variety of contexts.

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# Preface

The national laboratories participating in this report maintain research and technologydevelopment activities on observational capabilities from space, air, and land, as well as on modeling and data analysis of such data aimed at greenhouse-gas top-down measurements. Some serve as centers of bottom-up inventory reporting repositories. Collectively, these activities pertain to monitoring, reporting, and verification (MRV) goals that augment other national and international efforts.

Each laboratory accepted the larger problem that motivated this study as more complex than any one laboratory or agency could manage alone. Starting in 2008, the Laboratories began a partnership in Global Change & Energy (GC&E) aimed at cooperatively contributing their experience, skills, and capabilities towards a national program. A greenhouse-gas information system (GHGIS) emerged as an important goal of the larger activity.

In order to better understand broader national needs and obtain insights from science leaders, two workshops on GHGIS were hosted. The first was on the Caltech campus (15-16 October 2008) and organized by NASA/JPL.<sup>1</sup> The second was held at DOE/SNL (20-22 May 2009).<sup>2</sup> These workshops brought together government, academic, and national-laboratory experts from many organizations and agencies to address issues related to the understanding, operational monitoring, and tracking of greenhouse-gas emissions and carbon offsets. Proceedings and findings from these workshops are available at the sites indicated in the respective footnotes.

On 1 September 2009, the Directors of the four partner Laboratories at the time: Charles Elachi [JPL], Thomas O. Hunter [SNL], Michael R. Anatasio [LANL], and George H. Miller [LLNL] met with DOE Undersecretary for Science, Steven E. Koonin, and staff at JPL, to discuss a path forward. The need for a scoping study was identified that would focus on critical emissions-monitoring means and needs, and would develop a set of recommendations to deliver an operational GHGIS system, should it be decided that one should be developed. This led to a proposal to DOE and the support that yielded this report.

These workshops and meetings were followed by discussions at national and international meetings, and a one-day meeting at DOE Headquarters on 3 February 2010 on monitoring, reporting, and verification (MRV), hosted by Undersecretary of Science Steven Koonin for DOE and Sherburne (Shere) Abbott for OSTP. Speakers, participants, and invitees in those workshops included representatives from the CEQ, DOE, EPA, NEC, NASA, NIST, NOAA, NSF, USDA, US Navy, US State Department, US Treasury, other agencies, representatives from academic institutions, and representatives of the partner Laboratories. Many subtleties and complexities relevant to MRV emerged from this valuable exchange, pointing the way to issues that will need to be addressed in due course.

<sup>&</sup>lt;sup>1</sup> http://climate.nasa.gov/Documents/GHG\_workshop\_report\_final\_revA.pdf

<sup>&</sup>lt;sup>2</sup> http://climate.nasa.gov/Documents/GHGIS\_Workshop2\_Report\_final-CL09-3451.pdf

The present study is an outgrowth of those discussions. It was undertaken by the four national laboratories who submitted a proposal (13 April 2010) to the DOE Office of Science for a scoping study on GHGIS.<sup>3</sup>

- Jet Propulsion Laboratory, California Institute of Technology [JPL/Caltech], of NASA, with Paul Dimotakis as the Caltech/JPL study Co-PI and senior representative to the GC&E partnership;<sup>4</sup>
- Sandia National Laboratories [SNL] of DOE, with Bruce Walker as the SNL study Co-PI and senior representative to the GC&E partnership;<sup>5</sup>
- Los Alamos National Laboratory [LANL] of DOE, with Karl Jonietz as the LANL study Co-PI and senior representative to the GC&E partnership; and
- Lawrence Livermore National Laboratory [LLNL] of DOE, with Douglas Rotman as the LLNL study Co-PI and senior representative to the GC&E partnership.

The proposal was accepted and the study was commissioned by US DOE Deputy Secretary, Daniel B. Poneman, and Undersecretary for Science, Steven E. Koonin. It was executed by Nick Woodward of the Office of Science, who also served as Program Manager. W. Randall Bell of DOE/NNSA provided program management assistance throughout the study, aided by Donna Smith. The four proposing laboratories are the signatories on the title page of this report and bear full responsibility for its contents.

In this study and effort, they were assisted by three other DOE national laboratories that have since joined as partners in the greater GC&E effort and are listed below.<sup>3</sup>

- Lawrence Berkeley National Laboratory [LBL] of DOE, with Marc Fischer as the senior LBL representative to the partnership;
- Oak Ridge National Laboratory [ORNL] of DOE, with Gary Jacobs as the senior ORNL representative to the partnership; and
- Pacific Northwest National Laboratory [PNNL] of DOE, with Charlette Geffen as the senior PNNL representative to the partnership.

In addition, assistance to various parts of the study and report was rendered by

• Earth Science Research Laboratory [ESRL] of NOAA, with James Butler as the ESRL point of contact.

<sup>&</sup>lt;sup>3</sup> The listing of the national laboratories here, as well as on the cover and title pages, is in order of accession to the partnership that was formed. PNNL and ORNL acceded on the same day and are listed alphabetically.

<sup>&</sup>lt;sup>4</sup> JPL/Caltech participated in the DOE-OSC study as a subcontractor to SNL through an agreement with the National Aeronautics and Space Administration. Paul Dimotakis, who served as JPL's Chief Technologist at the beginning of this effort, has since returned as a full-time member of the Caltech faculty, continuing his association with JPL as a Senior Research Scientist. Valerie Duval of JPL served as Manager for the JPL contribution to this study. Initially, Michael Gunson served as GC&E and GHGIS Program Manager at JPL, and interface to NASA. Anthony Freeman of JPL has since taken over responsibility for GHGIS.

<sup>&</sup>lt;sup>5</sup> The senior SNL representative to the GC&E partnership was, initially, James Peery, whose leadership and guidance in the initial stages of this effort are hereby gratefully acknowledged. Robert Huelskamp of SNL recently replaced Bruce Walker as the senior SNL representative and as SNL Co-PI to this study. In his SNL representation to this study and report, he has been aided by Ethan Blansett of SNL.

This study and report could not have been completed without the support of and assistance by all participants throughout, and their contributions, as acknowledged below and in sections of the report.

To frame the present study, it should be noted that significant on-going work is in progress on global carbon and GHG emissions monitoring by national and international monitoring, archiving, and reporting agencies, scientific programs and efforts, and frameworks that, for the most part, rely on bottom-up inventory reporting. These include (not an exclusive list):

- A. For the US:
  - a. the Energy Information Administration (EIA) of the DOE,
  - b. the Environmental Protection Agency (EPA),
  - c. the Carbon Dioxide Information Analysis Center (CDIAC), operated by ORNL for the US DOE that includes the World Data Center for Atmospheric Trace Gases,

and others.

- B. For Europe:
  - a. the European Environmental Agency (EEA) that also maintains the Emissions Database for Global Atmospheric Research (EDGAR),
  - b. as part of activities in support of the European Union Greenhouse Gas Emissions Trading Scheme (EU ETS),

and others.

- C. Internationally:
  - a. the United Nations Framework Convention on Climate Change (UNFCCC),
  - b. the International Energy Agency (IEA),

and others, including scientific-research institutions and organizations.

Further, the present study and report on GHG monitoring and a proposed greenhouse-gas information system (GHGIS) comes in the wake of and has benefited from a considerable body of previous related work and studies, by various agencies, groups, and scientific programs and research. These include recent related and relevant work, compilations, reports, studies and publications in the last 15 years, or so, by the IPCC (e.g., 1996, 2007, and other work), the National Academy of Sciences (e.g., NRC 2004, 2007, 2008, 2010a, 2010c, and 2010d), the UNFCCC (2005), Gurney et al. (2008, 2009), Prather et al. (2008), EDGAR (2009), Gregg et al. (2009), Marland et al. (2009), periodic reports and postings on emissions by the US DOE (2010), the US EPA (e.g., 2011), the IEA (2010), the World Meteorological Organization in support of the UNFCC (WMO 2010), Boden et al. (2010), Ciais et al. (2009, 2010), GCP (2010), the US OSTP (2010), the UNFCCC (2010), the JASON group (2011), and many others cited throughout the report.

This study derives from the discussions and exchanges in the workshops listed, and others, and draws on the collective experience and expertise offered by the partner national labs. It focuses on GHGIS attributes that set it apart from other GHG and carbon-cycle monitoring systems, such as (not an exclusive list):

- the need for a GHGIS that must be operational, as required for decision-support, and
- designed and implemented as a system that meets specifications derived from imposed requirements;
- the need to adopt and maintain rigorous *calibration*, *verification*, and *validation* (CV&V) standards and records for all measurement and modeling/data-inversion data; and
- the need for the GHGIS to adopt a rigorous uncertainty-quantification (UQ) regimen imposed on all measurement and modeling data to allow GHGIS products to be subjected to third-party questioning, as well as scientific and other scrutiny.

Representatives from partner laboratories contributed material for, and edited, all sections. A complete list of contributors is included after the Executive Summary. Lead chapter-authorship responsibilities are as listed below:

- *Chapter 1. Introduction.* Lead authoring responsibility by Paul Dimotakis [JPL/Caltech], with contributions by Douglas Rotman [LLNL] on the section on SF<sub>6</sub> top-down measurements, Gregg Marland [ORNL] on inventories, and other material by Tony Freeman [JPL/Caltech].
- Chapter 2. Requirements Framework. Lead authoring responsibility by Joshuah Stolaroff [LLNL].
- *Chapter 3. Spaceborne Sensing.* Lead authoring responsibility by Paul Dimotakis and Tony Freeman [JPL/Caltech].
- Chapter 4. Airborne Sensing. Lead authoring responsibility by Jared Dreicer [LANL].
- Chapter 5. Ground-Based Sensing. Lead authoring responsibility by Tom Guilderson [LLNL].
- *Chapter 6. Measurement Data and Uncertainty Quantification.* Lead authoring responsibility by David Higdon [LANL].
- *Chapter 7. Modeling and Modeling Uncertainty Quantification.* Lead authoring responsibility by Philip Cameron-Smith [LLNL].
- Chapter 8. GHGIS Mission Operations Center (GMOC). Lead authoring responsibility by Marcus Chang and David Gallegos [SNL].
- *Chapter 9. Systems Engineering and Integration.* Lead authoring responsibility by Ethan Blansett [SNL], with material on the Observation Systems Simulation Experiment (OSSE) approach contributed by Kevin W. Bowman [JPL/Caltech] and material on Sensor Network Reliability Modeling and Analysis by Jaideep Ray [SNL].

Chapter 10. Conclusions. Lead authoring responsibility by Paul Dimotakis [JPL/Caltech].

Appendix authors are as indicated in each one.

Editing for content and reconciliation across the report was the lead responsibility of Paul Dimotakis [JPL/Caltech]. Copy editing and document integration was the lead responsibility of Ethan Blansett [SNL], with extensive support from Barbara Haschke [Ktech] and Leona Van Ostrand [Ktech].

The participating Laboratories, authors of, and contributors to this report would like to thank the DOE Office of Science for providing the opportunity and support to undertake this work.

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# Chapter 1. Introduction

This is a report on the interagency scoping study commissioned by the Department of Energy (DOE) Office of Science, for an initial design framework of a greenhouse-gas information system (GHGIS) that will:

- 1. support monitoring of national emissions-reductions and the efficacy of renewableenergy programs;
- 2. provide information on compliance with existing emissions agreements;
- 3. assist in the negotiation of and provide actionable information on compliance with possible future emissions and climate agreements;
- 4. provide Earth-science data presently not available at adequate space and time scales, on a sustained and traceable basis; and
- 5. provide monitoring and other data, and analysis for many other purposes.

The intended product of the proposed GHGIS is a set of reliable validated estimates of anthropogenic GHG emissions, reconciling top-down (GHG measurement) data with bottom-up (fossil-fuel inventory) data. Borrowing from Appendix A that discusses inventory data:

Disturbance of the natural, global cycling of carbon among the atmosphere, biosphere, and hydrosphere has been driven by human activities that release carbon from geologic deposits of fossil fuels and that change the amount of carbon contained in plants, plant debris, and soils. Carbon is released to the atmosphere in both cases, principally as carbon dioxide ( $CO_2$ ) but also as methane ( $CH_4$ ). While it remains a scientific challenge to understand and quantify the impact of human actions on the carbon stores of the biosphere, it seems straightforward in principle, if not in fact, to inventory the amount of carbon released from the oxidation of fossil fuels.

The proposed GHGIS, if successful, will be seen as a gold-standard for the world and an important projection of US soft power in the coming decades. It will provide a vehicle for further international collaboration on Earth-system monitoring; anthropogenic GHG emissions and emissions-mitigation actions, and climate change; and a monitoring, analysis, and information tool for global economic and energy- and industrial-production activity for both decision and policy support, as well as for science.

The main customers of the proposed GHGIS are likely to be US decision and policy makers. They may elect to contribute some or all of the GHGIS data and analysis in support of scientific research and international GHG monitoring efforts.

As noted in the 2010 Office of Science and Technology Policy report (OSTP 2010) and as this document discusses, there is a need for an authoritative source for greenhouse-gas (GHG) emissions and their dynamics, for both the decision- and policy-support, and science communities. Today, uncertainties that are sometimes significant accompany GHG data both in information extracted from bottom-up (reporting) activities (cf. Appendix A), proxy methods (JASON 2011), and top-down measurements. These are the consequence of the complexity of processes from which they derive, the diversity and disparity of data sources and methods, the incomplete understanding of the amount of carbon sequestered in terrestrial ecosystems,

unregulated activities in certain economic sectors, and a host of science and other issues with measurement, reporting, and verification (MRV), or, perhaps, as the discussion below suggests, what should more appropriately be termed as MRV&V (& validation) efforts. If and when GHG emissions are subjected to significant regulation, possibly associated with penalties for emissions above agreed limits, strong economic motivations for under- or over-reporting will likely further complicate the MRV&V process.

As stated in the National Academy of Sciences (NAS)/National Research Council (NRC) committee report (NRC 2010a):

The committee's recommendations fall into three broad categories: (1) strengthening national greenhouse gas inventories, which will likely remain the core of a global monitoring and verification system; (2) improving the ability to independently and remotely estimate national, annual fossil-fuel  $CO_2$  emissions and to monitor emission trends; and (3) developing the capability to make accurate estimates of national  $CO_2$ ,  $N_2O$ , and  $CH_4$  emissions and  $CO_2$  removals from sinks from agriculture, forestry, and other land uses, and to independently check self-reported estimates of  $CO_2$  emissions from deforestation, reforestation, and forest degradation.

The need for measurements and monitoring is also noted in the OSTP report (2010, p. 4) that states,

If the nations of the world were to limit the use of fossil fuels, the right to emit carbon dioxide could become an increasingly valuable traded commodity. In such a world, observations of the location, amount, and rate of carbon dioxide emission into the air, as well as the stock and flow of all forms of carbon on land and in the oceans, will be needed to manage a global carbon market fairly and efficiently. Finally, we need observations to characterize the location, magnitude, and rate of climate change impacts to strike an ongoing balance between investments in adaptation, and building the new energy infrastructure and systems for a sustainable future.

Similar points are made in the World Meteorological Organization (WMO) (2010, Executive Summary) report for the United Nations Framework Convention on Climate Change (UNFCCC) that also notes the need for an open global forum for such data:

Observations need to be recognized as essential public goods, where the benefits of global availability of data exceed any economic or strategic value to individual countries from withholding national data. In short, observations underpin all efforts by Parties to the United Nations Framework Convention on Climate Change (UNFCCC) to mitigate, and adapt to, climate change.

The proposed GHGIS products will include decision-, policy-, and science-relevant GHG and related monitoring information and will be developed relying on integrating data derived from the implementation of the first and third recommendations in the NRC (2010a) report. GHGIS will be releasing products that can be used to monitor the success and compliance with existing agreements; help formulate and negotiate future collaborative efforts to reduce emissions, as well as agreements and treaties, assess and verify future treaty compliance; deliver science information to researchers to improve understanding of carbon-cycle dynamics; and advance predictive large-scale-modeling capabilities.

Users of GHGIS data will include policy makers and those charged with treaty negotiation and verification; scientists, agencies, and administrators for climate-change analysis, adaptation strategies and planning; and for monitoring energy infrastructure, energy-intensive, and fossil-fuel-use, and related economic activities. The science need for such an observing system is also identified by the WMO (2010, Executive Summary) report:

Full implementation of the WMO/IOC-UNESCO/UNEP/ICSU3-sponsored Global Climate Observing System (GCOS)—and the evolving climate information services it supports—is required to ensure that countries are able to understand, predict, and manage their response to climate and climate change over the 21st century and beyond. This Plan, if fully implemented by the Parties, will provide observations of the Essential Climate Variables (ECVs) needed to make significant progress in the generation of global climate products and derived information; it will also provide support for the research, modeling, analysis, and capacity-building activities required by all Parties to the UNFCCC, as well as underpin most of the data and information needs of the "Acting on Climate Change: The UN System Delivering as One" initiative. The Plan also addresses the need for observational records to improve seasonal-to-interannual climate predictions.

The proposed GHGIS will fuse traceable data from multiple sources and observation sensors with attached quality control (QC), quality assurance (QA), and data-integrity parameters and metadata, and perform sensitivity analysis (SA) and uncertainty quantification (UQ) on processed data. This compilation will be used to compare with bottom-up inventory data (Appendix A) that at present are characterized by a considerable level of maturity, even if with uncertainties that vary with the country to which reports apply.

GHGIS will aim to reconcile and assimilate such data with state-of-the-art present and future modeling capabilities to produce reports relevant to decision and policy support, Earth science, and for other US national and international purposes. These include, but are not limited to, environmental and energy security, adaption planning and monitoring, and economic activity.

# 1.1 The GHGIS Environment and Its Elements

One effect of GHGs can be characterized in terms of their global-warming potential (GWP) that is referenced to that of carbon dioxide (CO<sub>2</sub>), the primary GHG. Table 1-1 lists the significant GHGs of interest and their relative GWP, per molecule, relative to  $CO_2$  for the stated time period.<sup>1</sup> When these values are multiplied by the mass fractions of each GHG in the atmosphere, the global-warming contribution over the stated period of that gas can be estimated. The last column in Table 1-1 normalizes the third column to produce the estimated relative contributions listed from each GHG in the 2009 US emissions. The IPCC (2007) produced a similar compilation from global GHG emissions, by GHG species, based on 2004 data. These are plotted in Fig. 1-1.

<sup>&</sup>lt;sup>1</sup> The GWP is a measure of how much a unit mass of a GHG is estimated to contribute to global warming. It is a relative scale that compares the radiative-trapping of the gas to that of the same unit mass of carbon dioxide, which is chosen as a reference and whose GWP, as a consequence, is equal to unity. A particular GWP is calculated over a specific time interval, as indicated in Table 1-1, and takes the gas molecule lifetime in the atmosphere into account.

Table 1-1. Global Warming Potential (GWP) for greenhouse gases, 2009 US emissions, and their relative contributions of the respective emissions. Numbers derive from the US Environmental Protection Agency (EPA) (2011), with GWP values based on Intergovernmental Panel on Climate Change (IPCC) (1996) values.

Gas	100-year GWP	2009 US emissions (TgCO2eq)	Fractional contribution to global warming (weighted %)
Total		6640	100.0
$CO_2$	1	5508	83.0
$CH_4$	21	687	10.3
N <sub>2</sub> O	310	300	4.5
HFCs	140 - 11,700	125	1.9
PFCs	6,500 - 9,200	6	0.1
$SF_6$	23,900	15	0.2



Figure 1-1. Anthropogenic emissions contribution to GWP by GHG gas, based on 2004 data (IPCC 2007, Fig. TS.1b and 1.1b. Copyright by IPCC Secretariat, World Meteorological Organization, Geneva, Switzerland).

 $CO_2$  from fossil-fuel use, deforestation, decay of biomass, and other causes is responsible for the overwhelming contribution (~77%). This provides the reason why this study and report, and other reports cited, primarily focus on a system that will detect and attribute sources (natural and anthropogenic) and storage/sequestration of this gas, or other forms of carbon, in general, that can be oxidized to form  $CO_2$ . While not close to  $CO_2$  in importance, methane (CH<sub>4</sub>) is the next highest contributor by that metric (cf. Table 1-1 and Fig. 1-1) with projections that indicate an

increasing future role for this GHG. Methane is a more powerful greenhouse gas than  $CO_2$  than its GWP in Table 1-1 (IPCC 1996) may suggest. More recently, its 100-yr GWP was increased to 25 and its 20-year GWP to 72 (IPCC 2007, Table 2-14).<sup>2</sup>

A useful graphical representation that illustrates the dominant role of  $CO_2$  is offered by the US World Resources Institute and tracks use/end-use activities. It is reproduced in Fig. 1-2.<sup>3</sup>



Figure 1-2. US GHG emissions flow chart, from sectors to emissions by GHG, scaled by the GWP of each gas (CO<sub>2</sub>eq). Data based on 2003 values by the US EPA (2005). From http://www.wri.org/chart/us-greenhouse-gas-emissions-flow-chart.

Figure 1-2 helps illustrate two important points. First, it enforces the previous data and their depictions as regards the dominance of  $CO_2$  in its global-warming potential. Second, it highlights

<sup>&</sup>lt;sup>2</sup> Methane is oxidized in the atmosphere (CH<sub>4</sub> +  $3O_2 \rightarrow CO_2 + 2H_2O$ ; this is the composite reaction equation – the primary oxidation path in the atmosphere is via OH radicals and involves a large number of chemical reactions) adding to GHG mass by contributing 44/16 = 2.75 tons of CO<sub>2</sub> per ton of CH<sub>4</sub> (e.g., Smith 2009). While the product CO<sub>2</sub> GWP is of course lower, this factor is not taken into account in the current GWP calculation.

<sup>&</sup>lt;sup>3</sup> The following commentary derives from http://www.wri.org/chart/us-greenhouse-gas-emissions-flow-chart, where Fig. 1-2 is posted: Emissions data in Fig. 1-2 derive from the U.S. EPA (2005) *Inventory of U.S. Greenhouse Gas Emissions and Sinks: 1990-2003*. Allocations from "Electricity & Heat" and "Industry" to end uses are WRI estimates based on energy use data from the International Energy Agency (downloaded 2005). All data are for 2003. Calculations are based on CO<sub>2</sub> equivalents, using 100-year global GWP from IPCC (1996), based on total U.S. emissions of 6,978 MtCO<sub>2</sub>eq. Emissions from fuels in international bunkers are included under Transportation. Emissions from solvents are included under Industrial Processes. Emissions and sinks from land-use change and forestry (LUCF), which account for a sink of 821.6 MtCO<sub>2</sub>eq, and flows less than 0.1% of total emissions are not shown.

the complexity of attributing emissions to economic sectors, which GHGIS may be asked to deliver as part of its goals. Attributing to country, or sub-country, regions is equivalent to geographic attribution, i.e., attribution to the location of surface fluxes, for which data-/model-inversion techniques are best suited. Attribution to economic and other activity sectors, however, would require unraveling the intertwining of emissions from the same, or neighboring, locations by other criteria. This may well require the combination of top-down (measurement data) and bottom-up (reporting data) to succeed.

Other gases are also important in fossil-fuel combustion and GHG emissions, such as carbon monoxide (CO), which even though is not itself a GHG, accompanies (is co-emitted with) fossil-fuel and forest-fire emissions. It can be used to help distinguish between natural and anthropogenic fluxes and attribute atmospheric  $CO_2$  concentration measurements to anthropogenic sources.

An important motivation for the proposed GHGIS is the augmentation of present monitoring, reporting, and verification (MRV) environments and methodologies in support of actions that mitigate climate change and anthropogenic greenhouse-gas (GHG) emissions. It is proposed that GHGIS support this environment by reliance on (top-down) measurement data to allow an independent assessment and validation of bottom-up reported inventory data. This need is illustrated by a case study of emissions of sulfur hexafluoride (SF<sub>6</sub>), an important, accumulating (increasing-concentration) greenhouse-gas discussed below.

The value of an independent GHGIS system is demonstrated through monitoring, reporting, and verification (MRV) activities surrounding international agreements via the Kyoto Protocol to reduce the emissions of SF<sub>6</sub> (sulfur hexafluoride). As noted in Table 1-1, SF<sub>6</sub> is an important gas within the suite of gases addressed by the Kyoto Protocol because of its extremely high Global Warming Potential (GWP) estimated as 23,900 (cf. Table 1-1, IPCC 2007, and Forster et al. 2007). Natural emissions of SF<sub>6</sub> are negligible (e.g., Harnisch and Eisenhauer 1998) with the vast majority of the SF<sub>6</sub> atmospheric burden caused by its use as an insulation gas in high-voltage installations and various manufacturing processes (Ko et al. 1993, Maiss and Brenninkmeijer 1998, and Olivier et al. 2005). The wide use of SF<sub>6</sub> in energy and industrial processes and its function that is difficult to replace with other materials, provide a motivation for under-reporting its emissions.

Because  $SF_6$  emissions are anthropogenic and because of its long mean lifetime in the atmosphere (~3200 years, Forster et al. 2007), direct inferences of its global anthropogenic emissions from measurements of  $SF_6$  concentration and accumulation in the atmosphere are possible (Maiss and Levin 1994).

Figure 1-3 depicts observational data of global concentration measurements of atmospheric SF<sub>6</sub>. These display increasing growth of its concentration and, therefore, emissions during the mostrecent 8-year period, following a period of reduced growth after passage of the 1997 International Kyoto Protocol. The difference between the North-Hemisphere (NH) measurements and those in the Southern Hemisphere (SH, labeled as CGO for the Cape Grim Observatory) is the result of the combined effect of the NH contribution that comprises the vast majority of SF<sub>6</sub> emissions and the one-year inter-hemispherical transport rate. Figure 1-4 shows inferred global SF<sub>6</sub> emissions based on atmospheric observations, along with SF<sub>6</sub> emissions reported by the ANNEX-1 nations to the UNFCCC. Also shown are global emissions from the Emissions Database for Global Atmospheric Research (EDGAR) emission database (Version 4, EDGAR 2009) and the EDGAR emissions attributable only to ANNEX-1 countries. EDGAR emissions are determined by combining bottom-up accounting with inferred emissions from global observations (P. Tans [ESRL], personal communication).



Figure 1-3. Global observations of tropospheric  $SF_6$  concentration and inferred growth/emission rate (Rigby et al. 2010).

Comparing observation-inferred emissions to those reported to the UNFCCC indicates that by 2005, 2/3 of all SF<sub>6</sub> emissions are "non-reported" (Levin et al. 2010). This is partly because only developed (UNFCCC Annex-1) countries report in the current system. However, estimates of the relative distribution of emissions by country (through the EDGAR database) and atmospheric observations both suggest that SF<sub>6</sub> emissions estimates for the countries that do report are also too low, by about a factor of 2.

The top-down measurements in this example constrain the global picture in an important way. As discussed in this report, atmospheric-transport models, coupled with regionally resolved global observations, can enable assessments not only of global emissions, but also of their regional distribution. Such a capability would allow the inversion of observational GHG concentration data and their attribution to surface GHG-emission sources.



Figure 1-4. Observation-inferred global  $SF_6$  emissions (solid black, 1 $\sigma$  uncertainty range), compared to (dashed red) total EDGAR estimated emissions, ANNEX-1 only (green dash-dot) EDGAR emissions, and (blue diamond) UNFCCC reported emissions (Rigby et al. 2010).

As noted above and discussed in Chapter 5,  $SF_6$  emissions are almost exclusively anthropogenic, and  $SF_6$  emission sources are fairly well understood. Yet under-reporting of this substance is significant, possibly because:

- 1. of uncertainties in emission sources (Maiss and Brenninkmeijer 1998),
- 2. emissions from non-ANNEX-1 countries that are not required to report their emissions may be rapidly increasing (RHGDP 2008, Levin et al. 2010), and
- 3.  $SF_6$  leakage from electrical/power/industrial installations and use that may be underestimated.

Because of the near-indestructability of this gas, its very low solubility in water (negligible absorption by oceans), and the fact that it is not produced naturally,<sup>4</sup> it mostly accumulates in the atmosphere. The large discrepancy between  $SF_6$  emissions reported to international-agreement bodies and atmospheric measurements demonstrates, by way of example, the need for a coordinated, independent, global- and regional-scale top-down observation and monitoring system, capable of reporting reliable GHG data to validate bottom-up inventory reporting, or highlight variances.

<sup>&</sup>lt;sup>4</sup> As discussed in Chapter 5, fluorocarbons, such as sulfur hexafluoride (SF<sub>6</sub>), perfluorocarbons (PFCs), and hydrofluorocarbons (HFCs), listed in Table 1-1, have virtually no natural sources. So much so that, if detected in atmospheric absorption spectra of distant planets, when the atmospheric limb of those planets cross the line of sight between Earth and their star, for example, the detection would be accepted as strong evidence of a humanlike technological civilization there. These gases are (almost) inert chemically and (mostly) accumulate in the atmosphere when released, hence the need to regulate their production and use.

At present, no economic penalties are associated with the continued emission of  $SF_6$ . Further complications and discrepancies with self-reporting can be anticipated once/if economic advantage can be derived from emissions under- or over-reporting.

# 1.1.1 The GHGIS Concept and Goals

The GHGIS concept is in response to broad requirements that would need to be met to monitor, verify, and validate anthropogenic emissions and emissions-mitigation actions, as well as the need for improved Earth-system monitoring. Verified and validated monitoring would be of value to track compliance with the Montreal Protocol of 1989,<sup>5</sup> compliance with the Kyoto Protocol that came in force in 2005,<sup>6</sup> quantifying contributions of anthropogenic GHG emissions, supporting negotiations, implementation, and compliance-monitoring of future agreements, and for scientific and other monitoring purposes.

Comparisons of bottom-up and top-down estimates of ozone-depleting species are illustrated in Fig. 1-5 (Kim et al. 2010). Three regimes are indicated by these data:

- 1. Top-down and bottom-up emissions estimates for some ozone-depleting species can be in substantial agreement, i.e., within their respective uncertainty bounds.
- 2. Bottom-up emissions estimates for some gases can be significantly lower than those indicated by top-down measurements, e.g., HFC-152a, HFC-32, HFC-125, HFC-143a, and  $C_3F_8$ .
- 3. Bottom-up estimates for some gases may not be available at all.

Experience with international agreements indicates that effective implementation and compliance is enhanced if a reliable monitoring system is available. Specifically, agreements whose compliance is monitored and the monitoring results shared are found to be more likely to succeed. The operational monitoring system developed and implemented in support of the Comprehensive Nuclear-Test-Ban Treaty (CTBT) provides a useful example and template, and is discussed elsewhere in this report.

<sup>&</sup>lt;sup>5</sup> The *Montreal Protocol on Substances That Deplete the Ozone Layer* (a protocol to the Vienna Convention for the Protection of the Ozone Layer), an international treaty designed to protect the ozone layer by phasing out the production of numerous substances believed to be responsible for ozone depletion. The treaty was opened for signature on 16 September 1987 and entered into force on 1 January 1989.

<sup>&</sup>lt;sup>6</sup> The Kyoto Protocol is an international agreement linked to the United Nations Framework Convention on Climate Change (UNFCCC). The Kyoto Protocol sets binding targets for 37 industrialized countries and the European community for reducing greenhouse gas (GHG) emissions. The targets average 5%/yr against 1990 levels over the five-year period, 2008-2012. The major distinction between the Protocol and the Convention is that while the Convention encouraged industrialized countries to stabilize GHG emissions, the Protocol commits them to do so. Recognizing that developed countries are principally responsible for the current high levels of GHG emissions in the atmosphere as a result of more than 150 years of industrial activity, the Protocol places a heavier burden on developed nations under the principle of "common but differentiated responsibilities." The Kyoto Protocol was adopted in Kyoto, Japan, on 11 December 1997 and entered into force on 16 February 2005. The detailed rules for the implementation of the Protocol were adopted at COP 7 in Marrakesh in 2001, and are called the "Marrakesh Accords." Material in this footnote derives from http://unfccc.int/kyoto\_protocol/items/2830.php (downloaded on 31 March 2011).

Measurements and monitoring in support of GHGIS activities, analyses, and reports would bestow other benefits, as well, both to the international community, in general, and the US government and economy, in particular. To cite an example, GHGIS monitoring can target information useful to gauge the effectiveness of adaptation measures in response to a changing climate, such as the adoption of dry-land farming practices and energy use and efficiency of various economic sectors, not only for the US but also globally.



Figure 1-5. Top plot: Chinese emissions from the Kim et al. (2010) study, referred to as "this study" in the top legend, and other studies are shown in the top plot. Results from Vollmer et al. (2009) are mostly higher than from the Wan et al. (2009) and Kim et al. (2010) studies. Differences between Yokouchi et al. (2006) and Kim et al. (2010) reflect increases in emissions since 2005. Emissions estimated by EDGAR (2009) are mostly lower. Bottom plot: Chinese emissions as percent of global emissions. Figure from Kim et al. (2010, Fig. 2).

Important side benefits of the proposed GHGIS are scientific. Their value is difficult to gauge in its absence,<sup>7</sup> much as the International Monitoring System (IMS) and its scientific extensions yielded for solid-Earth dynamics, seismic analysis, improved understanding of intense seismic events, etc. However, as discussed throughout this report, GHGIS does not target a science product, even though its value to science is manifest and will be considerable. A scientific system will have different goals and requirements. By way of example and as discussed in Appendix A,

<sup>&</sup>lt;sup>7</sup> The aphorism that one cannot gauge the future success of a bridge by counting people swimming across a river seems apt here.

a large uncertainty at one point may be of great importance for monitoring some future treaty compliance, but may be of little importance if it represents a small spatial error in the global carbon-cycle and scientific-modeling framework.

As alluded to above, reliance to date on estimates of GHG emissions has primarily been on reported inventories, i.e., bottom-up or proxy data, as discussed in Appendix A. The value of the proposed GHGIS would be a *validation* of, at best, otherwise *verified* reports (the distinction will be discussed below), with extractable information derived from variances between the two, in excess of their relative uncertainty bounds. For example, assume that Country A, or Region B, or Sector C emissions levels  $E_{bu}$ , derived from bottom-up estimates, are reported and regarded to be reliable to within  $X_{bu}$ %, i.e.,  $E_{bu} \pm X_{bu}$ %. A future GHGIS system based on top-down (direct) measurements reports emissions levels,  $E_{td}$ , with quantified uncertainties  $X_{td}$ %, i.e.,  $E_{td} \pm X_{td}$ %. Information can be derived if variances in  $E_{td} - E_{bu}$  exceed a compounded uncertainty, such as  $(X_{td}^2 + X_{bu}^2)^{1/2}$ %, if the processes that lead to the two estimates are independent and characterized by errors approximately described by Gaussian statistics, for example.

Anticipated needs lead to a vision for the proposed GHGIS concept depicted in Fig. 1-6, as described in the proposal that led to this study and discussed throughout this report. As indicated in Fig. 1-6, the proposed GHGIS is a requirements-driven system. A challenge at this writing is that requirements are difficult to set and depend on the intended use of the GHGIS products, their accuracy (uncertainty) bounds, and, not least, the cost and schedule of the proposed GHGIS project development, along with projected operations and maintenance (O&M) costs. Thus, needs along with feasibility, cost, and other considerations will define a future GHGIS, should the decision be made to implement it. JASON (2011) recommended an overall accuracy target of  $\pm 20\%$  for the larger emitting nations, acknowledging differences that would arise between cooperative and non-cooperative countries and complications such as the fact that emission levels per unit land area span a wide range, and an accuracy target for CO<sub>2</sub> emissions from fossilfuel use better than  $\pm 20\%$  at the 90% confidence level. A requirements framework for the proposed GHGIS that would provide decision support and consequences of particular accuracy choices is discussed below and in detail in Chapter 2.

Major technical challenges for the proposed GHGIS derive from the need for the GHGIS projectdevelopment and management of:

- 1. the complexity, inhomogeneity in measurement density and quality, and disparity of sensors and their platforms;
- 2. the diversity of (types of) data and their sources;
- 3. the need for measurement data uncertainty quantification (UQ);
- 4. the need to discriminate anthropogenic from the larger-amplitude natural/biogenic GHG emissions sources (as illustrated in Fig. 1-7);<sup>8</sup>

<sup>&</sup>lt;sup>8</sup> Natural/biogenic carbon fluxes are (or were) in quasi-equilibrium (in the pre-industrial era), i.e., are positive and negative and balance in the mean. The anthropogenic fluxes of interest in the GHGIS context are much smaller (~5%), posing a CO<sub>2</sub> measurement challenge, for example, but are (mostly) of one sign (positive). Altering the balance of the much larger natural fluxes, even by small fractional amounts, e.g., through feedbacks, can lead to large changes in atmospheric GHG accumulation rates, posing a second major challenge emissions monitoring and to the proposed GHGIS, as well as to national and international emissions policies.

- 5. reliance on imperfect models whose results must also be accompanied by UQ; and, as documented in this report;
- 6. the *operational*, as opposed to a *science/research*, nature of the proposed GHGIS;
- 7. the development of and adherence to *calibration*, *verification*, and *validation* processes leading to reliable, acceptable GHGIS products and reports that can stand up to scrutiny; and
- 8. the system engineering and integration of a GHGIS that meets these requirements.



Figure 1-6. The proposed GHGIS concept.

An important, perhaps the most important, technical challenge of the proposed GHGIS derives from the environment in which quantitative assessments of GHG concentrations and anthropogenic-emissions estimates must be made, in the presence of natural processes characterized by much larger natural (bidirectional) fluxes. This environment presents not only signal-to-noise ratio (SNR) measurement challenges, but more difficult signal-to-"clutter" ratio (SCR) challenges that derive from the magnitude of the natural background levels and fluxes in the presence of which the assessments must be made. The issue is also noted in JASON (2011). An assessment can be gauged in the fluxes depicted in Fig. 1-7, derived from a graphic in Houghton (2007), with numbers estimated based on 2005 data.

The partition between natural/biogenic and anthropogenic emissions is complex. For example, coal-seam/coal-mine fires are underground smoulderings of a coal deposit, often in a coal mine. Such fires, once started, are difficult to extinguish. When a coal seam reaches the surface, such fires can be started by natural causes, such as lightning, grass, forest fires. They can also be started by human actions, such as accidents during mining operations. Because they burn underground, they are extremely difficult and costly to extinguish, and are unlikely to be suppressed by rainfall.<sup>9</sup>



Figure 1-7. Terrestrial carbon flux estimates. Numbers are in Pg (Gt) or Pg/yr (Gt/yr). Net uptake estimates are differences of large numbers that can change (positive feedbacks): the green (bottom, left) and blue rectangles (bottom, right) indicate net absorption by the land and oceans. The red inserts (top right) provide rough 2009 updates of the indicated numbers. Graphic based on Houghton (2007, Fig. 1), with annotations for updated numbers and net uptakes by land and oceans.

Internationally, thousands of underground coal fires are burning now. Global coal-fire emissions are thought to comprise 3% of annual CO<sub>2</sub> emissions, with estimates as high as 7-14% of annual Chinese emissions, for example (Litschke 2005). Hundreds of such fires are burning in the US, with more than 100 burning beneath nine states, most of them in Colorado, Kentucky, Pennsylvania, Utah and West Virginia, with many that go unreported (e.g., Cray 2010). Attribution of coal seam fires to purely natural or anthropogenic causes would be incorrect, yet

<sup>&</sup>lt;sup>9</sup> Some of the material on coal seam fires here derives from http://en.wikipedia.org/wiki/Coal\_seam\_fire, where more details and references are available.

they must be tallied, one way or another, and are important considering the fraction of total  $CO_2$  and other (e.g., mercury) emissions they are responsible for.

An important issue that will almost certainly influence future mitigation agreements and, hence, monitoring-system requirements, can be appreciated in terms of global carbon movements as a result of international trade. Figure 1-8 from Davis and Caldeira (2010) depicts estimates of the largest interregional fluxes of emissions embodied in trade from dominant net exporting countries (blue) to the dominant net importing countries (red). Fluxes to and from Western Europe are aggregated to include the United Kingdom, France, Germany, Switzerland, Italy, Spain, Luxembourg, The Netherlands, and Sweden. As Peters et al. (2011) note:

A challenge with a territorial-based emission accounting system in the context of a mitigation architecture is that connections between economies are not directly considered. In particular, international trade and investment flows provide a link between production and consumption in different countries. Ignoring these connections might result in a misleading analysis of the underlying driving forces of global, regional, and national emission trends and mitigation policies.

As these analyses indicate, tools and means exist to estimate such movements, albeit perhaps not by top-down means. Should it prove necessary, such information would be incorporated as one of the bottom-up data streams that GHGIS will likely need to take into account in support of future agreements. Alternatively and probably preferably, exporting/importing countries could be responsible for emissions from their territories, regardless, with any related cost/onus that is attached to their products. Such a regime would obviate tracking emissions as they "move" by trade across national boundaries.



Figure 1-8. The largest interregional emissions fluxes as a result of international trade (MtCO<sub>2</sub>/yr). From Davis and Caldeira (2010).

Further complications arise from  ${}^{14}C$ :  ${}^{12}C$  isotope-ratio analysis of CO<sub>2</sub> samples. These rely on the fact that  ${}^{14}C$  is added to surface carbon stocks (primarily) by conversion of N<sub>2</sub> in the
atmosphere through cosmic-ray action. The <sup>14</sup>C half-life of ~ 5700 years implies that carbon deep underground, e.g., from mined fossil fuels, is depleted of it (cf. discussion in Chapter 5 and Chapter 7). However, volcanic CO<sub>2</sub> can also be depleted of <sup>14</sup>C so the <sup>14</sup>C:<sup>12</sup>C ratio is not as definitive if volcanic plume gases contribute to samples.

While an initial prototype GHGIS implementation would likely be capability-driven, i.e., rely on the collation, reconciliation, and integration of data derived from existing sources and methods, and, perhaps, the fielding of additional presently available sensors, this study and report concludes that the top-down (measurement) elements available today that were developed for other, e.g., primarily science, purposes are insufficient for the task. New purpose-built sensors and systems will be needed to meet anticipated operational GHGIS goals and requirements, with accuracy and precision that meet specifications stemming from the system requirements, if they are to be of value.

In view of this reality, the present study concluded that a GHGIS development effort could/should be undertaken in two phases that are focused on different deliverables. A Phase 1 effort would deliver a *prototype capability-driven* GHGIS that integrates available data sources and analysis methods to produce the best reports based on such data. It is estimated that this phase could be completed within three years from initiation of adequate funding and the beginning of this development effort. A Phase 2 effort would deliver an *operational requirements-driven* GHGIS, within an estimated ten years after initiation and sustainment of adequate funding. As the Phase 1 and Phase 2 deliverables are different, the two efforts could start concurrently, with the Phase 2 effort benefitting from experience gained by the Phase 1 effort, as discussed in further detail in this report.

Estimates of the necessary funding levels to achieve these deliverables depend on requirements agreed upon by GHGIS developers and its customers. Absent such agreements, meaningful estimates cannot be arrived at. Studies that would estimate such costs parametrically are possible, e.g., cost vs. performance, but such analyses are complex and beyond the scope of the present study and report.

#### 1.1.2 Estimating Surface Fluxes from Concentration Measurements

While it is possible to measure a local GHG species flux directly, e.g., by simultaneous measurement of its concentration (or mass fraction) and the three-dimensional velocity field at the same location, what are (and will be) typically measured are GHG concentrations in the atmosphere, even though what are sought are (anthropogenic) emissions from Earth's surface. The deduction of the latter from the former makes use of the species transport equation, augmented by the equations of motion of atmospheric flow.

As discussed in the proposal that led to this study, further in this chapter, and throughout this report, the total uncertainty in the final estimates is a composite of errors and uncertainties in measurement data as well as errors and uncertainties introduced by the data-inversion process that makes use of atmospheric-transport and other modeling. Quoting from the JASON (2011) report that also brings this issue to attention (square brackets ours),

... the performance of a measurement system for  $CO_2$  emissions (fluxes) depends both on the [quality of the] concentration measurements themselves and on what is called the "model inversion" [used] to go from the measured concentrations to the derived emissions.

The theory for performing this estimation is described in Appendix B. The *calibration*, *verification*, and *validation* processes, as applied to the methodology that provides these estimates, are described below and in Appendix C. As also discussed below and throughout this report, UQ must accompany all quantities that contribute to these estimates, ranging from UQ of measurement data (cf. Chapter 6) to UQ of the results of models used for these inversions (cf. Chapter 7). Appendix B also describes an approach that can be used to infer surface fluxes with an uncertainty that can be quantified and is traceable to that of the measurement data accuracy (and spatio-temporal resolution) and that of the wind field, albeit requiring a high measurement density in areas of significant interest.

#### 1.1.3 Top-Down Data and Modeling

The vision for the GHGIS sensing system is to rely on a suite of sensors whose output measurement data are fused and reconciled, and acquire attached estimated UQ metadata as part of the data-analysis step in the process. These data are provided as inputs to the modeling and data-inversion part of the process that combines these with other data and prior models of surface emissions to infer surface emissions sources, as discussed above and in Chapter 7. Distinguishing the anthropogenic from the natural/biogenic portions occurs largely in this step.

## 1.1.4 Bottom-Up Data

As discussed in Appendix A, bottom-up data derive from a large variety of sources and estimates of emissions on the basis of inventories of direct and indirect indicators, such as fossil-fuels used, night lights, population density, reporting by countries and economic sectors, etc. These data can exhibit small or large inconsistencies and uncertainties that lead to uncertainty estimates of  $\pm 5\%$ , for country-level reports for some of the more developed countries, but perhaps as high as  $\pm 16\%$ , or more, for local emissions estimates (cf. Appendix A). Uncertainties can be as large as  $\pm 15-20\%$  for some large emitters, such as China (e.g., Gregg et al. 2008), and possibly larger, especially for some smaller emitters (G. Marland [ORNL], private communication).

Bottom-up data compilations have been proceeding for some time, in support of international reporting agreements and for other reasons. However, estimated uncertainties in these figures are primarily the result of reconciliation between different reporting estimates and verification of the adherence to reporting standards and methods, and while perhaps providing the best emissions estimates available today, they are characterized by large variances in their estimated uncertainty levels depending on country, sector, year, etc.

A complication that arises is how one counts and where the separatrix between bottom-up and top-down data lies. By way of example, bottom-up inventory data can take into account measurements from sensors installed on power-plant stacks to improve estimates. For the purposes of GHGIS and as an operational definition, top-down data will be assumed to derive from GHG and other gas measurements taken after discharge into the atmosphere, i.e., some distance from exhaust stacks, for example.

Should a given country agree to reduce its GHG emissions, it may consider itself free to pick the base year against which to judge progress, even though the Kyoto Protocol prescribes the base year. Since reliable data on anthropogenic emissions for prior years is lacking, such a baseline will itself need to be estimated and will therefore be potentially subject to inaccuracy or manipulation. Furthermore, some nations declared their intent to reduce emissions on a per-capita or per-unit-GDP (Gross Domestic Product) basis relative to a baseline year. Since population and GDP are at best estimates (even US quarterly GDP figures are subject to significant revision in later quarters), these and additional uncertainties will complicate the analysis task.

#### 1.1.5 Top-Down/Bottom-Up Data Reconciliation

An important part of the GHGIS function is to reconcile bottom-up and top-down emissions data. As the  $SF_6$  emissions example illustrates above, there can be surprises that while almost certainly will not be as large for fossil-fuel emissions from developed countries as in that example, economic stakes of over- or under-reporting can be very large if future emissions agreements come in force, as the OSTP (2010) report notes and as discussed above. For the bottom-up/top-down reconciliation and comparison to be meaningful, uncertainty estimates between the two data streams must become comparable, placing a lower bound on requirements for the top-down-based GHGIS product. See also Chapter 2.

## **1.2 Requirements Framework**

No requirements for the quantification of anthropogenic emissions were set for this study and, perhaps, none can be set at this time. As a consequence, this study was conducted targeting, in part, the definition of a requirements framework. The actual framework would be defined as requirements are dictated by agreements, or for other monitoring purposes, from which specifications would flow.

Chapter 2 discusses a requirements framework that would be dictated by the need to detect, monitor, and ascertain *changes* in anthropogenic emissions over time. As intimated in parts of the discussion above and also throughout the report, this is somewhat less challenging than determining absolute emission levels. The weather and change in the weather are indicated by *changes* in barometric pressure, rather than *absolute* barometric pressure, which may be high, or low, for a variety of reasons.

Three important issues arise as regards requirements and derived specifications, which in combination will challenge a future GHGIS further.

Barring unforeseen circumstances such as global catastrophes,  $CO_2$  concentrations may well rise to twice their pre-industrial values, i.e., to values as high as 560-580 ppmv. Anthropogenic emissions at present add, approximately, 2 ppmv of  $CO_2$  per year. The annual increase may rise further before emission-mitigation measures, if not fossil-fuel costs/shortages and the development of alternative energy sources, improved energy efficiency, and new legal/regulatory environments start to bring new energy technologies within economic competitive reach, and start decreasing emissions. At present, annual  $CO_2$  emissions add about 2/380  $\cong$  0.5%/yr to global background concentrations. Even if the addition of 2 ppmv per year continues until the 560-580 ppmv levels are reached, fractional annual anthropogenic additions will drop to  $2/570 \approx 0.35\%/yr$ , rendering the top-down signal-to-background challenge even greater.

Second, however, if emissions-mitigation measures succeed, and anthropogenic emissions decrease by 80% of present levels, as some are suggesting, i.e., if they drop to 20% of present levels by the time a 570 ppmv level is reached, they will comprise 0.07% of background. While sensing technologies, modeling methodologies, and system integration would also evolve in parallel, such a signal-to-background ratio would render the goals of GHGIS daunting.

Third, GHG emissions may decrease over time. This may happen for any of a number of reasons, such as increasing cost/scarcity of fossil fuels, increasing cost-competiveness of alternative/renewable energy sources, a changing legal/regulatory environment, because climatic changes render this imperative at some time in the future, or for any combination of these (not mutually exclusive causes). If anthropogenic GHG emissions decrease by something like 80%, as some have called for, while accumulation has increased to the values above, then the anthropogenic signal will be even harder to discern amidst the background concentration levels. This makes the top-down challenge truly daunting and the requirements needed for a future GHGIS are not addressable any time soon. Most likely, then, there would be time to respond to evolving requirements. This issue was not addressed in our study and this report.

## 1.3 Measurement Data

The proposed GHGIS relies on measurement data from a suite of sensor subsystems to provide the top-down information, as described above (cf. Fig. 1-6, for example). These differ in the platforms that carry them, which determine many of their sampling characteristics, as well as the measurement instrument types (e.g., grating vs. Fourier-transform spectrometers for remote sensing) and technologies employed. The observational mix and the need and challenge for data fusion is noted in the OSTP (2010) report that states,

Observations are taken from space, and within the Earth system (in situ), from the air, in the water, and on and below the land and the oceans. They are measured by sensors and by people. The data they provide are interpreted, interpolated, and integrated. The myriad of observations taken today vary widely in purpose and scope and are appropriately distributed among hundreds of programs under the purview of Federal agencies and other institutions and individuals. To a large degree, these observations have been only loosely coupled, coordinated, and integrated, although there are notable exceptions such as the Global Energy and Water Cycle Experiment (GE WEX). GE WEX successfully integrates activities both nationally and internationally to better observe, understand, and model the hydrological cycle and energy fluxes in the Earth's atmosphere and at the surface, providing a great example of what can be done. The leap forward can only be achieved with a synergy between remotely sensed and in situ observations supported by robust, interoperable data systems that allow for long-term access and archive as well as the opportunity for long-term monitoring and assessment of status and trends. Increasingly, this promise is being realized, and seemingly disparate observations are combined in new ways to produce benefits across multiple societal areas. This recognition has led to the concept of an integrated Earth observing system as articulated by the U.S Group on Earth Observations (USGEO).

Generally, sensing and measurement specifications can be in response to different requirements, such as:

- 1. *Detection*: Can non-compliance be detected? Are proscribed or otherwise interesting gases being emitted?
- 2. *Attribution* to sources: Where are GHG and other gases emitted from?
- 3. *Quantification of concentrations and their uncertainties*: How much and how well do/can we know space-time resolved amounts (concentrations) in the atmosphere?
- 4. *Quantification of emissions and their uncertainties*: Where/what are the natural and anthropogenic GHG emission sources and rates?
- 5. *Quantification of offsets*: Are they because of actions in response to treaty obligations, would they have occurred anyway for other anthropogenic/economic reasons, or are they a result of natural variation, either induced or spontaneous?
- 6. *Quantification of baselines*: What are the baselines to be used in verifying an X% reduction in emissions?
- 7. *Reconciliation* between: Top-down data sources and top-down and bottom-up data.

As discussed above, data-inversion and attribution analyses need to rely on measurement samples captured/recorded at multiple points in space, at multiple times. Ground-sensor towers are the least expensive but must be deployed one per measurement site. Airborne platforms are more costly to operate, but are, or may be, also platforms of opportunity if hosted on aircraft that fly anyway. Space offers the most costly option per sensor. However, a single space sensor can provide global spatial coverage over time, if designed to do so. Determining cost-effectiveness can only be performed in a system sense, when all the considerations that are needed to produce the GHGIS products are taken into account.

Finally, the proposed GHGIS would likely target a tiered capability and end-use, i.e., international, select bi-/multi-lateral, and US-only, and requirements and specifications for each of these may differ.

The brief summary below is classified according to measurement platforms. Detailed discussions for each are included in topical chapters in this report.

#### 1.3.1 Spaceborne Sensing

Space provides an important arena for sensors for several reasons. Orbit choices can be made to control the atmospheric sampling that the sensor can provide. See Chapter 3 for a detailed discussion. Briefly, instrument and data-retrieval choices can determine which gas, or gases, are measured, their horizontal resolution, the vertical-sampling profile, and measurement precision/accuracy. There are also orbitology choices offered regarding ground-spatial resolution for a given collecting aperture, dwell time over the target area that could allow time-dependent data to be recorded, revisit frequency if not in a geostationary orbit, etc. By way of example, using passive IR sensing, the NASA AIRS instrument on the AQUA spacecraft returns, approximately, 15,000 verified  $CO_2$  concentration measurements per day, averaged over  $100 \times 100 \text{ km}^2$  ground pixels, i.e., roughly one quarter of what would be required to tile Earth at

this resolution, with a peak vertical sensitivity in the mid-troposphere.  $CO_2$  concentration precision and accuracy from this spaceborne instrument have been validated to be in the range of 1-2 ppmv. Other measurement choices are based on reflected sunlight (OCO-2, expected to fly in February 2013) and active methods (e.g., LIDAR) that are under consideration. Chapter 3 and Appendix C discuss other horizontal and vertical sampling options and choices.

Importantly, space provides an arena for which there is no denied access; an important factor considering that nations may decide they will not allow ground, or airborne sensors on, or over, their sovereign territory.

## 1.3.2 Airborne Sensing

Aircraft platforms can be used in two ways. The first is as hosts for in situ sensors that measure the concentration of select (GHG or other) gases in aspirated air, i.e., measurements of the air through which the aircraft platform flies, while the second is as remote-sensing platforms. These are discussed in Chapter 4 and Appendix F, respectively.

In situ aircraft sensors can exploit technologies developed over the years, primarily for in situ ground sensors that have been ruggedized for and interfaced to aircraft. These can return accuracies in  $CO_2$  concentration measurements in the range of 0.1-0.2 ppmv. Remote-sensing measurement technologies for airborne sensors are similar to those relied upon for space.

Airborne sensors can rely on continuous sampling and measurement technologies, or store aspirated air in flasks for more precise and sophisticated measurements, such as carbon-isotope measurements that provide an important criterion in discriminating between natural/biogenic and fossil-fuel sources of  $CO_2$ , as discussed in Chapter 5.

An important attribute of airborne sensors is that they can exploit the very dense flight patterns of aircraft trajectories. While measurements recorded at cruising altitudes may not be directly linkable to ground-surface emission attribution, frequent take-offs and landings in almost all parts of the world provide potentially important sampling opportunities within the planetary boundary layer (PBL), globally. A European effort (IAGOS) has been underway for some time that measures gas concentrations as part of a suite of meteorological measurements, world-wide. Aircraft can employ various altitude flight patterns to yield important vertical-profile and other in situ information to validate space-borne sensor data and calibrate/validate ground-based sensor data.

## 1.3.3 Ground-Based Sensing

Ground sensors and sensing technologies are discussed in Chapter 5. They have been under development and used for some time and represent the most mature GHG and other gasmeasurement technology components. Accuracies for such sensors are in the 0.1-0.2 ppmv range. Ground sensors are typically located on towers that could be quite high and sense at more than one height above ground-surface. These can provide vertical-profile data that help quantify planetary boundary-layer behavior, such as height, as well as data both below and above its ceiling, depending on its height, the time of day, topography/orography, and wind-field characteristics. While situated on a fixed tower, or other structure, ground sensors can sample different air parcels depending on their height above ground and on wind speed and direction, as discussed in Chapter 5, and Appendices B and C. As with airborne platforms, ground sensors can provide data on a continuous basis, or aspirate discrete air samples in flasks for subsequent analysis, such as for carbon-isotope measurements.

#### 1.3.4 Seaborne Sensing

This study concluded that  $CO_2$  exchanges between the atmosphere and the sea are important in many contexts. Sensing over oceans is also important in a global carbon-budget sense: oceans release to and absorb from the atmosphere a significant fraction of  $CO_2$ , as illustrated in Fig. 1-7 and discussed in context above. However, most anthropogenic emissions, by some margin, are on land. As a consequence, this study focused on ways best suited for such sensing. Further, sensing ocean-surface GHG activity with in situ sensors is not a mature technology at this writing and while it may prove important in the future and may provide important access to a country's emissions, if downwind, perhaps located off the country's coast, it did not rise to the level of the other three sensing modalities. This assessment can be reviewed in the future as system-integration considerations may indicate the need for select sensor deployment either on ships or on buoys.

# 1.4 Data Uncertainty Quantification

All data and derived numbers leading to GHGIS products must be accompanied by quantified uncertainties, if they are to serve the GHGIS purposes. Complexities arise because of the variety and diversity of sensor data, incommensurate uncertainties, sampling characteristics, and other considerations. Such data must be fused from all sources with attached UQ to provide input to analysis and data inversions downstream of that part of the process. These issues are discussed in Chapter 6 and represent one of the major challenges of the proposed GHGIS.

# 1.5 Modeling and Modeling UQ, Model-Based Data Inversions, and Attribution to Sources

The span of physical spatial and temporal scales that participate in atmospheric transport, ranging from centimeter-size viscous scales to thousands of kilometers of geophysical scales, makes a *direct numerical simulation* (DNS) of the fluid-dynamic equations of motion a challenge that cannot be met either today, or in the foreseeable future. Matters are further complicated by the interaction and exchanges of atmospheric air with complex orography that can induce local changes in wind direction and magnitude, as well as the nature of the ground surface, the sea, including disturbed seas, clouds and rain, and atmospheric chemistry. Not all of these interactions are known sufficiently well today to represent in numerical codes. Capturing the multi-physics processes and dynamics that contribute over the full range of scales in their detail is, thus, infeasible. Models can numerically resolve only a small fraction of the dynamic range of scales that contribute to transport, dispersion, and (molecular) mixing of GHG and other atmospheric species, as well as scales governing their interactions with Earth's surface. That necessitates abstractions, approximations, and modeling to represent dynamics and interactions

that cannot be resolved by computer codes that can generically be referred to as subgrid-scale (SGS) modeling.

An attempt to address this issue can be based on one of several approaches, or a combination of approaches. When explicit, a numerical model represents unresolved dynamics in terms of resolved quantities by embedding additional physics and assumptions. When implicit, it is based on the expectation that as long as fundamental quantities such as mass, momentum, energy, species, etc. are properly accounted for and conserved in the numerical simulation and the important physical processes are well represented, then contributions by unresolved dynamics can be ignored as an adequate approximation. In practice, models combine the two approaches, leaning more towards one end or the other, depending on implementation details, as well as available computational resources and required time-to-solution.

If the resolved scales were small enough, the second approach could be adequate, at least in the limit. However, models that simulate global transport cannot resolve scales below tens of kilometers, often not below 100 km (approximately, 60 nautical miles, or one degree of latitude), and no less than about 50 km in a code used in a production mode today. Spatial resolution in regional models is sometimes as fine as 10 km, or less, but such models must also address the challenge of inflow, outflow, and initial conditions that must be provided by other means.<sup>10</sup> Even at such grid resolutions, processes fundamental to atmospheric dynamics and transport must be modeled rather than directly simulated. These considerations dictate reliance on approximations in which the dynamics of complex processes are parameterized, i.e., (often) modeled by *ad hoc* relations with embedded adjustable constants, called *parameterizations*.

These fundamental challenges lead to the discussion in Chapter 7 on modeling that indicates that modeling and data-inversion methodologies, at least using presently available capabilities, are expected to contribute the preponderant fraction of estimated uncertainties in attributed local anthropogenic emissions by GHGIS. Appendices B and C include additional discussion in the context of estimating surface sources from atmospheric concentration measurements and attendant calibration, verification, and validation challenges.

# **1.6 GHGIS Missions Operations Center**

All GHGIS data from top-down measurements, modeling, and inversions will be stored and archived in the proposed GHGIS Missions Operations Center (GMOC). The GMOC will also perform the reconciliation with bottom-up and other all-source data, and be responsible for monitoring the operational and readiness status of all GHGIS components. It will also be responsible for tracking and assuring data integrity and security, and for overall cybersecurity of the computing, storage, and network components. The GMOC is discussed in Chapter 8.

<sup>&</sup>lt;sup>10</sup> A factor of 2 increase in spatial resolution imposes a factor of 16 increase in computational burden:  $2^3$  because of the 3D space and an additional factor of 2 because (in explicit codes) time steps must also be cut in half for numerical stability (CFL condition). The computational effort and computing resources required for a numerical simulation on a 100 km grid and the same simulation on a 100/8 = 12.5 km grid is  $2^4 \times 2^3 = 2^7$ , i.e., over *one hundred* times smaller. Capturing cloud dynamics or the effects of complex orography, for example, would require grid resolutions considerably less than 1 km.

# **1.7 Systems Engineering and Integration**

The need for data fusion, quality control, and integration was noted in the OSTP (2010) report that states,

In order to achieve the synergies and benefits of an integrated system of observations, USGEO identified the following needed elements.

- 1. A sustainable observing system of systems that focuses on enabling useful products for decision-makers and is achieved through a flexible, yet disciplined approach in coordination with all partners;
- 2. Data systems that utilize common data formats and information protocols for easy, timely, information sharing and system interoperability; and
- 3. Quality-control systems that ensure accurate, long-term data records for important environmental and climate parameters.

These elements collectively form the basis of the Global Earth Observation System of Systems (GE OSS), a multinational effort working to realize a future wherein decisions and actions are informed by coordinated, comprehensive, and sustained Earth observations and information.

These points were also discussed in the context of data UQ, above, and further below and throughout this report.

The complexity of the proposed GHGIS dictates a systems approach from the beginning. While, as discussed above, the proposed Phase 1 effort targets the delivery of a prototype system that is capability driven, the proposed Phase 2 effort will target delivery of the first operational prototype, with sensors and components purpose-designed and developed to meet specifications in a system sense. The systems engineering component of GHGIS will assess trades, such as the decision between more ground sensors, vs. new purpose-built space sensors, or the density of required measurements when assessed against the fidelity of existing and purpose-built models and codes. The systems engineering part of the proposed GHGIS is discussed in Chapter 9.

# 1.8 Calibration, Verification, and Validation

The proposed GHGIS must provide data and reports on anthropogenic emissions and emissionsmitigation actions, with quantified uncertainties, that can stand up to scrutiny by both scientists and policy analysts. This necessitates the adoption of rigorous processes in its operations that support a *calibration*, *verification*, and *validation* (CV&V) regime *for all GHGIS components*, in particular, a CV&V regime that would apply to the components listed below (not an exhaustive list):

- the design and implementation of GHGIS sensors and their maintenance, and of other sensors and measurement systems that provide, or may provide, data on which GHGIS relies;
- GHG concentration and other data analysis and retrieval from direct measurement data, and their quality tagging and tracking;

- sensor subsystem operating software, version and updates control, and quality tagging and tracking;
- data QA/QC and UQ;
- modeling and data inversion, and version and updates control; and
- GHGIS products and reports.

While a CV&V policy and process regime will apply somewhat differently to each component, all components share common considerations and criteria by which GHGIS must abide. Definitions for the three terms are summarized below and used throughout the report. They sometimes vary according to context, purpose, and sources, and are not uniformly interpreted by others. These definitions are familiar to the DOE/NNSA ASCI and ASC programs that were largely responsible for their development, adoption, and extensions to modeling.

*Calibration* refers to the process that leads to the adjustment of constants, parameters, and models, such that the output of a particular component matches, to the extent possible, the representation of reality the component targets. This relies on comparisons with the reality to be matched and must be performed correctly, reliably, and be documented, both for sensors that are purpose-built for GHGIS, or ones operated for other purposes, as well as for data analysis, interpolation and reconciliation, models and data-retrieval methodologies, etc.

*Verification* refers to the process that, if successful, ascertains that the hardware and software suite that is part of an instrument, sensor system, data analysis and its uncertainty quantification process, model and data inversion/retrieval process, etc., are consistent with and conform to the intended design of those components. In the case of hardware, a verification step would assert that the hardware has been built as designed and intended. In the case of software that operates an instrument, spacecraft, etc., a verification step would assert that the code that implements the logic and logic-sequence requirements does so correctly, i.e., inter alia, asserting that the software has no "bugs". In the case of a numerical model, such as an atmospheric-transport model that would be relied upon to attribute GHG concentration measurements to (anthropogenic) GHG surface sources, successful verification would assert that the fundamental equations of motion embedded in the model are correctly and consistently solved by it, i.e., that the code/model, "solves the equations right." In practice, of course, one can never be certain that verification is complete, so an incomplete operational practice of subjecting a sensor, data-analysis process, or code to a suite of finite verification tests must be adopted, as discussed in Appendix C.

Ideally, *validation* must await successful verification and refers to the process that ascertains that the hardware and software suite that is part of an instrument, sensor system, data analysis and its uncertainty quantification process, or model and data inversion/retrieval process, etc., performs the intended task successfully and achieves the intended goal, when compared with (known) reality. In the case of hardware, a validation step would assert that what was built as designed, i.e., what was verified, achieves its measurement or other objectives, within required uncertainty bounds. In the case of software that operates an instrument, spacecraft, etc., a validation step would assert that code that was verified, per above, achieves the intended goal, e.g., that the software specifications that were verified to have been met are correct. A piece of software can

be "bug-free" but fail to deliver on its intended goal, if the algorithmic, or logic, or logic-sequence functions were incorrectly specified.

In the case of a numerical model, such as an atmospheric-transport model relied upon to attribute GHG concentration measurements to (anthropogenic) GHG surface sources, successful validation would assert that the fundamental equations of motion embedded in the model were verified to be correctly and consistently solved by it, and simulate reality as it is best known, *without any further adjustments*, i.e., that the code/model, "solves the right equations."

In simple terms, in the context of codes and modeling, verification is the process for determining if the equations, logic, etc., were coded correctly and validation is the process for determining if the correct equations have been solved; the word *process* should be stressed here because one is never done in these exercises.<sup>11</sup>

We add here that models that cannot be verified, i.e., models that do not successfully pass the verification test suite, can still be useful. As noted in Appendix C, most weather models used today are not likely to pass these tests, yet they usefully forecast weather for us. The special (and perhaps new) challenge for GHGIS is the need for traceability of the uncertainty quantification that must accompany all numbers. Future models that are relied upon for data inversions, as described above, in Appendix B, and in greater detail in Chapter 7 on modeling, may well need to pass all of these tests, if GHGIS is to deliver quantified uncertainties in its reports.

In the context of monitoring, reporting (of bottom-up data), and verification (MRV) in support of climate and emissions agreements, the *verification* part describes those activities aimed at ascertaining that the reporting and reported results are consistent with agreed processes. From the vantage point of the definition offered above, *verification* implies that the results are the product of a correct implementation of the agreement.

Reported bottom-up numbers are, presumably, *verified*, in this sense, but not *validated*, i.e., not confirmed by reality as captured by independent (top-down) measurements. The important example of  $SF_6$  emissions discussed above illustrates the point. As a consequence, while an agreed-upon process may have been followed in generating the reports, adherence to that process offers no guarantees that its reports are correct, i.e., that they represent reality. Variances may either arise because of misreporting that is a consequence of errors of omission, or errors of commission. As noted in a recent report:<sup>12</sup>

It is already an agreed principle (since the Bali meeting) that any international agreement on climate change must be monitorable, verifiable, and enforceable. Such a treaty is bound to have immense economic impact, and with that there is bound to be a high incentive for cheating on the behalf of at least some signatories. Even where signatories intend to be in compliance, and actually believe themselves to be in compliance, there are cases where faulty or dishonest internal reporting leads central authorities into error. The President will need the highest quality information available in order to make sensitive decisions about compliance by other parties.

<sup>&</sup>lt;sup>11</sup> J. Peery [SNL], private communication.

<sup>&</sup>lt;sup>12</sup> This passage derives from the (unclassified) appendix to the CIA/MEDEA report, (U) *The Contribution of National Security Systems to Understanding Global Climate Change. Phase I Final Report* - Volume II. The GHGIS study team did not have access to the full report.

# 1.9 Concluding Remarks

In the context of the proposed GHGIS concept and goals, the study team recommends that a more appropriate approach to supporting climate and emissions-monitoring and -reduction agreements would be captured by a process best described as one of *monitoring*, *reporting*, *verification*, and *validation* (MRV&V), as proposed by the study team in the February 2009 interagency meeting on monitoring emissions, forests, land-use, and carbon stocks. A GHGIS will be required if it was decided that *validation* of national, sub-national, or by economic sector anthropogenic emissions estimates is necessary. While errors and uncertainties in fossil-fuel reports are unlikely to lead to the magnitude of the variances that experience with  $SF_6$  measurements indicates, the truth is (1) we do not know, and (2) the consequences of large uncertainties and errors are high. In this event, means of ascertaining that emissions uncertainties and their estimation are within acceptable limits are indicated.

The proposed GHGIS is characterized by a host of challenges ranging from those in science, technology, engineering, systems engineering and design, development-project management, operations-system management, and product integration, and, not least, transitioning from what has largely been a science-research effort to date into an operational activity characterized by long-term stability and reliability. As also noted in the OSTP (2010, p.15) report,

Development of an integrated climate observing system continues to stand as a large and urgent challenge. One part of the challenge is that the required observing system must deliver multi-decade data records with the accuracy and precision needed to distinguish long-term climate changes from natural variability and other environmental influences.

Other operational monitoring systems, such as the one developed and operated in support of the CTBT and for other US-government purposes, provide a useful template. However, the broad spectrum of sensing modalities and platforms that GHGIS will likely encompass; the complex project-development and inter-agency challenges; the integration of all-source data for at least some of the reports; the requirement for calibrated, verified, and validated sensors, processes, and procedures throughout; and the need for data and software quality-control, quality-assurance, and quantified uncertainties that must accompany all measurement and analysis data, render this a technical, management, and operations challenge that may, *in toto*, be unprecedented.

# **Chapter 2. Requirements Framework**

# **Chapter Summary**

The present study on a proposed greenhouse-gas information system (GHGIS) was undertaken without the benefit of requirements and specifications that will ultimately drive its choices and architecture. The discussion in this chapter attempts to develop a *requirements framework* that can be relied on to make choices between desired accuracy, precision, and confidence, vs. cost, schedule, and other elements.

The accuracy or precision of the GHGIS (top-down) components required to *validate* reporting and international commitments depends on factors determined by the nature of the commitments as well as the goals of the users. The present study focuses on the task of measuring GHG emissions and attributing anthropogenic surface fluxes. This chapter explores possible emissions pathways that depart from targets and makes a number of assumptions about the needs of users to detect and quantify such departures, regardless of whether they are the result of inadvertent or willful reporting errors. Such user needs would be used to set GHGIS requirements.

# Findings

- 1. GHGIS requirements from which specifications on accuracy, precision, data and modeling uncertainty quantification (UQ) can be derived have not been set.
- 2. Based on assumptions documented below, if GHGIS is to validate total, country-level GHG emissions against annual targets, then *accuracies* will likely need to be in the range of  $\pm$  5-18%, depending on emissions pathways and the required levels of confidence. These estimates would be refined or adjusted, accordingly, in response to requirements.
- 3. If GHGIS must quantify *changes* in emissions relative to a baseline year and based on the same assumptions as in Item 2, above, then the required *precision* is  $\pm 5-18\%$ .
- 4. High *precision* is easier to achieve than high *accuracy* and may require a GHGIS that is operational in the *baseline year*.
- 5. The need for high precision could be somewhat relaxed if top-down GHGIS components are used in combination with bottom-up inventories, however, at the cost of losing some benefits of (independent) validation.

# **Recommendations (Phase 1 Development)**

- 1. GHGIS development should include the ability to establish reliable baseline estimates in regions of interest early on.
- 2. GHGIS should supplement the lower precision of results from its early development phase with capabilities to validate mitigation actions and support and incorporate all-source information.

## **Recommendations (Phase 2 Development)**

- 1. As a guideline, GHGIS should adopt a methodology that will yield an overall precision of anthropogenic emissions of  $\pm 10\%$ , or better.
- 2. GHGIS should be capable of measuring multiple greenhouse gases, including  $CO_2$ , methane (CH<sub>4</sub>), nitrous oxide (N<sub>2</sub>O), as well as carbon monoxide (CO), and a number of fluorinated gases.
- 3. GHGIS should aim to also attribute emissions by economic sector.
- 4. GHGIS should be designed to provide periodic emissions estimates, such as quarterly and annually, covering specific countries, emitters, industries, or economic sectors in response to GHGIS-customer needs.

## **Recommendations Overview and Reasoning**

GHGIS includes an important top-down component based on measurements, which aims to monitor country-level greenhouse-gas (GHG) emissions to provide independent *validation* of emissions declarations, mitigation measures, and as well as treaty commitments and compliance. Current state-of-the-art, bottom-up estimates are based on engineering calculations ("inventories"). The top-down GHGIS component does not rely on self-reported bottom-up data. These can be used either as independent input, or to augment top-down estimates to improve both. At present, inventories provide the only estimates. They are likely to remain better-suited for emissions estimates by sector than may be achievable by top-down measurements alone, at least in the near and intermediate term. The top-down and bottom-up components that GHGIS will integrate should be viewed as best used in conjunction.

The accuracy or precision required of GHGIS to monitor and validate international commitments depends on a number of factors, including:

- 1. the specificity of the commitment and whether it is conditioned on other estimated data that must be taken into account, such as emissions per unit GDP;
- 2. the magnitude of the departure from target emissions that must be detected and quantified;
- 3. how quickly the departure must be detected;
- 4. the probability of detection, if departures from emission agreements occur; and
- 5. the required confidence level before reporting that a departure has occurred.

Further, the commitment can take various forms. It may be on total GHG emissions or a subset of gases and sectors. It may be on absolute emission levels or on a compound metric like carbon intensity (i.e., emissions per dollar of Gross Domestic Product [GDP]), or national per capita emissions. Uncertainties in these denominators (GDP or population) would need to be taken into account. The commitment may also be the implementation and maintenance of specific mitigation actions, such as slowing or reversing deforestation, or even afforestation.<sup>1</sup> The present study focuses on the task of measuring GHG emissions and attributing anthropogenic surface fluxes that will be an essential component in almost any case.

In support of estimations with the required precision or accuracy of GHGIS reports, it is proposed that the system be capable of detecting departures with a greater than 50% probability, within four years of the start of the departure, and a 95% confidence level that the departure is occurring when reported. Four reasonable emission pathways were explored that depart from target emissions (see Fig. 2-1). If GHGIS is framed as a tool to validate total, country-level GHG emissions against annual targets, then the required accuracy is in the range of  $\pm 5-18\%$ , depending on the emissions pathway (see Table 2-1). If GHGIS must establish *changes* in emissions relative to a baseline year, then the required *precision* is  $\pm 5-18\%$ . This scenario requires a GHGIS that is operational in the baseline year, but has the advantage that a  $\pm 5\%$  precision, for example, is easier to achieve than  $\pm 5\%$  accuracy because certain systematic errors will not exert the same influence on the former.



Figure 2-1. Potential emissions trajectories for the hypothetical country Midlandia. According to an emissions reduction agreement, "Target" emissions drop by 2% per year, relative to the baseline year 2010, achieving a 20% reduction by 2020 and an 80% reduction by 2050. If no mitigation actions are taken, Midlandia follows the Business as Usual (BAU) path, increasing emissions by 1% per year. Each scenario is described in detail in the text.

<sup>&</sup>lt;sup>1</sup> *Reforestation* refers to restoring a forested area and forest growth, i.e., where a forest has previously existed. *Afforestation* refers to the establishment and maintenance of forests in areas not forested previously, or not forested in a given reference year.

Scenario	Accuracy required
Under-report	+/-5%
Partial mitigation	+/-6%
Inflated baseline	+/-12%
BAU	+/-18%

Table 2-1. Required measurement accuracy to achieve proposed detection criteria for the departure scenarios shown in Fig. 2-1: 50% probability of detection at 95% confidence within 4 years.

The need for high precision could be relaxed if the top-down GHGIS components are used to provide a validation check on bottom-up inventories that, in turn, would be compared to target emissions. Inventory reporting provides multiple points of comparison for emissions, e.g., by gas and sector instead of a single, annual total. To exploit the full information, GHGIS must be capable of measuring multiple gases, attributing anthropogenic emissions by sector, and potentially attributing anthropogenic emissions by region and for relatively short time periods, while accounting for seasonal variations. This capability will enable integration of a variety of external and all-source information and improve reliability and flexibility in the detection process. The proposed GHGIS should have these capabilities with an overall precision for the quantification of anthropogenic emissions of  $\pm 10\%$ .

To measure total emissions trends with this precision, several GHGs must be monitored and measured. In particular, the proposed GHGIS should include fossil-fuel carbon dioxide ( $CO_2$ ), biogenic  $CO_2$ , methane ( $CH_4$ ), nitrous oxide ( $N_2O$ ), and a number of fluorinated gases.

On the question of which countries to cover, one may chose to cover 80% of global emissions. This can be adjusted in the future, as policy and other needs evolve along with GHGIS capabilities. The particular countries to include is a separate question, also a matter of policy, but will likely include at least eight emitters (with the European Union [EU] considered as a single emitter) and may reasonably include tens of countries, ranging widely in size and geography. The required spatial scale/resolution for GHGIS will then vary from country to country.

As an initial benchmark, a horizontal spatial resolution in the range of 10 to 50 km for reporting anthropogenic emission sources is proposed, with planning to refine this further as experience is gained and future GHGIS requirements dictate and evolve. This would allow sub-national emissions estimates in some larger countries, although, at this resolution, smaller countries may not be distinguishable from their neighbors. A higher (finer) horizontal spatial resolution for *measurements* and localized anthropogenic source retrievals is likely to be necessary to support the horizontal resolution in GHGIS reports, depending on emitter types and the geographical details and distribution of the anthropogenic emission sources (e.g., localized power plants vs. distributed transportation corridors).

The GHGIS envisaged provides anthropogenic emissions estimates quarterly and annually for comparison with inventory reports, and certain economic data to be released quarterly or monthly. However, both anthropogenic and natural GHG emissions vary substantially, both geographically and temporally, i.e., on seasonal, hebdomadal (weekly), and diurnal (daily) cycles, so GHGIS must internally aggregate emissions estimates on shorter time scales.

The discussion above summarizes the high-level requirements framework to help the GHGIS design if it is to be used as a tool to monitor and validate national and international emissions targets and treaty commitments. Since the nature and specifics of such future commitments are not known at this time, and perhaps not for some time to come, a general requirements framework was defined for the present study, although additional assumptions were necessary to arrive at some quantitative conclusions.

## 2.1 Introduction

Monitoring, reporting, and verification (MRV) is an essential component of international environmental treaties (Barret 1998). Recently, the Bali Action Plan called for "measurable, reportable, and verifiable" GHG mitigation actions and commitments (Ellis and Moarif 2009). The Copenhagen Accord included a provision for transparency of GHG emissions and the effectiveness of mitigation actions for both developed and developing countries (Houser 2010). Effective MRV will allow countries to agree to and implement actions with confidence that they will know if other countries comply and abide by their agreements. It also allows both individual countries as well as the international community to track the effectiveness of mitigation measures and forecast whether implemented measures will suffice to meet policy goals.<sup>2</sup>

GHGIS is envisaged as having the capability to provide monitoring of country-level and subnational level GHG emissions, and the independent validation of emissions declarations, mitigation measures, and treaty commitments. Specific design and significant resources are required to develop a GHGIS that can perform these tasks. The desired monitoring precision and the nature of the commitments to be validated will dictate the ultimate form and cost of GHGIS.

## 2.1.1 Bottom-Up GHG Inventories

Bottom-up estimates based on reporting and engineering calculations ("inventories," or "emissions inventories") provide the current methodology for GHG estimation (International Energy Agency [IEA]/Organization for Economic Cooperation and Development [OECD] 2010). Under the United Nations Framework Convention on Climate Change (UNFCCC), Annex-1 parties (developed countries) must submit annual inventories of GHG emissions to the UNFCCC Secretariat. Procedures and guidelines on how to prepare inventories are provided by the UNFCCC, and the submissions are subject to review by independent experts to assess their correctness and compliance. However, no policies or procedures exist at this writing to enforce compliance, or address non-compliance, other than the exchange of information and attempts at reconciliation.

Estimates of national GHG emissions are calculated by summing up emissions from dozens of individual "source categories." Each source category, for example, "steel mills" or "wastewater treatment," has a defined procedure for calculating emissions. In general, the calculation starts with "activity data," which typically derive from economic reports or business surveys, and include such figures as the number of gallons of gasoline sold and the number of tons of cement produced. Activity data are then multiplied by "emissions factors," such as the average number

<sup>&</sup>lt;sup>2</sup> By way of example, if a particular set of mitigation actions is undertaken to decrease emissions by a certain percentage, an MRV system would reveal if the mitigation actions have achieved the intended target(s).

of tons of  $CO_2$  released per ton of cement produced and the average mass of carbon emitted per gallon of gasoline burned. Emissions factors are derived from engineering models of various processes (such as cement manufacture), chemical analysis of fuels, and emissions measurements at particular representative sources, such as vehicle tailpipes and boiler smoke stacks (EPA 2010).

Uncertainties in national GHG emissions estimates are introduced by uncertainties in activity data, emissions factors, and by the definitions of source categories that may either overlap (double-count) or omit certain sources. In some cases, source categories are intentionally omitted because procedures or data with which to estimate associated emissions are not agreed upon, or are incomplete. At present, the US GHG Inventory reports a 95% confidence level in the uncertainty of net GHG emissions of -2 to +7%. The uncertainty range for  $CO_2$  emissions from fossil fuel alone is -2 to +5% (EPA 2010). However, these uncertainty ranges should be viewed as *consistency* estimates of reported inventories. The ranges do not account for omitted source categories and are not *validated*, i.e., they are not confirmed by independent means at this time.

Bottom-up inventories with a precision similar to that reported by and for the United States require significant infrastructure and expertise. Non-Annex-1 parties to UNFCCC (developing countries) currently provide GHG emissions estimates of varying frequency and quality, with associated uncertainties that are accepted as being much larger (NRC 2010a).

In this chapter, *accuracy* refers to the uncertainty of absolute emissions measured by GHGIS, e.g., for a given country in a given year. The term *precision* refers to the uncertainty range in *differences* in emissions and, in particular, differences relative to a baseline year. Unless otherwise noted, all uncertainty ranges (such as  $\pm 10\%$ ) correspond to a 95% confidence interval. When a bottom-up inventory report is provided in the context of a treaty, or some other commitment where it serves as an official statement of country-level emissions, it will be referred to as a *declaration*, or *declared emissions*. The terms *verification* and *validation* are used as defined in the Introduction (Chapter 1) and amplified in Appendix C.

## 2.1.2 The Value of Independent Methods

Bottom-up inventories hold the promise of high precision and can provide substantial detail about GHG emissions sources. However, emissions inventories are the product of self-reporting. Errors and ambiguities may arise that are either inadvertent (i.e., the result of human error, or an inability to compile and report accurate data that represent a complex undertaking), result from the omission of certain sources, or even willful misreporting. Some checks may be made for internal consistency and against other data sources, but inventory reports that have not been independently verified and validated may not be and need not be accurate, or accepted as such.

If and when consequences are attached to the emission of GHGs, either in the form of charges for over-target emissions, or in the form of incentives to reduce emissions, emitters and those who aggregate and report inventories may have incentives to slant what they are prepared to report. Thus accurate inventories depend on both the *ability* to collect accurate data and analyze it correctly and the *willingness* to issue accurate reports. This is not to say that inventories are not without value, but rather that they need to be seen as one part of a system, which in its entirety allows for verification and validation.

Because GHGIS will depend on measurements and data that are independent from inventories, e.g., atmospheric measurements, it can provide a means of validation of emissions estimates not available through current methods or other means. Additionally, because atmospheric measurements can be made in and by countries or organizations not controlled by the country being monitored, GHGIS can provide independence in a way not available through self-reporting. It is this feature – the potential to provide independent validation – that makes GHGIS particularly valuable in supporting the assessment of mitigation actions and compliance of international commitments, in addition to its many science and other uses.

## 2.1.3 Use of GHGIS Products

GHG emissions estimates and other GHGIS products can serve many useful purposes, including substantial contributions to Earth science and climate science, monitoring of economic and other activities that depend on fossil-fueled energy production, and for other purposes, as discussed in the Introduction (Chapter 1) and throughout this report. However, the primary purpose of GHGIS is in the context of MRV, or MRV&V, and the facilitation and monitoring of climate-change and emissions-mitigation actions. The goal is to hold countries to their commitments and allow countries to make stronger commitments with confidence that others' commitments are also monitored and honored. Accordingly, the primary benefit of GHGIS is not achieved by accurate outputs alone, but from the expectation that GHGIS outputs will be accurate and definitive and, in turn, induce behavioral change by governments or international actors.

This chapter primarily focuses on the required accuracy and scope of GHGIS estimates. However, estimates derived from GHGIS products must also be convincing to outside parties. This may be achieved through features such as transparency, traceability, and independent review, with the inclusion of relevant stakeholders in those aspects of GHGIS design and operation that are best shared. Existing multilateral regimes generally rely on expert and peer review as part of the MRV, or MRV&V, process, and the automatic public release of inputs and outputs of review (e.g., Pew Center 2010). Of course, the particular approach to transparency and assurance is a matter of policy and cannot be addressed here in broad terms. Later chapters will discuss specific issues in assuring quality and credibility of GHGIS inputs and outputs.

## 2.1.4 Goal of this Chapter

The goal of this chapter is to lay out the requirements framework for a GHGIS that is useful for monitoring of country-level GHG emissions and the independent validation of mitigation commitments. Currently, there is no authoritative source dictating requirements for a top-down GHG monitoring system. This chapter attempts to define a starting place that bridges a reasonable expectation of what will be required to achieve policy goals, on the one hand, and projected technical capabilities of such a system, on the other.

The proposed requirements framework does not address sovereignty issues and the political ownership of GHGIS. Ground-level and airborne measurement in the country of interest are assumed to be available, i.e., we assume local access. Further, remote-sensing measurements from space are not subject to denied-territory limitations. This issue is discussed further in subsequent chapters. Neither is the legal status of GHGIS addressed, e.g., whether it exists

within a treaty framework or whether its findings may initiate sanctions or proceedings, or whether it is intended to serve the purposes of US policy-makers alone.

The type of commitments made and the type of validation desired has a substantial impact on the specific GHGIS requirements. The next section discusses a number of possible framings of GHGIS and its role in validation. The section concludes with a set of working assumptions about how GHGIS could be used. The following sections address six high-level design criteria: country coverage, coverage by greenhouse gas, spatial resolution, temporal resolution, accuracy, and sectoral attribution. The chapter concludes with a summary of findings.

# 2.2 Potential Framings of GHGIS and Validation

GHGIS requirements depend on how validation and top-down emissions measurements are framed in the context of global climate-change and emissions mitigation. Traditionally, commitments are thought of in terms of cuts to total, country-level GHG emissions over time. The Kyoto Protocol provides the prime example. However, other types of commitments may take hold, such as "GHG Intensity," i.e., GHG emissions per unit of GDP. Intensity targets were set voluntarily by the United States during the Bush administration (Pizer 2005) and recently by China, in advance of the Copenhagen conference (Worthington 2009). GHG emissions per capita have also been frequently proposed (Baumert et al. 2005). To verify either type of commitment, one would need to verify both GHG emissions and either GDP or population, as appropriate, each with associated uncertainties and, possibly, manipulation. The focus of this report is the measurement of the anthropogenic GHG emissions component, the need for which is not diminished by composite metrics, such as GHG intensity. However, the need for complementary efforts to monitor and verify other components is also acknowledged. It is assumed that these components will be provided, or be integral, to GHGIS, which will integrate them into an overall top-down and bottom-up reconciliation and reporting to meet specific requirements.

Even focusing on GHG emissions, commitments may take a variety of forms that dictate expected roles of GHGIS. Such alternative "framings" are discussed below. Each has implications for the accuracy, precision, and scope required of GHGIS. It is also possible that countries may commit to particular mitigation activities, without reference to emissions metrics *per se*. Verification of activities is discussed as one of the framings below and, more generally, in the Introduction (Chapter 1) and in Appendix C. We conclude this section with a summary of our working assumptions and conclusions regarding some useful GHGIS framings.

## 2.2.1 Top-Down and Bottom-Up Measurement Components

Framing the bottom-up and top-down measurements as methods of contributing to the same goal—monitoring (a country's) GHG emissions—then GHGIS must accept as an uncertainty quantification (UQ) requirement an integration of top-down measurements that meet precision and accuracy uncertainties that are comparable to, and ideally better than, those of bottom-up inventories. Otherwise,

1. one might elect to choose inventories, if only one system could be chosen, or

2. GHGIS may offer little additional information when the products of the two systems are combined.

If one wished to validate one system against the other, GHGIS would need accuracy comparable to that of inventories, otherwise inconsistencies may be difficult to distinguish from known errors (this problem is statistically analogous to detecting departures for validation purposes, discussed in the next section). In short, *information from bottom-up and top-down reconciliation flows from variances between the two that exceed their combined uncertainties.*<sup>3</sup>

Framing bottom-up and top-down measurements as components of equal significance would be appropriate if the goal is to validate the two types of measurements against each other, whether both are made in good faith or not. For example, if the United States develops a GHGIS for domestic monitoring to detect systematic errors for its own purposes, this framing would apply. However, in terms of international commitments, there is a qualitative difference between the measurement systems. The feature of independence, either from control of the country being measured or simply from bottom-up inventory methods, is important.

On a related note, objections to strong MRV requirements at the recent Copenhagen conference cited "intrusiveness" (Eilperin 2009). Thorough review of an inventory requires a volume of reliable economic data that may be considered intrusive to a country, such as fuel sales and detailed records of the development and operation of industrial facilities. Depending on the GHGIS structure, it may be considered intrusive in terms of measuring emissions within a country, but this exposes information of a different sort. In US law, emissions to the environment are considered public information and not subject to privacy restriction or trade-secrets protections. On the other hand, some inputs to bottom-up accounting methods, such as the types of equipment used within industrial facilities, are considered confidential business information and shielded from public view (e.g., EPA 2009). If international law follows this precedent, GHGIS may achieve a more palatable scrutiny than alternative methods of verification and validation using inventories alone.

For these two reasons, i.e., independence and less economic intrusiveness, GHGIS can provide a qualitatively different function than that provided by bottom-up inventory reporting systems.

## 2.2.2 GHGIS to Detect Departures from Absolute Emissions Targets

The most direct use of GHGIS for monitoring or treaty verification (validation of emissions and mitigation actions) would be to measure total, country-level GHG emissions and compare them with applicable emissions targets on an absolute scale. GHGIS would detect departures from targets or from declared emissions, regardless of whether departures are unintentional (mistakes), intentional (cheating), or within the uncertainty bounds of the reported values; *the lower the GHGIS uncertainties, the smaller are the departures that could be detected.* In this framing, GHGIS alone could trigger procedures for corrective action when departures are detected, or it could supplement and trigger other means of validation.

<sup>&</sup>lt;sup>3</sup> Top-down (GHGIS) uncertainties could be larger than those of inventories and still useful. By way of example, if the (claimed) inventory uncertainty was 5% and the assessed top-down uncertainty was 10%, valuable information would derive from a variance between the two of 20%.

Figure 2-1 shows a simplified set of GHG emissions trajectories for a hypothetical industrialized country, Midlandia, with emissions in 2010 of 100 MtCO<sub>2</sub>e (million tons carbon dioxide equivalent; cf. Chapter 1). The trajectories represent a range of potential scenarios. Target emissions are based on an assumed 20% emissions reduction by 2020 and an 80% reduction by 2050, i.e., a reduction of 2% each year relative to the baseline year 2010. The BAU trajectory increases by 1% each year relative to the baseline, which is roughly the emissions growth of the United States in the period 1990–2008. Other scenarios are also shown for which emissions depart from targets. None of the scenarios are meant to represent accurate predictions of a particular country's emissions pathway, but rather are meant to illustrate the scale of departures that GHGIS could be called upon to detect.

Emissions pathways for a developing country could show much higher growth rates. For example, China's emissions grew at an average rate of 5.4%/yr over the period 1979–2006 (Zheng et al. 2008). In contrast, *relative* reduction targets for developing countries may be modest. For example, one estimate finds that China's commitment before the Copenhagen conference to a 40-45% reduction in GHG intensity by 2020 amounts to only a 12% emissions reduction by that year from BAU (Worthington 2009). Thus relative changes in emissions that must be detected are not necessarily larger than for developed-country scenarios.

Assume that Midlandia commits by treaty to the target emissions trajectory shown in Fig. 2-1, but actually follows the BAU trajectory. This may be the easier detection problem for GHGIS. In the first year covered by the treaty, there is a 3% discrepancy between target and actual emissions. Figure 2-2 illustrates this at the end of the first year. The curves in this figure assume that GHGIS measurement uncertainties are  $\pm 5\%$  (as defined by a 95%, or  $2\sigma$  confidence interval), which is a rather ambitious assumption.

Figure 2-2 shows that the probability distribution of measurements one would expect to make if Midlandia's emissions are on target (the "noise" distribution) overlaps substantially with the distribution of measurements one would expect to make if Midlandia is instead following BAU (the "signal" distribution).

As with most signal-detection systems, a "decision threshold" is required, above which action is triggered if GHGIS reports emissions above this threshold. The action could range from initiating further investigations, to starting discussions with Midlandia to better understand the "discrepancy," to imposing sanctions on Midlandia for violating the treaty. Wherever the threshold is set, there is a chance that one would detect Midlandia as above target, when it is not, i.e., a "false positive," or that Midlandia would depart from targets undetected, i.e., a "false negative."

The choice of a decision threshold depends on the seriousness of the action that will be taken – imposing sanctions would likely require a very high threshold, for example, while a secondary investigation triggered by a less-strict threshold might be routine. *A priori* beliefs about the likelihood of emissions departures could be taken into account as well.

Formal treatment is not possible here, so it is assumed for illustrative purposes that a 95% confidence level that Midlandia is off target is required before taking any action. Equivalently, one could say that there should only be a 5% chance of accusing Midlandia of a departure when

they are actually on target, i.e., a "false-positive rate" of 5%. The 95% confidence decision threshold is also shown in Fig. 2-2. The red-hatched area to the right of it demarks the 5% false-positive rate. The larger, blue-hatched area to the right of the decision threshold indicates the probability of detecting a departure if it occurs, i.e., the "true-positive rate." In this case, the detection probability is 32%. That is, if Midlandia is above target, the probability that GHGIS will return a measurement that allows us to say so with 95% confidence is 32%.



Measured Emissions [Mt CO2/yr]

Figure 2-2. Distribution of measured values given compliance (at emissions = 98, the "target") and noncompliance (at emissions = 101, "actual") with a measurement uncertainty of  $\pm 5\%$  and a decision threshold of 95% confidence (5% false-positive rate).

Whether a 32% probability of detection is sufficient is a question whose answer is a matter of policy. If one is concerned with intentional departures from targets (cheating), a reasonable goal may be to create a "culture of compliance" where cheating would generally be rare. This has been the case with most past environmental treaties (Barret 1998). A reasonable means of supporting a culture of compliance is if detecting cheating becomes more likely than not (probability of detection > 50%). By this criterion, the hypothetical detection problem depicted in Fig. 2-2 is not tenable. However, considering the time scales involved, it may not be necessary to detect departures the first year they occur. Measurements and integrated assessments can be performed over several years to build confidence by statistical accumulation, or other information, to discriminate between one trend versus another. In the BAU example, as time progresses, one gains both through repeated measurements and an ever-widening gap (strengthening signal) between actual and target emissions. Figure 2-3 shows the cumulative probability over 10 years of detecting a departure for several different GHGIS uncertainty levels. In this figure, GHGIS can be seen to meet the proposed requirements in the second year, with a  $\pm 5\%$  uncertainty, in the third year with a  $\pm 10\%$  uncertainty, and in the fifth year with a  $\pm 20\%$ uncertainty.

An alternative approach to presenting the detection problem depicted in Fig. 2-3 (and Figures 2-4 through 2-6, discussed below) is in terms of ROC (Receiver-Operator Characteristic) curves. The ROC curve plots the probability of detection versus the false positive rate. The area under the ROC curve (AROC) is technically a better characterization of a detection system than the probability of detection because it does not require an a priori establishment of a decision threshold. However, AROC is more difficult to relate to policy goals. For interested readers, several ROC curves analogous to Figs. 2-3 through 2-6 are presented and discussed further in Appendix D.



Figure 2-3. Cumulative probability of detecting a departure from target emissions, if actual emissions follow the BAU scenario (Fig. 2-1). The decision threshold is set at 95% confidence (5% false-positive rate, as in Figure 2-2). Each curve is labeled by the GHGIS measurement uncertainty (accuracy), represented by the relative 95% confidence interval. Each year, the probability of detection increases because of repeated measurements and the increasing discrepancy between target and actual emissions.



Figure 2-4. Cumulative detection probability for the "partial mitigation" scenario shown in Figure 2-1.



Figure 2-5. Cumulative detection probabilities for the "inflated baseline" scenario shown in Figure 2-1.



Figure 2-6. Cumulative detection probabilities for the "under-report" scenario shown in Figure 2-1.

The examples in Fig. 2-3 illustrate that required GHGIS uncertainty levels (accuracy) depend on how soon departures must be detected. High-level treaty targets may be made with a 10-year time horizon (e.g., the Kyoto Protocol). Validation of such high-level targets would certainly be an important function of GHGIS. However, substantial emissions growth and near-irreversible environmental damage can occur over a 10-year period, if countries are off target and unchecked. Most likely, one would wish to receive warnings, identify and notify emitters (domestic or international), and correct emissions departures on shorter time scales. If departures are the result of willful actions (cheating), one would wish to hold the administration accountable that committed the violation, or at least have a chance of doing so. A time horizon of 4 years in which to achieve the required detection probability may then be desirable. Table 2-1 summarizes the proposed accuracy requirements that flow from this consideration.

#### 2.2.3 Emissions Scenarios

The discussion thus far focused on the detection of the BAU scenario. Figure 2-1 shows other emissions scenarios that depart from target emissions. These are discussed below.

**BAU Scenario** – This follows a 1%/yr growth in emissions, roughly the average for the United States over the period 1990–2008. If the country of interest does nothing to reduce emissions, the gap between actual and target emissions will grow. This would present the easiest detection problem.

**Partial Mitigation Scenario** – Emissions are reduced under this scenario, but at half of the needed rate (1%/yr instead of 2%/yr, relative to the baseline). This scenario is interesting because it would be difficult to detect based on infrastructure data and policies; the country is clearly undertaking mitigation measures and making reductions. The difference is in magnitude.

*Inflated Baseline Scenario* – In this scenario, the country of interest misrepresents emissions in the baseline year (year zero), inflating them by, say, 8%. This allows the country to delay action for 4 years before beginning to reduce emissions at the target rate. Since GHGIS is framed as monitoring emissions relative to a *measured* baseline, it is not sensitive to what the target country declares as baseline emissions. An interesting feature of this scenario is that, for GHGIS, detection of the original baseline inflation becomes increasingly easy over time. In contrast, for many bottom-up methods, the best chance for detection occurs in the first year, when the absolute difference between stated and actual emissions is largest, and detection becomes increasingly difficult over time, and nearly impossible after Year 4.

**Under-Reporting Scenario** – In this scenario, the country of interest under-reports emissions by, e.g., 2% each year, relative to the baseline, but after the first year, reduces emissions at the target rate. If the treaty framework allows for some kind of trading on emissions credits based on annual allowances, then the financial motivation for this scenario is clear. It poses a difficult detection problem for bottom-up methods as well as top-down GHGIS components, since it may fall within the uncertainty range of bottom-up inventory methods in any given year.

Figures 2-4 through 2-6 show the probability of detecting the departure for each of the additional scenarios. Implications in light of the proposed uncertainty/accuracy requirement are summarized in Table 2-1. Once again, it is a policy choice as to which scenarios are important to detect, but all of these may be of interest. If indeed all of the scenarios are of interest, and if GHGIS is framed as a system to measure absolute, total GHG emissions to be compared with country-level targets, then GHGIS must achieve uncertainties that are not much higher than  $\pm 5\%$ . Although many assumptions were made to reach this conclusion, and reasonable alternative assumptions can certainly be made, it is unlikely that the general need to detect changes in emissions of, at most, a few percent per year can be avoided, which requires a GHGIS (as a tool to verify total, country-level emissions targets on an absolute scale) is centrally characterized by low-uncertainty (high-accuracy) requirements. As discussed in Chapter 7 and elsewhere, such uncertainty levels may be difficult to achieve. Other framings, discussed below, may allow this requirement to be relaxed to some extent.

#### 2.2.4 A GHGIS Framed to Detect Departures from Relative Emissions Targets

Emissions targets are often stated as a fractional reduction relative to a baseline year. Emissions commitments of this type can be framed in terms of a relative reduction in emissions that does not necessarily depend on knowledge of baseline-year emissions with great accuracy. In this case, the GHGIS figure of merit is (integrated) measurement precision from one year compared with another, rather than accuracy on an absolute scale. Focus on precision mitigates sensitivity to year-to-year systematic errors. Another advantage is that such a GHGIS would not be sensitive to inflated baselines, i.e., over-reported emissions in a baseline year.

However, if GHGIS is to be relied upon to detect relative changes, it is advantageous from a monitoring perspective that it be operational in the baseline year. Existing treaties, such as the Kyoto Protocol and Montreal Protocol, have relied on historical baseline years. An advantage of this choice is that it is more difficult for participants to game the system (and further damage the environment) by ramping up emissions in the baseline year. However, baselines in the past pose measurement challenges and the choice of the baseline year is subject to some manipulation. For GHGIS to be used in this mode, a future agreement would need to use or somehow be linked to a baseline for which GHGIS could collect or had collected data, in which case the precision of the baseline-year measurements is particularly important.

In this context, GHG measurements from existing sensors and especially from space (because of their near-continuous extensive coverage) can play an important role, for example, from sensors such as Atmospheric Infra-Red Sounder (AIRS) (Chapter 3) that have been operating since 2002. While such measurement assets were not designed to support an operational GHGIS, year-to-year *changes* in detected GHG concentrations, even though not attributable by themselves to anthropogenic sources, can help reveal inconsistencies between declared emissions and measured concentrations in the reference baseline year. Similar benefits accrue an integrated system that can perform retrospective analyses of archived all-source data.

In the present framing, GHGIS measures total, annual emissions and compares them to singlevalue targets, much as in the previous framing. The analysis above of required accuracy still applies, except now one may replace "accuracy" with "precision" and can place the emissions trajectories in Fig. 2-1 on a relative scale (% change instead of MtCO<sub>2</sub>e). Thus, an analogous conclusion as for the previous framing can be drawn: that this framing demands a high measurement *precision* to meet requirements. As stated above, the difference is that high precision will likely be easier to achieve than high accuracy because of common-mode rejection of certain systematic errors. However, this benefit may be diminished by year-to-year changes in infrastructure, population density, industrial activity, transportation-sector modalities, etc., and, not least, the environment itself. The remainder of this report primarily focuses on precision rather than accuracy.

## 2.2.5 GHGIS as a Check on Bottom-Up Inventories

In the previous two framings, measurements made by GHGIS each year are compared to another estimate, e.g., a target. Bottom-up inventories encompass a wealth of information, not just a single, annual emissions total. If the bottom-up inventory is considered as the "declaration," i.e., what the country reports to be true and its best estimate, then inventory verification and

validation becomes equivalent to target verification and validation. In this framing, the declaration, once verified, validated, and certified, becomes the official emissions record for that year, against which consistency with treaty obligations may be judged. Declared emissions need not match target emissions, but if the country declares emissions higher than target, they may be expected to undertake appropriate actions, such as buy emissions credits to make up the difference, undertake other verifiable offset/mitigation actions, or pay some penalty.

A consequence of this framing is that GHGIS must allow for uncertainties and errors inherent in the inventory process. That is, one would expect an inventory made in good faith to sometimes miscount, or undercount emissions. This effectively broadens or shifts the "noise" distribution against which GHGIS attempts to detect errors (intentional or not) in the inventory. Suppose that Midlandia submits an inventory with  $\pm 5\%$  uncertainty, as is reasonable for a well-developed inventory. Per above, the uncertainty would best be narrower if the interest is year-on-year changes rather than absolute accuracy.





Figure 2-7. Distribution of measured values given compliance (at emissions = 98) and noncompliance (at emissions = 101, "actual"), with an estimation uncertainty of  $\pm 5\%$  and a decision threshold of 95% confidence (5% false-positive rate, analogous to Fig. 2-2), adding  $\pm 5\%$  uncertainty in the bottom-up inventory (the declared emissions value) for an inventory to be verified. Departure detection is less likely (compared with Fig. 2-2) because some high measured values result from random underreporting within the inventory uncertainty range.

Figure 2-7 shows a detection problem analogous to that depicted in Fig. 2-2 with this inventory uncertainty factored into the noise distribution. The wider noise distribution compels setting a higher decision threshold, reducing the probability of detection to 13%, compared with 32% if the inventory value was accepted as error-free. When GHGIS is used as a check on declared emissions, improving the accuracy of bottom-up inventories increases the value of GHGIS by making detection easier. This conclusion may run counter to intuition that GHGIS is less

valuable when good inventories are available, which stems from framing top-down and bottomup methods as equally important components, as discussed above.



Measured Emissions [Mt CO2/yr]

Figure 2-8. Distribution of measured values given compliance (at emissions = 100, "Reported") and noncompliance (at emissions = 105, "Actual") with a measurement uncertainty of  $\pm 10\%$ .

Although detection may be more difficult in the presence of inventory uncertainty in this framing, the wealth of inventory information can render detection easier. At least, one has information about economic-sector (sectoral) emissions. GHGIS could also estimate sectoral emissions and then compare values with inventory reports, yielding improved chances to identify inconsistencies. One can also make multiple measurements in the same year.

Suppose, for example, that GHGIS can attribute Midlandia's emissions into four sectors: coal, petroleum, natural gas, and non-CO<sub>2</sub>. For simplicity, assume that measurements of these sectors are independent and that the total is calculated by summing them (in reality, measurement of ratios among the sectors and the total to make the attribution is more likely, but the conclusions are similar in either case). Suppose also that Midlandia's reported emissions from each of the four sectors are equal, e.g., 25 Mt/yr each for a total of 100 Mt/yr, and consider the detection scenario of determining whether Midlandia's total emissions are 5 Mt (5%) above target.

If each sector is measured with a relative uncertainty of  $\pm 20\%$  and if, for the purposes of illustration, uncertainties are dominated by random uncorrelated (independent) errors with an equal probability of being positive and negative, then estimated total emissions would have a relative error of  $\pm 10\%$ , since, for *n* equal sectors (n = 4 in this example) with such uncertainties, the relative error of the sum would decrease by  $1/\sqrt{n} = 1/2$ . However, if inventory errors are all of one sign and correlated, e.g., from inadvertent or intentional underreporting, then the fractional uncertainty of the sum remains that of the (relative) uncertainty of each component and, in

particular, does not decrease with n. The important issue and consequences of the apportionment of uncertainties (errors) into random (aleatoric) and systematic (epistemic) is discussed later in this report in the context of spaceborne sensor data (Chapter 3), data uncertainty quantification (Chapter 6), and modeling and modeling uncertainty quantification (Chapter 7).

Figure 2-8 illustrates the detection problem when considering only total emissions. However, sectoral attribution allows the incorporation of external pieces of sector-specific information. Suppose, for example, that independent information is available that leads one to believe that Midlandia's emissions are off-target by 5 Mt/yr because of growth in their coal-sector emissions. Figure 2-9 illustrates the detection problem sector by sector. In three sectors, target emissions match reported emissions, so measurements trigger no detection. In the coal sector, however, departure from reported emissions is larger relative to GHGIS precision than for the total. There is then a 62% chance of detecting this scenario at the 95% confidence level, as opposed to 25% if one considers total emissions alone.

Absent information identifying the sector in which the departure is occurring, localizing emissions departures to one sector would not be as helpful as it appears. One would expect such a measurement to occur by chance four times as frequently, so one would have to set a higher decision threshold for similar confidence.

Although currently not required by the UNFCCC process, bottom-up inventories could be expanded to break out emissions by region. Many states and provinces already produce GHG inventories. Inventories could also resolve emissions on a shorter time scale, perhaps quarterly or monthly. These expansions would allow GHGIS to make comparisons with regional and temporal emissions values, providing additional comparisons to certify inventory consistency.

An advantage of such a framing of GHGIS would be its incorporation of external information to constrain the detection problem (as in the example above), to confirm inferences from other means of detection, or to focus further investigation to a particular sector, region, or time period. Verification methods of bottom-up inventories, e.g., audits of economic data, could be triggered by measurements of high emissions in a particular area. Thus, this framing provides substantially more flexibility and potential for integration with other methods, somewhat reducing thereby the burden on GHGIS of high precision. However, a trade is made between integration of other information to constrain and improve assessments and detection, and treating other information as independent, to be used as a consistency check of GHGIS assessments.



Figure 2-9. Representation of the detection problem in Fig. 2-8, broken into four sectors, given external information that the departure occurs in the coal sector. Each sector is measured with a relative uncertainty of  $\pm 20\%$ . The departure is more easily detected than for the scenario in Fig. 2-8 (no sectoral attribution).

#### 2.2.6 Framing GHGIS to Verify Mitigation Actions

Previous framings focused on GHGIS providing quantitative measures of GHG emissions, the primary focus of this report. However, elements of GHGIS can be used to validate mitigation activities, or commitments, such as construction and operation of renewable-energy sources, reforestation and afforestation, or shuttering of coal-fired power plants. For example, Brazil committed to reduce deforestation by 80% by 2020, as measured by land area (Tollefson 2010). Similarly, elements of GHGIS may be used to verify mitigation actions that, in turn, signal compliance with an emissions commitment, such as the absence of new coal-fired power plants.

Satellite imagery in particular can be used to assess reports of large-scale mitigation measures. Large power plants will show up as hot spots in a  $CO_2$  concentration map, signaling their operation and when they are taken off line. Trends in certain non- $CO_2$  tracers may also signal the presence or absence of mitigation measures, such as electric-vehicle use, or ethanol fuel blends in vehicles.<sup>4</sup> Such signals may be important during Phase 1, when quantitative measurements will not be sufficiently precise. Validation of mitigation actions was discussed in Chapter 1 and will be covered further in Chapter 3.

#### 2.2.7 Conclusion and Working Assumptions

A challenge of validating single-point emissions targets is the high precision required  $(\pm 5\%)$  to meet detection goals. For this reason, a GHGIS may best be used in conjunction with bottom-up inventories that provide multiple comparisons and aid integration of external information into the detection process. As a consequence, GHGIS should (also) be capable of providing sectoral attribution and, potentially, regional and sub-annual emissions estimates in addition to country-level totals. Such capabilities can enhance detection probabilities with lower precision levels.

To characterize the usefulness of an integrated system, the probability of detection provides a better metric than high-level uncertainty (accuracy or precision). However, such a metric depends on factors that cannot be quantified in this report, such as how well anthropogenic emissions can be discriminated in a background of (large-amplitude) natural/biogenic emissions and how well economic/energy/industrial sectors can be distinguished, what external information is available, and how reliable that information is. As an initial benchmark, a goal of  $\pm 10\%$  precision for annual emissions from high-emitting countries can be considered. This goal recognizes the value of a reliable total emissions estimate and of not relying too heavily on external information. Note also that the term "precision" is used because the proposal is to focus on relative changes in emissions rather than absolute totals.

# 2.3 Spatial Resolution

GHGIS data analysis and reporting will be characterized by a number of spatial scales. These need not be the same for measurements and reporting. They include the data-retrieval horizontal resolution dictated by the density of a ground-sensor network, the horizontal and vertical resolution of measurements from airborne and space sensors, the horizontal resolution and quality of local and regional emissions-inversion models ("the retrievals"), and the scale on which local, sub-national, and national emissions are estimated for reporting. A GHGIS goal of emissions estimates is retrieval at the country level. However, when sub-national information is available for comparison, retrievals at sub-national scales add value. This may include state- or province-level emissions in larger countries, or emissions from particular metropolitan areas, or regions of intense industrial activity.

Metropolitan areas offer an opportunity because they produce high local  $CO_2$  concentrations compared with background emissions, yielding strong signals in atmospheric samples. They also represent distinct and contained emissions sources compared with an entire country. These two

<sup>&</sup>lt;sup>4</sup> Ethanol fuel blends result in a different emissions profile at the vehicle.

features together may allow for greater precision in emissions measurements. While metropolitan area emissions are not surrogates of country-level emissions, they can provide useful year-by-year comparisons and a bellwether of national emissions trends.

As a consequence, required horizontal spatial scales will likely vary from country to country. As a benchmark, an initial horizontal spatial resolution for anthropogenic emissions estimates in the range of 10 to 50 km may be adopted for reporting purposes, with refinements, as necessary, to capture sub-country (regional) emissions. A 10- to 50-km horizontal resolution would allow subnational emissions estimates for larger countries, although at this scale, some smaller countries may not be readily distinguishable from their neighbors. Higher-resolution measurements and retrievals could address stricter monitoring and reporting requirements.

For comparison with bottom-up inventories, GHGIS measurements of most interest are in the lower part of the atmosphere, particularly the part of the troposphere known as the planetary boundary layer (PBL). The PBL is typically contained below an altitude of 0.5 to 1.5 km.<sup>5</sup> Measurements made at higher altitudes in the atmosphere, e.g., at mid-troposphere or stratosphere altitudes, can provide year-to-year tracking of emissions trends, constraining transport models, and improving understanding and characterization of the carbon cycle, but are not as useful as lower-troposphere, near-surface, or ground-level measurements are for constraining surface fluxes or emissions attribution directly.

# 2.4 Temporal Resolution

Similar to spatial resolution, GHGIS measurements and reports will be characterized by a number of temporal scales: the temporal resolution of measurements by the various sensors, of the inversion model, and the resulting emissions estimates. It would be desirable if the frequency of official reported emissions estimates matched the temporal scales of other reported data against which they will be compared – chiefly, the schedule of emissions targets and release of bottom-up inventories. Both of these are, at present, typically annual. Other information of interest may include economic reports, many of which are released quarterly, and energy statistics (such as fuel sales) that are sometimes available monthly. GHGIS should provide official emissions estimates on an annual basis, along with quarterly interim reports that could be subject to subsequent updates and revision. Quarterly reports would provide a comparison with sub-annual economic data and energy statistics and serve as early indicators of emissions trends in any given year, helping stabilize future carbon markets.

Another time scale of interest is the lag time between the completion of a measurement year and the release of the official emissions estimate. A variety of factors will contribute to lag time: some in situ samples must be physically shipped and analyzed, data must be vetted for quality assurance and quality control (QA/QC), data UQ analysis must be performed and passed through various organizations, and instrumentation may need to be checked and recalibrated. Bottom-up

<sup>&</sup>lt;sup>5</sup> Transport within and through the PBL presents great emissions retrieval challenges. Mixing within it is rapid during daylight hours, so retrieval of upwind emissions information is made difficult because of the enhanced dispersion. Further, night-time transport occurs in a stratified atmosphere governed by totally different, if perhaps more tractable, dynamics. Finally, PBL height and behavior within it depends on orography and upwind-terrain details, all of which contribute complexity and uncertainty in the face of modeling and wind-field uncertainties.

inventories against which the top-down estimates are to be compared also have a significant lag time. Inventories are currently submitted to the UNFCCC, by legal requirement, with a lag time of about 16 months. While a future international agreement may stipulate shorter lag times for inventories, a significant delay is still expected. Inventories depend on surveys and reporting by businesses and various organizations. The data must be checked, compiled, and reviewed. It may prove difficult for this process to be completed in much less than a year. All considered, the proposed GHGIS should not add to this delay and should accept a goal of no more than a one-year lag time.



Figure 2-10. Average relative monthly variation in GHG emissions by sector (EDGAR 2009).



Figure 2-11. Average relative day-of-the-week variation in GHG emissions by sector (EDGAR 2009).

While emissions estimates are reported annually and quarterly, GHGIS must internally aggregate emissions-related measurements on a variety of shorter time scales. GHG emissions vary substantially on seasonal, weekly, and daily cycles. Figures 2-10 through 2-12 illustrate the variation of these cycles in the Emissions Database for Global Atmospheric Research (EDGAR). GHGIS instrument systems will need to resolve these cycles (e.g., with hourly measurements), average over them in a manner that minimizes bias, or normalize/compensate for them using time profiles of emissions like those shown. Profiles would need to be developed for each area measured and, if based on self-reports by target countries, would need to be verified and

validated to address the possibility of manipulation. Handling the temporal cycles is an important issue. Proposed approaches will be discussed in the sensor chapters



Figure 2-12. Average relative diurnal (hourly) variation in GHG emissions by sector (EDGAR 2009).

# 2.5 Country Coverage

The choice of which countries should be monitored by GHGIS is influenced by which countries make commitments, which countries allow access, and which contribute significantly to global emissions. In order to stabilize atmospheric concentrations of  $CO_2$ , global emissions cuts of *at least* 80% will be required (NRC 2010b). Thus, if GHGIS is to support stabilization, GHGIS would eventually need to cover countries that contribute the vast majority of global emissions. A Phase 2 goal of covering at least 80% of emissions, by country, is proposed.

The picture of how many and which countries must be covered is slightly different depending on which gases are included, whether emissions related to land-use change are included, and whether the EU is considered as a single entity with a collective emissions target (following the model of the Kyoto Protocol), or whether its 27 member countries are considered individually. Figures 2-13 and 2-14 show, in a sense, the two extreme perspectives. Figure 2-13 shows only fossil CO<sub>2</sub> emissions with the EU considered as one entity, and Figure 2-14 shows total GHG emissions including land-use change with the EU disaggregated. In the former case, the top eight emitters cover 80% of the global total, and in the later case, 28 countries must be measured.

In light of the varying perspectives, a list of countries that must be covered, which will also be driven by other considerations, is not proposed here. However, the figures illustrate the size and type of countries that GHGIS should be capable of monitoring. Further, these rankings will change, evolving with time, albeit slowly.



Figure 2-13. Top fossil CO2 emitters and cumulative emissions coverage (red line), with the European Union considered as one emitter. Based on emissions data for 2005 (WRI 2010).



Figure 2-14. Top GHG emitting countries and cumulative emissions coverage (red line) with the EU disaggregated into member countries. Based on emissions data for 2005 (WRI 2010).
## 2.6 Coverage by Gas

Figure 1-1 in the Introduction (Chapter 1) shows the share of total global GHG emissions by gas, in  $CO_2$  equivalents, based on the global warming potential of each gas.  $CO_2$  is further broken into fossil-derived emissions and natural/biogenic emissions.  $CO_2$  from fossil sources comprises only about 60% of emissions. Countries may make commitments to total GHG emissions, as they have in the Kyoto Protocol. Coverage of non- $CO_2$  GHGs and non-fossil  $CO_2$  will be required if the GHGIS is to achieve meaningful validation of targets.

The share of non-fossil CO<sub>2</sub> and non-CO<sub>2</sub> gases varies by country, with fossil CO<sub>2</sub> being relatively more important in industrialized countries. For example, in the United States, fossil CO<sub>2</sub> represented 84% of gross GHG 2005 emissions. However, CH<sub>4</sub> and N<sub>2</sub>O are significant, comprising 8% and 6% of emissions. In China, CH<sub>4</sub> and N<sub>2</sub>O represent 12% and 10% of emissions in the same year, a somewhat larger share. Fluorinated gases (hydrofluorocarbons [HFCs], perfluorocarbons [PFCs], and sulfur hexafluoride [SF<sub>6</sub>] together) generally represent than 2% of national emissions. Of the top emitters, the United States has the largest share attributed to fluorinated gases, comprising about 3% of total emissions (WRI 2010).

Assuming an interest in relative *changes* in emissions, a gas contributing a significant share, but which does not change much over time, could perhaps be omitted from the monitored list.  $CH_4$ and HFCs would not be good candidates, however, because they represent opportunities for nearterm, low-cost mitigation efforts (EPA 2006). An argument might be made to omit N<sub>2</sub>O on this basis; N<sub>2</sub>O emissions have been essentially flat in the United States since 1990, for example (EPA 2010). Mitigation opportunities and their efficacy for N<sub>2</sub>O (primarily associated with agriculture) are hard to quantify and less well-developed than for other gases. Whether N<sub>2</sub>O must be included to achieve the overall required precision depends on expectations on the future role of N<sub>2</sub>O mitigation. To maintain maximum GHGIS functionality, N<sub>2</sub>O should be included.

In summary, a GHGIS is proposed that covers all GHGs necessary to allow confident measurement of total anthropogenic emissions trends, with  $\pm 10\%$  precision. In particular, GHGIS must monitor fossil CO<sub>2</sub>, biogenic CO<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>O, and the majority of fluorinated gases.

## 2.7 Attribution by Sector

As discussed above in the section on framing, attribution of emissions to sector (that is, attribution either by the type of emitting source or the type of fuel used) offers a number of potential benefits. Sectoral attribution allows detailed comparison with bottom-up inventories, the incorporation of sector-specific external information, and detection of departures even with lower monitoring precision. For effective comparison with bottom-up inventories, GHGIS should be capable of attributing emissions to, at least, the following sectors, or categories:

- biogenic (non-fossil) CO<sub>2</sub>,
- coal-power CO<sub>2</sub>,
- petroleum-based transportation CO<sub>2</sub>,
- natural-gas CO<sub>2</sub> from heating and cooking,

- discrete events, such as forest fires or oil-spill burning, and
- select large-scale natural events, such as volcanic eruptions.

As discussed in later chapters, sector attribution is possible by measuring isotopes, such as <sup>14</sup>C and <sup>13</sup>C, and co-emittants, such as carbon monoxide (CO). Different source types and fuels have different isotopic and co-emittant signatures. High spatial resolution of the sensor network and of emissions estimates can also aid attribution when combined with information about the geographic distribution of certain source categories (e.g., emissions in an urban grid square are more likely associated with transportation, while emissions in a rural grid square are more likely biogenic). Specific techniques and capabilities for attribution will be discussed in later chapters.

## 2.8 Conclusions

A high-level requirements framework for GHGIS as a tool to monitor and verify international emissions targets and treaty commitments has been discussed. Since the nature of future emissions-mitigation commitments is unknown, an attempt was made to keep the discussion general, with necessary assumptions made to reach the quantitative conclusions above. In the analysis of alternative framings of GHGIS, the conclusion was reached that the most practical framing is to consider GHGIS as a tool to measure relative *changes* in emissions and compare those with reported changes in bottom-up inventories.

The required precision with a number of quantitative examples was explored, which, although simplified, illustrates a robust conclusion, i.e., that the precision eventually required for monitoring anthropogenic emissions for an operational GHGIS is close to  $\pm 10\%$ . This assumes a GHGIS capable of multiple comparisons with bottom-up inventories or other information.

The ability to compare GHGIS results with inventories and external information drives several other requirements: GHGIS should be capable of attributing emissions to at least a handful of separate sectors, resolving emissions regionally in larger countries, and resolving emissions on a variety of time scales.

The choice of which gases to cover is driven by the assumption that future commitments will be made on total GHG emissions and not on  $CO_2$  alone. To achieve high-precision measurements of the total,  $CO_2$  (both fossil and non-fossil),  $CH_4$ ,  $N_2O$ , and the majority of fluorinated gases (HFCs, PFCs, and SF<sub>6</sub>) must be monitored. However, the primary focus of this report is fossil  $CO_2$ .

On the question of which countries to cover, covering 80% of global emissions is proposed. The choice of the particular countries to cover represents a separate (political/policy) issue. However, the list may reasonably include tens of countries, including countries on every continent except Antarctica and with every type of terrain, with countries ranging in area from  $36 \times 10^3$  km<sup>2</sup> (Taiwan) to  $17 \times 10^6$  km<sup>2</sup> (Russia), and ranging in latitude from 83°N (northernmost tip of Canada) to 56°S (southernmost tip of Argentina).

# Chapter 3. Spaceborne Sensing

## **Chapter Summary**

This chapter addresses the space segment of the proposed Greenhouse-Gas Information System (GHGIS). Global space-borne measurements of GHGs in the atmosphere, including the lower troposphere and with sensitivity to the planetary boundary layer (PBL), sampled at space and time scales that can resolve the variability attributable to natural and anthropogenic processes, represent a component that cannot easily be replaced, especially in view of the advantage that space bestows with respect to denied-territory limitations. While existing and planned-for space-borne capabilities will play an important role in early and prototype GHGIS implementations. New, purpose-built space sensors will be needed to meet GHGIS requirements. Options and concepts to achieve these are discussed in this and other parts of this report.

## Findings

- 1. Satellite observations can deliver a critical GHGIS capability with global GHG observation coverage, including over denied territories.
- 2. Flexible options in satellite orbits provide global coverage at known frequency of overpasses (low Earth orbit [LEO]), near global coverage at 24-hour overpass periods providing a combination of broad coverage with long dwell times over particular areas (middle Earth orbit [MEO]), and continuous coverage of specific geographic domains (geosynchronous orbit [GEO]).
- 3. Satellites can provide critical data to assess actions taken to mitigate or adapt to climate change (including land-use/land-use-change, and installations of energy-production facilities).
- 4. Space-borne sensors can measure GHG concentrations to accuracies that are adequate for flux attribution (e.g., 1-2 ppmv for CO<sub>2</sub> for the AIRS instrument).
- 5. Currently, GHG observations from space derive from sensors designed to support science/research goals and cannot meet the proposed GHGIS operational requirements of measurement density and revisit frequency, lacking adequate measurement density and do not yield near-surface information with sufficiently low uncertainties; however, data-retrievals based on vertical-sampling kernels targeting near-surface data are being developed.
- 6. Satellite observations of combustion co-products, in combination with observations from land and aircraft systems, will be important to discriminate anthropogenic from biogenic emissions of GHGs.
- 7. Development and deployment of satellite systems can take 6 years, or more, from design to validated data delivery; hence, satellites specifically aimed at achieving GHGIS goals will need to be started well in advance of GHGIS operations.

- 8. OCO-2 will be ready for launch by February  $2013^1$  and will measure CO<sub>2</sub> with groundlevel peak sensitivity. It can provide valuable additional information on carbon fluxes, even though its accuracy and validated sampling yields must await its launch, and calibration and validation phases.
- 9. Retrospective analysis of space-borne sensor data can provide information to establish economic/energy sector and forestry baselines.
- 10. Existing imaging space-borne sensors and planned space-borne sensors targeting soilmoisture and other Earth-science data can provide significant contributions to land-use and carbon-cycle modeling that can help with discrimination of anthropogenic vs. natural/biogenic GHG fluxes.

## **Recommendations (Phase 1 Development)**

- 1. Use existing data sets of GHG observations (e.g., AIRS, GOSAT, SCIAMACHY) and, when available, OCO-2, coupled to aircraft and land observations, to improve global CO<sub>2</sub> surface flux maps.
- 2. Develop a robust calibration system for future OCO and other missions using upward-looking FTS measurements from the TCCON network.
- 3. Use existing land cover and imaging data to improve international assessments of land-cover, land-use-change, agricultural productivity, and economic/energy activities.

## **Recommendations (Phase 2 Development)**

- 1. Begin a 2-year design/analysis study to assess choices of orbit, instrument, sampling, resolution, and other options for one, or more, dedicated, GHGIS-specific satellite platforms; included in this study would be improved Observation Systems Simulation Experiment (OSSE) capabilities.
- 2. Design and field purpose-built GHGIS space-borne sensors to augment the current national and international fleet of proposed satellites to meet GHGIS requirements and specifications.
- 3. Rely on the GHGIS Mission Operation Center (GMOC) to control the flow of GHGIS space observations (as well as GHGIS aircraft and land observations), and coordinate with other international observation campaigns

## 3.1 Introduction

The chapter discusses the context for spaceborne observations, followed by a summary of current, planned, and potential satellite sensors that can measure greenhouse gases (GHGs). Next, space-segment capabilities for Phases 1 and 2 are discussed, followed by generalized space-segment architecture information. Finally, risk mitigation and recommended next steps are discussed.

<sup>&</sup>lt;sup>1</sup> The second failure of the Taurus XL launch vehicle that would have been used to loft OCO-2 has resulted in a launch-schedule uncertainty. See http://www.spacenews.com/civil/110623-nasa-suspends-payments-orbital.html.

The nature and role of satellite observations, i.e., the contribution that spaceborne sensors can provide as part of a GHGIS, is global, precise, and synoptic. In addition to space-borne measurements of GHGs, satellite observations of non-GHG atmospheric trace gases and parameters associated with terrestrial and ocean carbon fluxes will also be necessary to support attribution of anthropogenic (vs. natural) activity and reduce errors in the transport and carbon cycle models employed by flux inversion systems, as also discussed in Chapters 1, 2, and 7, and Appendix B. Achieving this will require significant new capabilities not offered by the current, or currently planned, suite of research-oriented spaceborne and other sensors, as also discussed elsewhere in this report. Observations using spaceborne instruments will complement other data from airborne, land-based, and possibly future seaborne sensors as an integral part of the GHGIS.

Satellite observations can offer near-global coverage with spatial and temporal sampling and resolution characteristics that can be designed to the GHGIS task and specifications, such as dense spatial sampling and, in some cases, dense and continuous temporal sampling, for a wide range of biogeophysical parameters as well as of anthropogenic activities relevant to energy, industrial, urban, and GHG/carbon monitoring. In the case of GHGs, spaceborne data would typically be of mole-/mixing-fractions or concentrations of select gases, versus space and time, but could also extend to other relevant quantities, such as thermometry and barometry, and water-vapor, clouds, and precipitation that influence atmospheric chemistry and transport.

A spaceborne-sensor constellation can be designed to offer sustained global observations over all Earth's surface. Global coverage is important to minimize errors in global flux inversions associated with either limited access or boundary conditions. The integration of observational data from spaceborne sensors with those from airborne and land-based sensors in a GHGIS will be critical to tracking carbon stocks and natural biogenic cycling between carbon reservoirs in Earth's atmosphere, oceans, and terrestrial ecosystems, as well as the anthropogenic contributions that GHGIS must monitor in the context of future emissions-mitigation agreements.

An important characteristic of spaceborne sensors is that of cross-calibration and traceability to standards. Comparing the cost of spaceborne sensors relative to hundreds, or perhaps thousands, of less-costly land-based sensors, for example, can only be realized in the context of operations and maintenance (O&M) costs to sustain calibration and stability of many independent sensors to a single stable standard, versus the cost of more costly but many fewer independent spaceborne sensors that incorporate means of on-board National Institute of Standards and Technology (NIST)-traceable calibration.

Finally, spaceborne sensors that rely on high-resolution imaging can also contribute information on land-use/land-use-change (LULUC), such as reforestation/afforestation, as well as renewableenergy installations, nuclear power plants, and large wind-farm or photovoltaic installations that would need to be assessed for the verification and validation of mitigation actions agreed to in the international effort to limit the increase of GHGs in the atmosphere, in support of various types of agreements and mitigation actions that may well differ for different signatories of such agreements.

#### 3.1.1 Greenhouse Gases, Surface Fluxes, and Spaceborne Sensors

The effect of GHGs can be characterized in terms of their global-warming potential (GWP) that is referenced to that of carbon dioxide (CO<sub>2</sub>), the primary GHG. As discussed in the Introduction (Chapter 1), CO<sub>2</sub> represents and is responsible for the overwhelming contribution, and provides the reason why this study and report primarily focuses on detecting and attributing sources (natural and anthropogenic) and storage of this gas, or carbon, in general.

If the desired data product is surface fluxes of these gases, referenced, for example, to carbonequivalent, e.g.,  $gCeq/m^2/yr$ , or CO<sub>2</sub>-GHG-equivalent, e.g.,  $gCO_2eq/m^2/yr$ ,<sup>2</sup> the relation between space and time sampling and resolution requirements and those of the transport models that will be relied upon to deduce surface fluxes from concentration measurements is paramount. For a final product of surface fluxes, requirements on quality/uncertainty, type, and sampling characteristics of data derived from spaceborne sensors can only be set in conjunction with the type, quality/uncertainty, and sampling characteristics of data from other (air, land, and possibly sea) sensors, as well as uncertainties propagated forward by modeling, in addition to other possible contributors to overall uncertainty, as discussed elsewhere in this report.

A major challenge for a GHGIS is addressing lateral fluxes of atmospheric carbon in estimating anthropogenic contributions and attribution, and discriminating against natural/biogenic surface fluxes. Space-based observations of trace gases, combined with appropriate land- and air-based fossil-fuel combustion-product observations, offer an important element in addressing this problem. Space- and air-based observations can also be used to estimate energy activity associated with key emission sectors, and in the synthesis and reconciliation of such (top-down) data with inventory and other energy and economic (bottom-up) data.

#### 3.1.2 Synergy with Air- and Land-Borne Sensors

Spaceborne-sensor observations typically return radiances that can be used to retrieve columnaveraged sounding samples. These are weighted by a vertical sampling function (kernel) that depends on the type of measurement, e.g., reflected sunlight in the visible and near-infrared (VNIR) or thermal emission in the infrared (IR). At this writing, demonstrated column- and footprint-averaged concentration accuracies can be as low as 1 to 2 ppm, as for the data from the mid-tropospheric spectral channel of the Atmospheric Infra-Red Sounder (AIRS) (e.g., Chahine et al. 2005, 2008) that are updated every 30 days. By comparison, land-based in situ sensors provide fixed-point measurements that can be continuous in time with accuracies that can be about one order of magnitude better, i.e., 0.1 to 0.2 ppm, or better in some instances (cf. Chapters 4 and 5), but are confined to the air sampled by a fixed sensor.

One can also perform total-column  $CO_2$  sampling from the ground, using VNIR instruments that more-closely approximate reflected sunlight measurements from space, as performed by the Japanese Greenhouse gases Observing Satellite (JAXA) (GOSAT) and the National Aeronautics and Space Administration's (NASA's) planned OCO-2 mission. However, the vertical sampling functions for the two (space vs. ground) are not identical and, as a consequence, require some

<sup>&</sup>lt;sup>2</sup> The two quantities are in the ratio of the molar masses (gram-formula weights) of C and CO<sub>2</sub>, referenced to the abundant carbon and oxygen isotopes, i.e., <sup>12</sup>C and <sup>16</sup>O, i.e., 1 gCeq =  $(12/44) \times gCO_2$ eq.

degree of modeling, interpretation, and validation, depending on the vertical concentrationprofile uniformity of the gas of interest. Airborne measurements can be of either type, i.e., soundings from high-altitude aircraft that can approximate spaceborne measurements,<sup>3</sup> or onboard analysis of continuously aspirated gas samples acquired in situ during flight, as discussed further in Chapter 4.

Generally speaking, spaceborne measurements can achieve high *precision*, e.g., for estimates of spatial gradients that are less subject to systematic errors that may vary between different measurement sites, as well as for temporal changes that are important in tracking and monitoring the efficacy of mitigation actions, more easily than achieving high *accuracy* that requires low systematic errors for every point measured. Precision is of particular value where spatial-contrast information comes at a premium, while measurement accuracy, i.e., referenced to stable standards, is required in establishing small but long-term trends. As discussed in Chapter 2, the former is accepted as the more appropriate target measurement and data-analysis uncertainty metric for GHGIS.

Within these considerations, a GHGIS will likely be integrating global satellite and airbornesensor data with in situ (locally sampled) data in a common data validation, assimilation, and modeling framework to minimize estimation errors and perform uncertainty quantification, as also discussed elsewhere in this report.

Spaceborne and airborne sensors can measure GHG concentrations over the ocean quite readily. This is significant because the technology for long-lived in situ ocean-borne sensors is currently not sufficiently mature.<sup>4</sup> While measurements over the ocean are and will be essential to advance the state of knowledge of Earth's carbon cycle, this study focuses on measurements and data retrievals over the land surface, where the majority of anthropogenic emissions take place. To repeat, however, this does not preclude measurements of carbon stocks and carbon-flux estimation, and GHGs over the ocean that can be realized from space, or by remote sensing from airborne platforms, as discussed in Chapter 4 and Appendix H, that can be made more reliably and easily, in many cases, than on land.

#### 3.1.3 Driving Requirements

Chapter 2 discusses the general GHGIS requirements framework. However, overall requirements for GHGIS represent work in progress. At the time of this writing, the top-level objectives that map the requirements framework (Chapter 2) to a space segment are:

- 1. GHGIS shall produce country, or sub-country (regional), level estimates of total emissions of  $CO_2$ ,  $CH_4$ , and nitrous oxide (N<sub>2</sub>O) from fossil-fuel consumption, no less frequently than annually, for the largest emitters, with sufficiently low uncertainties to allow detection of variances from reported, or agreed-upon, values.
- 2. GHGIS shall provide country, or sub-country (regional), level estimates of changes in total anthropogenic emissions over time of CO<sub>2</sub>, CH<sub>4</sub>, and N<sub>2</sub>O for the largest emitters,

<sup>&</sup>lt;sup>3</sup> Approximately  $15/16 \approx 0.94$  of the atmosphere's mass is between sea level and an altitude of ~60 kft (~18 km).

<sup>&</sup>lt;sup>4</sup> John Orcut, UCSD/SIO, private communication (July 2010).

with sufficiently low uncertainties to allow detection of variances from reported, or agreed-upon, values.

As with the other parts of this study and report, the discussion of the space segment in this chapter will primarily focus on the portion of the requirements pertaining to  $CO_2$ , with some discussion on  $CH_4$  and some other co-combustion gases discussed in Chapter 2.

Method	Instrument	CO <sub>2</sub> Measurement	CO <sub>2</sub> Precision <sup>a</sup>	Sample Aggregation <sup>b</sup>	Other Gases Retrieved	
Reflected Sunlight	SCIAMACHY	Total column	3-10 ppm	Monthly average; ~700×700 km <sup>2</sup>	CH <sub>4</sub> , N <sub>2</sub> O, CO, O <sub>3</sub> , NO <sub>2</sub> , H <sub>2</sub> O, SO <sub>2</sub> , others	
	GOSAT on IBUKI	Total column	4 ppm (est.) <sup>d</sup>	Monthly average; (10.5 km IFOV)	$\begin{array}{c} CH_4, O_2, O_3, \\ H_2O \end{array}$	
		Stratospheric <sup>e</sup>	TBD <sup>e</sup>	TBD <sup>e</sup>	TBD <sup>e</sup>	
	AIRS	Mid-trop	1-2 ppm	Biweekly average; ~100×100 km <sup>2 c</sup>	CH <sub>4</sub> , CO, O <sub>3</sub> , H <sub>2</sub> O, SO <sub>2</sub> , others	
Thermal Emission		Near-surface <sup>e</sup>	TBD <sup>e</sup>	TBD <sup>e</sup>	TBD <sup>e</sup>	
Linission	IASI-A	IASI-A Mid-trop		Monthly average; (~100 km IFOV)	CH <sub>4</sub> , N <sub>2</sub> O, CO, O <sub>3</sub> , H <sub>2</sub> O, others	
	TES	Mid-trop	~5 ppm	Monthly average; ~1500×1500 km <sup>2</sup>	CH <sub>4</sub> , N <sub>2</sub> O, CO, O <sub>3</sub> , H <sub>2</sub> O, HNO <sub>3</sub>	

Table 3-1. GHG Measuring Satellites Currently in Orbit.

<sup>a</sup> Precision estimates represent expected/hoped for uncertainty goals and include random errors, but no systematic/bias/calibration errors that are difficult to estimate a priori.

<sup>b</sup> Other spatial sample aggregations can yield similar precisions.

- <sup>c</sup> AIRS native resolution is 13.5 km. The mid-tropospheric CO<sub>2</sub> product is released with a 100-km grid resolution.
- d GOSAT data analysis indicates uncertainties with an estimated random component of ±5.5 ppm and a -7 ppm systematic/bias component (Baker 2010), for sample data at present, with ongoing work to improve calibration, validation, and data retrievals. See also Avis (2010, Figure 4 and related discussion).
- <sup>e</sup> AIRS stratospheric and near-surface channel data retrievals are presently under development with uncertainty estimates that are, as yet, undetermined.

#### 3.1.4 Background

Spaceborne systems can estimate  $CO_2$  abundances in the atmosphere using a variety of passive or active remote-sensing techniques, as listed in Table 3-1. One passive technique, VNIR spectroscopy, relies on reflected solar light and the normalization of two  $CO_2$  VNIR bands with an  $O_2$  band, where  $O_2$  is used as a reference molecule of known mole fraction, to estimate the total column of  $CO_2$  (or potentially also other gases, such as  $CH_4$ ) concentration (mole fraction), by comparing absorption features in the selected spectral bands during daylight hours. The Japanese GOSAT mission<sup>5,6</sup> and NASA's OCO-2 mission rely on this method (Figure 3-1, left). A second passive method uses emissions by GHG molecules in the mid-wave (3 to 5  $\mu$ m) or thermal IR (8 to 16  $\mu$ m) spectral bands. Under the right conditions, contributions to the detected spectrum from such molecules can be differentiated from background atmospheric radiation and the Earth's surface based on detailed forward-modeling and data-retrieval techniques (Figure 3-1, right).



Figure 3-1. Left: Reflected-sunlight passive sensing of a select molecule, best realized from a sensor on a sun-synchronous orbit (e.g., SCHIAMACHY, GOSAT, OCO instruments). Right: Passive sensing based on thermal IR emissions (e.g., AIRS, IASI-A, TES instruments). Graphic from a JPL OCO presentation.

Passive-IR sensing does not rely on sunlight and can provide 24-hour sensing coverage, as demonstrated using the AIRS sounder on NASA's AQUA spacecraft. AIRS data are currently used to generate a global mid-troposphere  $CO_2$  product (Figure 3-2) and, along with data from other spaceborne sensors, provide valuable insight into the global  $CO_2$  exchange and transport, as well as  $CO_2$  surface-flux information, both directly and via data assimilation into global models (e.g., Chahine et al. 2008, Jiang et al. 2008, Imbiriba et al. 2010, Lia et al. 2010, Liu et al. 2010, Tangborn 2010).

A comparison between the OCO vertical sampling kernel and the AIRS mid-tropospheric sampling kernel is depicted in Figure 3-3. The difference between the two is important in the context of a GHGIS that is primarily focused on near-surface behavior and surface fluxes.

<sup>&</sup>lt;sup>5</sup> The GOSAT instrument flies on the IBUKI satellite at an altitude of approximately 666 km (not part of the A-train orbit) and completes one revolution in about 100 minutes. The satellite returns to the same point in space in three days. See http://www.gosat.nies.go.jp/eng/gosat/page2.htm for more information and additional discussion below.

<sup>&</sup>lt;sup>6</sup> At this writing, GOSAT data are available in HDF5 format, along with documentation, from the Goddard Earth Sciences Data and Information Services Center Atmospheric Composition Portal through the GOSAT/ACOS page at GES DISC, http://disc.sci.gsfc.nasa.gov/acdisc/documentation/ACOS.shtml, or directly through the search and download software interface Mirador: http://mirador.gsfc.nasa.gov/, or, by using the keyword: http://mirador.gsfc.nasa.gov/cgi-bin/mirador/collectionlist.pl?keyword=ACOS.

Weighted-column averages of OCO-type kernels have a peak, or near-peak, sensitivity near the ground and, as a consequence, can provide data to constrain atmospheric-transport models to infer surface fluxes. Such measurements, however, are also sensitive to high-altitude  $CO_2$  concentrations and require high-fidelity vertical-transport modeling, or other information vs. altitude, to enable reliable inference of surface concentrations and fluxes.



Figure 3-2. AIRS July 2003 mid-tropospheric  $CO_2$  monthly average (450,000 soundings), global-coverage measurements. Color legend indicates  $CO_2$  concentration in ppm, on a  $1^{\circ} \times 1 (100 \times 100 \text{ km}^2)$  grid (M. Chahine, private communication). Approximately, 64,000 such grid cells are required to tile the globe.

Reliance for near-surface behavior on the proven AIRS mid-tropospheric channel data (alone) that have a very low sensitivity to near-surface concentrations (Figure 3-3) would require an even greater reliance on atmospheric vertical-transport modeling and wind-profile data. Reliable modeling and simulation of the relevant dynamics is beyond today's capabilities, by some margin, and expected error propagation will result in unacceptably high surface-behavior uncertainties.



Figure 3-3. Direct comparison between the near IR (NIR) (OCO: blue, 1.61 μm) and the mid-tropospheric thermal-emission (red, near 14.3 μm IR) sampling kernels, vs. altitude (M. Chahine, private communication).

In addition to the mid-tropospheric channel, the AIRS team is developing both stratospheric and, importantly in the context of GHGIS requirements, near-surface  $CO_2$  products, based on kernels derived from different parts of the IR spectrum. A preliminary plot is depicted in Figure 3-4. This part of the work on AIRS data is in progress at this writing and data retrievals have yet to be validated.



Figure 3-4. Three passive thermal IR vertical-sampling kernels for CO2. These rely on different parts of the spectrum and exploit the difference in atmospheric transmissivity vs. wavenumber. The mid-tropospheric kernel (blue) is the same as the one identified with AIRS in Figure 3-3. A first stratospheric data product is available and pending validation. The near-surface kernel is presently under development (M. Chahine, private communication). Further details are discussed in Appendix E of this report. To appear in Pagano et al. (2011).

Both OCO and AIRS fly on the same (A-Train) sun-synchronous orbit (705-km altitude) and a combination of the two types of data could provide near-surface estimates that are better than from any one space sensor alone, though the spatial resolution of the two sensors is quite different (~2 km for OCO vs. ~90 km for AIRS). A more detailed discussion on vertical-sampling kernel options offered by passive thermal IR sounding is included in Appendix E and was also discussed in the recent JASON report (2011).





Figure 3-5. Top: TES global CO map from September 2007. Image from TES (NASA data). Bottom: AIRS August 8-11, 2010, mid-tropospheric (505 mb) CO global map in ppbv (http://aqua.nasa.gov/highlight.php?id=44, downloaded November 5, 2010). Image from AIRS (NASA data). Figures courtesy NASA.

VNIR and IR spectroscopy can also measure some of the other, if not most, gases discussed above and in Chapter 2 that are important in monitoring anthropogenic carbon emissions. Figure 3-5 depicts a global map of CO concentration (ppbv) generated by the Thermal Emission Spectrometer (TES) instrument (top) and by the AIRS (bottom), by way of example. CO is not a GHG, but is co-produced in combustion and important in monitoring fossil-fuel and other combustion of carbon, such as in forest fires, and other phenomena important to global anthropogenic emissions. As with  $CO_2$  measurements, the distribution of CO is determined by its sources and horizontal and vertical transport dynamics in the atmosphere, so while important qualitative and semi-quantitative conclusions can be drawn from measurements of CO concentrations, reliable attribution to surface fluxes requires additional information and modeling. Further, CO is oxidized in the atmosphere, with a relatively short chemical-kinetic life, so it does not accumulate, as does  $CO_2$ , and its presence indicates relatively recent combustion activity corresponding to emissions sources not far upstream of where the measurement is made.

Currently, five satellites measure  $CO_2$  (Table 3-1). The European SCIAMACHY is a VNIR instrument that generates total-column  $CO_2$  maps, which are degraded by the low yield as a consequence of the large SCIAMACHY footprint (e.g., Houweling et al. 2005). Another VNIR instrument, the Japanese GOSAT on the IBUKI satellite, is returning radiances converted to column- $CO_2$  products. Thermal IR sounders, such as AIRS and IASI, measure  $CO_2$  primarily in the middle and upper troposphere, as discussed above, with stratospheric and near-surface spectral channel data retrievals currently under development for AIRS. TES is an IR Fourier-transform spectrometer (FTS) on board the EOS-Aura spacecraft (July 5, 2004, launch).

TES has higher spectral resolution than AIRS and can have a longer dwell time in its step-andstare mode, but it yields many fewer samples than AIRS because of its limited field of view (FOV). TES measurements are sensitive to  $CO_2$  in the lower troposphere, but are characterized by a relatively high ppm uncertainty.  $CO_2$  concentrations derived from TES data have been used to estimate  $CO_2$  fluxes, albeit on very coarse "TransCom" spatial scales (Figure 3-6).



Figure 3-6. Carbon flux estimates from TES CO<sub>2</sub> data on TransCom spatial scales (Kulawik et al. 2010).

Currently, GHG measurements from space suffer from inadequate measurement density, i.e., are seriously under-sampled, both temporally as well as spatially, and do not yield near-surface information with sufficiently low uncertainties. Possible future passive systems such as Carbonsat, OCO-WF, ARIES, and PanFTS (Tables 3-2 and 3-3) are designed to significantly increase measurement density by having a wider cross-track swath (or FOV), along with high spatial resolution. These systems can generate 2 or 3 orders of magnitude more samples of atmospheric  $CO_2$ , per orbit, than the current GOSAT and AIRS instruments.

Method	Sensor	CO <sub>2</sub> Measurement	CO <sub>2</sub> Precision <sup>a</sup>	Sample Aggregation <sup>b</sup>	Swath Coverage	Other Gases	Planned Launch
	OCO-2	Total column	1-2 ppm	2.3 km	8 km	O <sub>2</sub> , CO <sub>2</sub>	2013
Reflected Sunlight	Pre-Sentinel-5	Total column	TBD	10 km	5-50 km	$\begin{array}{c} CH_4, CO,\\ O_3, NO_{2,}\\ SO_2 \end{array}$	2014
	CarbonSat	Total column	1-2 ppm <sup>a</sup>	2 km	500 km	O <sub>2</sub> , CO <sub>2</sub> , CO, CH <sub>4</sub>	2018
	MicroCarb	Total column	TBD	2.3 km	TBD	$CO_2$	2016
Thermal Emission	IASI-B	Mid-trop	2 ppm	100 km	100 km	CH <sub>4</sub> , CO, O <sub>3</sub> , H <sub>2</sub> O, SO <sub>2</sub>	TBD
	IASI-C	ASI-C Mid-trop		100 km	100 km	CH <sub>4</sub> , N <sub>2</sub> O, CO, O <sub>3</sub> , H <sub>2</sub> O, others	TBD
	JPSS/NPOESS CrIS	Mid-trop <sup>c</sup>	Mid-trop <sup>c</sup> TBD ~ 5		50 km	CH <sub>4</sub> , N <sub>2</sub> O, CO, <sup>c</sup> O <sub>3</sub> , H <sub>2</sub> O, HNO <sub>3</sub>	NPP 2011 JPSS-1 '15 JPSS- 2 '18
Active	ASCENDS	Lower-trop	2-4 ppm	~100 km	50 m	СО	2020

Table 3-2. Planned Future GHG Measuring Satellites.

<sup>a</sup> Precision estimates represent expected/hoped-for uncertainty goals and include random errors, but no systematic/bias/calibration errors that are difficult to estimate a priori.

<sup>b</sup> Other spatial sample aggregations can yield similar precisions.

<sup>c</sup> The JPSS/NPOES CrIS sensor is listed here for completeness. It is not expected to yield CO<sub>2</sub> retrievals and, possibly, also no CO retrievals.

It is noted here that for successful assimilation of the data these new systems will provide, bias/systematic/epistemic uncertainties (not removable by averaging) must be reduced to <0.5 ppm, with random/aleatoric errors (removable by averaging) that must be reduced to <2 ppm (Baker 2010).

Active spaceborne GHG sensing measures the absorption of laser radar (LIDAR) signals in discrete bands generated by a (frequency-modulated continuous wave, or pulsed) on-board laser transmitter in the VNIR bands (typically around 1.6 or 2  $\mu$ m). The planned NASA ASCENDS and the potential European A-SCOPE missions both rely on this technique. Active sensors share an advantage with IR sounders in that they can provide 24-hour coverage, and pulsed LIDARs offer the potential for generating CO<sub>2</sub> profiles vs. altitude by gating returns in time bins (2-ns intervals of round-trip time per foot).

The potentially smaller footprint of LIDAR measurements confers an advantage over lowerresolution passive systems by increasing the number of observations that can be considered cloud-free. However, eye-safe considerations may dictate how small the size of the laser ground spot can be for a given laser power, so, without further detailed study, it is not possible to say whether future active sensors can/will return higher horizontal-resolution data than passive sensors.

Given the limitations of current spaceborne data, the carbon-flux community has only just begun to include satellite data in flux inversion or synthesis experiments (e.g., NASA Carbon Monitoring System Flux Pilot). Planned passive systems will generate considerably more GHG measurements than current systems, but data-retrieval/-reduction efforts may still be limited by insufficient data to constrain inversion and transport models.

For GHGIS planning purposes, development time (design, build, test, and launch) for the simplest satellites using mature technology is 3 to 4 years. Sensors that rely on new technology demand even longer schedules. On-orbit checkout and commissioning of a new satellite can take 1 to 6 months or more. Validation of new satellite data products typically requires 1 to 2 years, at a minimum. These times should be borne in mind when considering implementing and incorporating GHGIS spaceborne sensors, as well as when considering replacements of existing of future space assets.

Method	Sensor	CO <sub>2</sub> Measurement	CO <sub>2</sub> Precision <sup>a</sup>	Sample Aggregation <sup>b</sup>	Swath Coverage	Other Gases Retrieved	Planı Laur
Reflected Sunlight	OCO-WF	Total column	1-2 ppm	2.3 km	360 km	O <sub>2</sub> , CO <sub>2</sub> , CO, CH <sub>4</sub>	TB
Thermal Emission	ARIES	Mid-trop	Same as AIRS	1-2 km	1650 km	CH <sub>4</sub> , N <sub>2</sub> O, CO, O <sub>3</sub> , H <sub>2</sub> O, HNO <sub>3</sub>	TB
Pan- spectral	Geo FTS	Total-column to lower-trop	TBD	10 km	500 km	CH <sub>4</sub> , N <sub>2</sub> O, CO, O <sub>3</sub> , H <sub>2</sub> O, HNO <sub>3</sub> , others	TB
Active (LIDAR)	ASCOPE <sup>b</sup>	Lower-trop	2-4 ppm	~100 km	50 m	СО	TB

Table 3-3. Possible Future GHG Measuring Satellites.

<sup>a</sup> Precision estimates represent expected/hoped-for uncertainty goals and include random errors, but no systematic/bias/calibration errors that are difficult to estimate a priori.

<sup>b</sup> Other spatial sample aggregations can yield similar precisions.

The next generation of European, Japanese, and US GHG-measuring satellites is currently under development, with launches in the 2013 to 2020 timeframes (Table 3-2). Other potential missions that are in the conceptual stage (but have no planned launch) are summarized in Table 3-3.<sup>7</sup> These sensors are envisioned as research-based (not operational) with a commensurate acceptance of single-string implementations, irregular data releases, and, for some, relatively

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<sup>&</sup>lt;sup>7</sup> This listing includes LEO and GEO satellites, as presently considered for science/research purposes, but not possible future sensors in MEOs.

short expected lifetimes. These limitations are not necessarily inherent and could be overcome by suitable design and implementation, albeit at the expense of schedule and cost. Opportunities (may) arise for implementations to be hosted on board future satellites (e.g., on JPSS-1 or -2) with an eye to meeting GHGIS operational requirements.

As a general and important observation, acceptable random and systematic uncertainties, as they enter into overall precision and accuracy, are coupled to (validated) data yield. By way of example, it may be possible to impose sufficiently tight consistency and environmental requirements on measurements based on remote-sensing data retrievals to meet a particular set of uncertainty specifications. An example of such a requirement is optical attenuation from atmospheric aerosols and clouds. However, if the probability of meeting the consistency and environmental requirements is small, the number of valid measurements per orbit will be correspondingly low. In designing sensing technologies for the purposes of a GHGIS, it is important to keep such opposing accuracy and yield considerations in mind. Similarly, there is a trade between accuracy and spatial resolution. One may lower (random) errors by averaging over many ground pixels; however, this is realized at the expense of horizontal spatial (grid) resolution in the reported product from the space sensor. Such trades can only be made in concert with the modeling that receives such data, in a system sense.

#### 3.1.5 Orbit Options

The discussion above focused primarily on LEO options on which Earth-observing systems largely rely today. The centerpiece of NASA's current Earth Observing System (EOS) is the A-Train (for *afternoon train*). This is a sun-synchronous orbit that places the nadir point around ~1:30 pm local solar time, enabling periodic observations that rely on sunlight reflected with a fixed sun-aspect angle. A-Train measurements span the electromagnetic spectrum from the ultraviolet (UV) to microwave wavelengths. Having many satellites occupy the same orbit that follow each other by fixed time intervals enables synergies since they observe the same nadir point on Earth only a few minutes apart; measurements from one satellite can be correlated with data from another. Figure 3-7 illustrates the A-Train LEO sequence.

An advantage of the A-Train orbit sequence is that it provides global coverage that repeats every 16 days, or 233 orbits, with observations at a single local (solar) time. This is important in the context of monitoring carbon and GHG emissions in that there is a significant diurnal variation in the carbon cycle driven by photosynthesis (carbon absorption/sink), during the day, and respiration (carbon emission/source) at night by plant life on land and algae on ocean surfaces. A-Train data suffer from a systematic bias, but could be used to extract emissions trends over time, since such samples are synchronized to important natural and anthropogenic cycles.



Figure 3-7. The A-Train LEO sequence (705 km altitude). Inset figure courtesy NASA.

The GOSAT instrument operates on the same principle as  $OCO^8$  and is hosted on the IBUKI satellite. It is in a 666-km-altitude orbit with a 1300 ±15 min nadir local solar time (also sun-synchronous) and observes with a repeat rate of 3 days (72 orbits).

The Joint Polar Satellite System (JPSS) is the civilian portion of the former National Polar-Orbiting Operational Environmental Satellite System (NPOESS) and is managed by NASA for the National Oceanic and Atmospheric Administration (NOAA). JPSS will consist of a LEO constellation of two sun-synchronous spacecraft in different orbital planes with afternoon equatorial ascending nodal-crossing times. The JPSS will carry a payload similar to the NPOESS Preparatory Project (NPP) mission, to fly in 2012, that can potentially be augmented for additional climate monitoring. The currently confirmed payload for JPSS is the Visible/Infrared Imager/Radiometer Suite (VIIRS), the Cross-track Infrared Sounder (CrIS), and the Ozone Mapping and Profiling Suite (OPMS). The JPSS-2 and JPSS-3 missions are planned to launch in 2015 and 2017/2018, respectively.

In summary, sun-synchronous LEO choices bestow many advantages, but also disadvantages. The latter may prove to be acceptable if only *changes* in GHG emissions are the goal of a GHGIS, based on comparisons at fixed local solar time, but they do not help in the characterization and quantification of the diurnal behavior of the natural carbon cycle, or of anthropogenic emissions activities that vary (significantly) between day and night, with variations that differ, in turn, seasonally or over years. Current LEO satellites also provide

<sup>&</sup>lt;sup>8</sup> See http://www.jaxa.jp/projects/sat/gosat/index\_e.html for additional information on the GOSAT instrument and http://www.gosat.nies.go.jp/eng/technology/technology.htm for the IBUKI/GOSAT path calendar, and GOSAT Standard Mesh Point (sampling strategy). Some differences between GOSAT and OCO: GOSAT relies on an FTS instrument that senses two polarization components. OCO is a (more stable) grating spectrometer that senses only one (principle-scattering-plane) polarization.

limited temporal revisit sampling, though this will be partly addressed by future systems with much wider swath capabilities, and possibly through constellations of multiple satellites.

Moving to a higher vantage point, MEO options can be chosen with shorter revisit times and can provide both diurnal sampling as well as global coverage. An illustrative example is a ~12-hr orbit at about 18,000-km altitude depicted in Figure 3-8. Indicated ground coverage for this orbit corresponds to a single 24-hour period coverage with a ground swath chosen with target-elevation (local zenith-complement) angles (TEAs) limited to values above 60°.<sup>9</sup> An advantage of such an orbit is that the sensor is over a particular target area for hours, allowing both high spatial-resolution and essentially continuous (temporal) data to be acquired over particular targets of interest, such as power-plant stacks, industrial plants, etc., for long times. The latter can be used to increase dwell time and hence improve the signal-to-noise ratio (SNR) and to construct time series of measurements. A further advantage is that a single sensor in such an orbit would provide global coverage, with no part of the Earth unmonitored, with optimum (near-nadir) soundings over any location every 30 days, and soundings within the indicated ground coverage every 4.5 days or so, or less if lower minimum TEAs prove acceptable.



Figure 3-8. Illustrative MEO, with ground swath corresponding to a minimum TEA of 60° and a 24-hr coverage that samples almost all of the land mass. Circular region marks the field of view (FOV), corresponding to TEAmin = 60°. Orbit and FOV are indicated in the inset figure on bottom, left.

Surface coverage from such a MEO is indicated in Figure 3-8 and can be seen to provide significant advantages. At this phasing, it affords *near-total global land coverage in a single 24-hour period*. Disadvantages include larger apertures that would be required for a given ground resolution (relative to LEO, for example), or a given required photon flux. Both of these can be maintained by scaling aperture diameter with orbit altitude, albeit at higher cost. An issue

<sup>&</sup>lt;sup>9</sup> Nadir corresponds to TEA = 90°. Soundings at lower TEAs require traversal of the atmosphere at shallower angles, complicating data retrieval and data validation, possibly beyond the point where acceptably small uncertainties (random and systematic) can be realized. Insufficient experience exists at this time to provide a quantitative assessment of this issue, even though useful first assessments could be derived from analyses based on forward-modeling techniques, such as those part of OSSE tools.

of MEO options stems from the (much) higher radiation levels at such altitudes. MEO options are not sun-synchronous and, as a consequence, opportunities to exploit reflected sunlight, especially sunglint off the ocean, are limited. As a consequence, such orbits are better suited to host sensors that rely on IR emissions. As with LEO options, multiple spacecraft in intercalated MEO choices would decrease revisit times by the ratio of their number, or better, since cloud-cover statistics would be less correlated over longer revisit times/locations, or by lowering altitude, or both in any combined manner.



Figure 3-9. Illustrative GEO choice, with three spacecraft and corresponding ground coverage for a minimum TEA of 30°. Scaled orbit and spacecraft locations for three continental region coverage are depicted in the inset figure on bottom, left. Major emission regions are highlighted in red.

A third choice is offered by GEO options, as illustrated in Figure 3-9. GEO confers its own advantage in providing persistent monitoring and surveillance over portions of the globe within the instrument's FOV, but presents some unique calibration challenges. A scanning instrument in GEO can provide very short revisit times, diurnal sampling that is critical for characterizing the exchange of trace gasses with the atmosphere (e.g., Sitch et al. 2003, Rayner et al. 2008), and wide area coverage. Three such platforms would cover most of the global land surface, though coverage would be poor to non-existent in the high arctic and polar regions as a result of a lack of the viewing geometry. Figure 3-9 depicts three such regions corresponding to a minimum TEA of 30°, similar to the angular range of the current AIRS and IASA-A instruments. The viewing geometry will allow sunglint observations over the ocean in only a few select locations. As for the MEO case, increased dwell time can improve the SNR to make retrievals more robust. One unique feature of a GEO vantage point is its very wide field of regard, which means that measurements can be targeted at areas that are relatively clear of aerosol and cloud contamination, increasing the yield (at the expense of coverage).

A given spatial pixel resolution for a sensor in GEO dictates apertures roughly twice as large as for the 18,000-km MEO. This means that GEO observations are best suited for instruments with modest resolution, of say 4 to 10 km. Dedicated GEO spacecraft are relatively costly, but the

commercial communication satellites crowding that vantage point offer numerous opportunities to fly a GHG sensor as a hosted payload. An example of such a sensor is included in Table 3-3.

## 3.2 Phase 1

#### 3.2.1 Space Segment Goals

Based on requirements identified in Chapter 2 and at the beginning of this chapter, four principal goals can be identified for the GHGIS space segment:

- A. Monitoring of country-level and sub-country/regional-level CO<sub>2</sub> and CH<sub>4</sub> atmospheric concentrations, including area source/sinks associated with Agriculture, Forestry, and Other Land Use (AFOLU);
- B. Monitoring fossil-fuel CO<sub>2</sub> emission trends of the largest urban areas (population centers) and power plants;
- C. Earth-system monitoring to improve related science and atmospheric-transport models;
- D. Monitoring emission-mitigation activities including energy, transportation infrastructure, and AFOLU projects.

#### 3.2.2 2014: Phase 1 Baseline Products

Given the development and deployment times indicated above for new spaceborne sensors, satellite observations that could contribute to an initial capability in Phase 1 (through calendar year 2014) are limited to validated data sets available in the 2013 timeframe. The current state of the art in generating higher-level products from spaceborne observations to address goals A through D is summarized below.

# 3.2.3 Global CO<sub>2</sub> 100-km-Resolution Surface Flux Maps With ~200 gC/m<sup>2</sup>/yr Uncertainty

Anthropogenic and biogenic emissions cannot be resolved or distinguished using current spaceborne remote sensing capabilities alone. Global  $CO_2$  surface flux maps can be generated that rely on multiple observations of the quantity of  $CO_2$  in the atmosphere, with estimates of the amount contained within the PBL, fed into a model to yield  $CO_2$  surface-flux estimates.  $CO_2$  flux models used are strongly dependent on underlying weather model and wind-profile data to track atmospheric transport, in general, and the movement of  $CO_2$ , in particular. Ground-based measurements and modeling would be used as a calibration capability for space-based measurements. For Phase 1, baseline products could be generated using GOSAT satellite observation data, if systematic and random uncertainties can be driven low enough, as discussed above. Further information on  $CO_2$  vertical profiles, and in particular on  $CO_2$  concentrations in the boundary layer, could be provided by combining VNIR measurements with those at longer wavelengths in the thermal IR as currently measured (Christi and Stephens 2004). During the Phase 1 period, additional important data could be derived on 100-km scales from the AIRS near-surface channel, if/when that data retrieval is validated, which could occur within the

Phase 1 timeline. Surface-flux estimates would then be inferred through assimilation of these and other data, with appropriate prior estimates, in a chemical-transport model to produce a targeted uncertainty of ~200 gC/m<sup>2</sup>/yr, globally (e.g., Baker et al. 2010 and references therein).

#### 3.2.4 CarbonTracker

Observations of  $CO_2$  mole fraction by NOAA Earth System Research Laboratory (ESRL) and partner laboratories are at the heart of CarbonTracker. They provide information on changes in the carbon cycle, whether regular (such as the seasonal growth and decay of leaves and trees), or irregular (such as the release of tons of carbon by a wildfire). CarbonTracker results depend on the quality, number, and location of available observations. The detail at which the carbon cycle can be monitored reliably increases with the density of the observing network. At present, only land-based data are integrated into CarbonTracker. Comparisons with AIRS data have begun (Baker 2010) and more could be done during the Phase 1 period to help improve and validate this approach.

Figures 3-10 and 3-11 show the components of the present NOAA ESRL  $CO_2$  flux-mapping capability. These data imply that the continental United States, characterized by the denser ground network, is a net carbon sink (natural + anthropogenic), but that estimated uncertainties are comparable to (or locally even greater than) estimated values, i.e., the sign of the net flux could be in error.



Figure 3-10. Current CarbonTracker CO<sub>2</sub> observational network. Graphic from http://www.esrl.noaa.gov/gmd/ccgg/carbontracker/summary.html.



Figure 3-11. An example global carbon-flux and carbon-flux uncertainty map. Graphic from http://www.esrl.noaa.gov/gmd/ccgg/carbontracker. Note that uncertainties at this time are comparable to estimated values, or higher.

#### 3.2.5 Augmented Capability with OCO-2 (by 2014)

An improved map of global  $CO_2$  abundances should be available within about a year of the OCO-2 mission launch (scheduled for February 2013). These data will augment modeling and data-integration capabilities and are expected to produce a global  $CO_2$  flux map with lower uncertainty levels, at a spatial resolution of  $100 \times 100 \text{ km}^2$ , with estimated flux uncertainties better than 200 gC/m<sup>2</sup>/yr (Miller et al. 2007). The current plan is to generate monthly updates to that map when the full OCO-2 capability is achieved. In addition, the benefits of estimating  $CO_2$  profiles with greater discrimination of the PBL using OCO-2 will be explored, in combination with near-simultaneous IR radiance data retrievals from AIRS and possibly TES.

#### 3.2.6 Calibration and Validation

Satellite CO<sub>2</sub> measurement calibration requires a standards-based approach. For OCO-2, a set of upward-looking FTS measurements from the Total Carbon Column Observing Network (TCCON) network will be used to estimate column-averaged CO<sub>2</sub>. Periodically, TCCON measurement sites will be overflown by aircraft with CO<sub>2</sub> measurement systems that will perform spiral flight patterns over a range of altitudes to obtain vertical-profile information. Their sampling systems will be calibrated against known reference standards in the laboratory. Aircraft overflights will be used to calibrate the ground-based FTS systems. Measurements will also be made over TCCON sites by OCO-2 during the "target" mode observations, where the instrument is pointed to the ground-based FTS containers. These measurements will be made at least monthly for each ground site. The data will be used to provide sustained calibration of the satellite column-averaged mole-fraction ( $X_{CO2}$ ) measurements. Additional radiometric calibration data can also be collected, such as moon views, solar calibrations, and vicarious calibrations of specific earth targets.

#### 3.2.7 Augmented Capability with OCO-3 (2015)

NASA is developing a copy of the OCO-2 instrument called OCO-3 that could be deployed on a mission of opportunity as early as 2015 if a host spacecraft and launch vehicle can be identified. Depending on the effective lifetime of the OCO-2 satellite and observational priorities for the OCO-3 satellite, the combined capabilities of the two satellites in appropriately phased orbits would offer improvements in CO<sub>2</sub> flux uncertainties over a OCO-2-only product—perhaps a  $1/\sqrt{2}$  reduction from a 4-OCO simulation, depending on correlation between yield and cloud statistics.

#### 3.2.8 Augmented Capability with SMAP (2015)

NASA's Soil Moisture Active/Passive (SMAP) mission, a combined synthetic aperture radar (SAR) and microwave radiometer is scheduled to launch in 2015 and will offer high space-/timeresolved estimates of soil-moisture and freeze/thaw states. One of the planned SMAP data products will include estimated net ecosystem exchange (NEE) of CO<sub>2</sub> using model assimilationbased soil moisture, temperature, and F/T inputs from SMAP retrievals, along with ancillary information on global land cover and vegetation productivity (GPP), which should result in significant improvements in carbon surface source/sink strength estimation.

#### 3.2.9 Global Land-Cover Map Product (5-m Resolution – TBR)

In the initial phase, satellite sensors can contribute to improved estimates of country-level sources and sinks (part of Goal A) based on a global land-cover map generated using existing multi-spectral and imaging satellites. As with existing GHG-measuring spaceborne sensors, most of these have been developed for research purposes.<sup>10</sup> In the case of LANDSAT<sup>11</sup> and the Moderate resolution Infrared Sounder (MODIS), operational agencies such as the US Geological Survey and US Department of Agriculture rely on the NASA-provided data from these sensors to generate land-cover, land-use-change, and agricultural productivity assessments.

Land-cover maps for the 2011–2013 time frame can be derived from the MODIS land-cover product, now offered with a 1-km resolution, in conjunction with one or more high-resolution  $(\sim 1 \text{ m})$  imaging products. MODIS produces 25-m-pixel native-resolution data currently downgraded to 1 km. A higher-resolution land-cover map product would be possible during this period.

Well-developed land-cover maps are presently generated at the 1-km level, derived from MODIS (Strahler et al. 1999) and Defense Meteorological Satellite Program observations. However, higher spatial-resolution observations (250 m) are available from MODIS but have not been used for high-spatial resolution land-cover maps. Both rely on a 1-km gridded database composited from MODIS Level 2 and Level 3 products. Data are composited over a one-month period to produce a globally consistent, multi-temporal database on a 1-km grid as input to classification and change-characterization algorithms. The land-cover parameter recognizes 17 categories following the International Geosphere-Biosphere Program (IGBP) scheme. For higher resolution,

<sup>&</sup>lt;sup>10</sup> This, of course, refers to civilian satellites only.

<sup>&</sup>lt;sup>11</sup> http://landsat.gsfc.nasa.gov/about/etm+.html.

a data-fusion approach (or synthesis product) could produce an intermediate product that approaches a 5-m resolution land-cover product using the 1-km MODIS product in conjunction with 1- to 5-m images in non-MODIS bands in imagery from other sources. See Table 3-4.

Satellite	Sensor Package	Scene Size	Pixel Resolution
LANDSAT 7 ETM	Multi-spectral (RGB, NIR) plus panchromatic (450 – 900 nm)	8 km × 8 km	15 m
KOMPSAT-2	Multi-spectral (RGB, NIR) plus panchromatic (450 – 900 nm)	TBD	1 m
RapidEye	5 satellites: (RGB, NIR) (440 – 850 nm)	TBD	5 m
QuickBird	Multi-spectral (RGB, NIR) plus panchromatic (450 – 900 nm)	16.5 km × 16.5 km	~0.6 m–2.9 m
ASTER	IR radiometry (520 nm – 11.65 µm)	120 km × 150 m	~15 m–90 m
IKONOS	Multi-spectral (RGB, NIR) plus panchromatic (450 – 900 nm)	11 km × 11 km	~1 m–4 m
OrbView	Multi-spectral (RGB, NIR) plus panchromatic (450 – 900 nm)	8 km × 8 km	~1 m–4 m
SPOT	Multi-spectral (RGB, NIR) plus panchromatic (450 – 690 nm)	60-km swath width	Multi: 10 m Pan: 2.5 m–5 m

Table 3-4. Current Civilian Imaging Satellite Systems and their Capabilities.

#### 3.2.10 Imaging Data

In addition to the MODIS land-cover maps, other imaging satellites can provide surface imaging for LULUC analysis to address Goal A, and to assess economic/sector activity (Goal D). These satellites range from government (National Technical Means) assets to commercial satellite imagery providers, and provide different products based upon their primary objectives and customers. Table 3-4 summarizes some of the significant civilian imaging assets that will be available during Phase 1.

## 3.3 Phase 2

Phase 2 provides an opportunity to meet Goals A through C by deploying new spaceborne sensors.<sup>12</sup> Detailed system and design studies are required before moving forward with a specific observing scenario, or active/passive or VNIR/thermal-IR instrument technologies, and orbitology. Such planning cannot take place in isolation: it must balance the contribution from ground and airborne sensors, modeling capabilities, and uncertainties with data-sampling density requirements, for example, in an integrated GHGIS.

Factors that will be relevant in the selection of a Phase 2 space segment as part of a sustained GHGIS monitoring capability include:

<sup>&</sup>lt;sup>12</sup> It is assumed here that meeting Goal D in Phase 2 will be achieved using national observing assets, which will be addressed in an addendum to this report.

- 1. The mix, possibly tiered, of the observation set (vantage points, orbits, and sensor types).
- 2. The range of retrieved parameters, both direct quantities of interest, such as CO<sub>2</sub> and CH<sub>4</sub> total column mole fractions and vertical profiles, as well as correlative or attribution gas tracers, such as CO, nitrogen dioxide (NO<sub>2</sub>), sulfur dioxide (SO<sub>2</sub>), transport tracers, and land/ocean carbon parameters such as vegetation indices, Leaf Area Index (LAI), Fraction of absorbed Photosynthetically Active Radiation (FPAR), Net Primary Production, soil moisture, freeze/thaw state, land cover, biomass, fire counts, etc.; other auxiliary data such as improved thermometry and barometry, the latter important for improved modeling of wind-field data, as required for transport modeling.
- 3. Timelines for sensor and satellite development, launch, commissioning, and validation, versus GHGIS system and timeline needs.
- 4. Robustness, reliability, and a sustained-replacement strategy.

The space segment will provide observations of the atmosphere, land, and oceans. A complete, optimal evaluation warrants analysis and modeling beyond the reach and resources provided for the present scoping study. The material in this section is based on a rough extrapolation from existing analyses and intended to illustrate some of the space segment trade space. A suitable design effort, including cost/risk/performance trades and integration with other GHGIS elements, as alluded to above, would require 12 to 24 months of analysis to assess and compare the various orbit, instrument, sampling, spatial and temporal resolution, gas-sensing, and other options, in concert with other GHGIS components.

#### 3.3.1 Country-Level Emissions

To address Goal A, the space segment of GHGIS will need to contribute to the estimation of total atmospheric carbon fluxes on a global scale as part of the discrimination of anthropogenic from the (larger) natural fluxes at country or sub-country levels, as also discussed in Chapter 2. Projected maximum uncertainties that are required for such estimates are under discussion. Three challenges are highlighted below and are identified as standing in the way of meeting Goal A.

#### **Reducing Transport-Model Errors**

Global flux estimates are significantly impaired by errors in the wind fields, or atmospherictransport errors (Baker et al. 2006, Prather et al. 2008, Baker et al. 2010, Houweling et al. 2010). In particular, Houweling et al. (2010) showed that *transport errors contribute the primary uncertainty for fluxes estimated from CO*<sub>2</sub> *measurements by the next generation of space-based sounders*. Forward-modeling atmospheric-transport errors increase with distance from the location of the primary data and the uncertainty in the three-dimensional wind profiles. Using flux estimates from an ensemble of models driven by slightly different wind fields, Houweling et al. (2010) showed that errors in transport placed a lower bound on the final uncertainty of 100 gC/m<sup>2</sup>/yr, or worse. Significantly, bias errors in wind-field data were *not* considered, which would further increase this uncertainty. This performance floor would need to be addressed by improved transport models, increased sample density, or both. Generically, such uncertainty levels are not peculiar to the inversion of data derived from spaceborne sensors.

#### Reducing Errors Attributable to Incorrect Process

In view of the large natural flux amplitudes and variations, improved modeling and parameterization of the biosphere-atmospheric exchange (e.g., Sitch et al. 2003; Baker, Doney and Schimel 2006; Rayner et al. 2008) is important and will factor in determining the overall uncertainty budget. However, for the purposes of meeting the GHGIS goals, it is important to differentiate modeling and parameterizations, as needed to close retrievals via transport modeling, from those needed for long-term climatic forecasting. The two are different and should not be confused with each other.

#### Reducing the Impact of a priori Assumptions on Flux Estimates

Baker et al. (2010) and work documented in references therein indicate that relatively minor differences in a priori assumptions used to regularize flux estimates can have a significant impact on final estimates. This is a problem common to attempts to solve a seriously underdetermined problem (e.g., Rodgers 2010); prior knowledge of the system may be inadequate. For robust results, the impact of prior errors must be minimized and, in particular, should not dominate the uncertainty. Currently, the choice of regularization significantly affects both convergence and calculation of a posteriori errors. This issue can be addressed by:

- a. improved algorithms for regularizing the inverse problem and for calculating the impact of a priori assumptions on a posteriori errors,
- b. better assessment of a priori statistics,
- c. increased/improved sampling of high-information content retrievals to reduce the impact of a priori assumptions on final flux estimates, and
- d. improved atmospheric-transport modeling.

Space-based observations can play a key role in items (b) and (c), and help validate item (d).

#### 3.3.2 Urban Domes

To address Goal B, fossil-fuel  $CO_2$  emission trends from the largest emitting countries can be estimated by proxy – that is, by tracking the evolution in  $CO_2$  variations in the planetary boundary layer over and near approximately 1000 large cities (urban domes) and/or large power plants. In situ observations and analysis of the  $CO_2$  concentrations in urban domes indicate that peak diurnal enhancements of 20 to 80 ppm above background are not uncommon for the largest cities (Wunch et al. 2009, Riley et al. 2008, Pataki et al. 2006).

Modeling and airborne remote sensing of plumes from moderate size power plants suggest  $CO_2$  enhancements of 20 ±10 ppm above background, depending on distance from exhaust flues and surface winds (Bovensmann et al. 2010). These signals suggest that monitoring systems must be capable of detecting trends in these enhancements with a precision and accuracy (stability) of 2 ppmv, or less, in the boundary layer, integrated over several years as also noted by Baker (2010). This uncertainty target is consistent with the ability to detect a 10% change in anthropogenic emissions, discussed in Chapter 2.

The NRC (2010a) report on this topic suggests that this concept will require an integrated network involving intensive in situ monitoring of a statistically representative subset (perhaps 100 cities and power plants globally), together with satellite observations of all 1000 targets. The design and implementation of such a monitoring component will also require detailed modeling and simulation. To assist with attribution and transport-error reduction monitoring tracers that are co-emitted with  $CO_2$  will likely be required. For example, as discussed in the NRC report, sulfur hexafluoride (SF<sub>6</sub>) data can be regressed onto  $CO_2$  PBL data to help discriminate the relative contribution of  $CO_2$  from natural versus anthropogenic sources (Turnbull et al. 2009). However, this approach will only work directly if the tracer is co-emitted with fossil-fuel combustion and there are no other nearby sources. For example, Wunch et al. (2009) measured  $CO_2$  above Los Angeles and found co-variations of the measured  $CO_2$  with transport of air from outside the Los Angeles area.

Simple regressive approaches could be performed in conjunction with regional CO<sub>2</sub> emission estimates, ideally using PBL CO<sub>2</sub> data, along with attribution tracers from within or from nearby larger emitters. Such tracers could include, for example, SF<sub>6</sub> and <sup>14</sup>C, as discussed in the Turnbull et al. (2006, 2007, 2009) studies, or CO as a combustion and transport tracer (Palmer et al. 2006, Wang et al. 2009, and recall also Figure 3-4 and related discussion), or methanol, formic acid, or formaldehyde as biogenic tracers (e.g., Beer et al. 2008, Millet et al. 2008a, Razavi et al. 2010). NO<sub>2</sub> and SO<sub>2</sub> are also useful tracers for combustion or coal burning (e.g., Lin et al. 2010). However, care must be taken in the reliance on tracers for information on CO<sub>2</sub> because the ratio of these species to CO<sub>2</sub> depends on changes in combustion efficiency, fuel type and details (e.g., sulfur content), or the (possibly variable) scrubbing effectiveness of combustion-system exhausts. While the qualitative value of such co-monitoring is clear, it will likely require independent monitoring of such changes and variations to reliably integrate tracer information in a manner that leads to reliable quantitative assessments.

#### 3.3.3 Flux Error Reduction and Attribution

To address the stringent uncertainty and measurement requirements associated with Goals A and B, a space segment that monitors PBL  $CO_2$  as well as data needed to characterize transport error, biosphere/atmosphere exchange, and the sampling needed to characterize and reduce the impact of a priori assumptions on the fluxes could be implemented. Such measurements may also provide inputs to decrease transport errors as well as provide correlative and corroborative tracers to help reduce  $CO_2$  flux uncertainties.

Characterizing and mitigating transport errors with space-based measurements to address Goal C will require dense spatio-temporal sampling of  $CO_2$  profiles along with useful transport tracers such as CO. Water vapor isotopes also have the potential for characterizing air-parcel mixing, especially between the free-troposphere and the PBL, and can usually be measured in spectral regions where  $CO_2$  and CO are measured (e.g., Worden, Noone, and Bowman 2007; Frankenberg et al. 2009; Lee et al. 2009). Profiles of these species with vertical discrimination of the PBL from the free troposphere is possible by combining reflected sunlight (or column measurements) with the profiling capability available to high spectral resolution (~0.1 to 0.2 cm<sup>-1</sup>) thermal-IR measurements (e.g., Christi and Stephens 2004, Worden et al. 2007, Landgraf and Hasekamp 2007, Worden et al. 2010). Biogenic tracers, such as methanol, formic acid, and formaldehyde, can also be measured in the PBL with thermal IR sensing (e.g., Beer et al. 2008, Razavi et al.

2010), or ultraviolet radiance measurements (e.g., Millet et al. 2008b). These tracers can be used to help characterize air parcels affected by biogenic sources.

For both the area-flux and urban-emissions goals (A and B), producing an optimal flow-down of performance allocations on the various observations requires rigorous formulation and analysis of error budgets that will, in turn, depend on numerical simulations such as those that rely on OSSE tools. This will further define the measurement requirements for the GHGIS space segment in Phase 2. These will likely include:

- 1. global daily atmospheric soundings (over most of the land and ocean surfaces) to enable area flux estimation of CO<sub>2</sub>, CH<sub>4</sub>, and ancillary tracers (CO, NO<sub>2</sub>, SO<sub>2</sub>, etc.);
- 2. higher spatial and temporal resolution atmospheric soundings focused on high-priority urban areas and power plants with a sampling frequency to be determined by modeling and experiment, plus periodic sampling of area sources to enable fossil-fuel CO<sub>2</sub> tracking and to address transport-model errors; and
- 3. other remote-sensing observations to address various land- and ocean-carbon parameters needed to assess misparameterizations of biosphere inputs to the atmosphere, enhance discrimination of natural vs. anthropogenic sources, and identify flux errors in priors. Since the largest uncertainties in the natural carbon cycle are in the contribution of forests to atmospheric CO<sub>2</sub>, one area to focus on is improving the quality of inputs to models of forest carbon stocks and dynamics (Table 3-5).

Finally, they will also need to include remote-sensing inputs to models that estimate carbon sequestration through altered farming practices, as discussed below.

Table 3-5. Observations for Carbon Stocks and Stock-Change Mapping Products in Support of GHGIS. NASA's DESDynl mission, planned to launch in 2017 (as of this writing), is expected to significantly improve the quality of some of these products.

Poquirod	MAPPING PRODUCTS									
Observation	Global Carbon Stock Maps	Global Maps of Disturbed Areas	Post-Disturbance Biomass Change							
3D Forest structure	•		٠							
Forest Extent	•	•	•							
Disturbance Maps	•	•								
Forest Composition	•	•	•							
Forest Type	•	•	•							
Tree volume	•	•	•							
Slope/aspect	•	•	•							

#### 3.3.4 Soil Organic Carbon

Sequestration of organic carbon in agricultural soils by changing tillage practices is one proposed approach to help reduce  $CO_2$  and other GHGs, with the potential to offset ~13% of US and ~17% of global  $CO_2$  emissions (Lal 2004). Remotely sensing the levels of soil organic carbon (SOC) to monitor such activity and address Goal A presents two challenges: sensing below-ground is difficult, if not impossible, and SOC levels at the surface can only be inferred indirectly.

According to Brown et al. (2010): "Remote sensing can provide data on vegetation characteristics that relate to plant productivity, tillage practices, and measures of crop residue quantity and coverage, which are needed as inputs into models that estimate SOC and predict future SOC changes." Remote sensing from space is therefore useful in generating key indices as input to models that estimate SOC. LAI is one such parameter, which can be estimated reliably from multi-spectral VNIR observations of the surface, such as those made by the spaceborne LANDSAT series. The Cellulose Absorption Index (CAI), derived from imaging spectrometer measurements in the short wave IR bands, is another, which has recently been used to estimate the percentage of crop residue cover, from which it is possible to infer the amount of carbon left as a residue in the soil (Serbin et al. 2009). NASA's HyspIRI mission, currently slated for launch post-2020, is expected to provide measurements with the right spectral, spatial, and temporal coverage to estimate CAI (and LAI), and hence SOC.

Table 3-6. Int	ternational Satellite	Program of	f Record (as	of this writing).
----------------	-----------------------	------------	--------------	-------------------

	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020
ATMOSPHERE																,
GHGs (total column) - US									0CO-2		000-3		Maaaa	aaaaaa	annan a	ASCENDS
GHGs (total column) - international	SCIAMA	ACHY	9//////							Sentine	el-5 Precu	rsor				Sentinel-5
GHGs (total column) - international					GOSAT					Merlin			Microca	arb		
GHGs (free trop) - US	AIRS, T	ES			<i>.</i>		Cris			CrIS						
GHGs (free trop) - international		IASI-A				111111		ASI-B				IASI-C				
Atmospheric Chemistry (CO, NO2, etc) LAND	MOPPIT	¥////////							8							
Soil Moisture	TRMM/	AMSR-E	111111							SMAP				MIS		
Vegetation Index	MODIS	9000					VIRS			VIIRS						
Primary Productivity	MODIS	Mana and a start of the second					VIIRS			LDCM,	VIRS					
Land Cover/Land Use	MODIS						VIIRS			LDCM.	VIIRS					
Top & Sub Canopy Biomass - US	ICESAT						1		1		<b>ICESAT</b>	-2	DESDyr	ป		
Sub Canopy Biomass - International		ALOS F	ALSAR			Shillin		Sentine	F1							
Fires	MODIS	111111					VIIRS			VIRS						
Freeze/Thaw Transition									1.0	10	SMAP			111111		
Land Surface Composition	Landsa	t-7	111111							LDCM						
OCEAN																
Ocean Color - US	MODIS	"anna														PACE
Ocean Color - international	Envisat	MERIS							Sentine	I-3 OLCI						
	12	NASA	Farth Obs	erving Sv	stem	1115				117	1		-			
		foreign	partner													-
		Landsa	t Data Co	ontinuity M	dission (L	DCM): Jo	int Polar	Sensing 5	System (.	JPSS)						
		NPOES	S Prepara	tory Proje	ct (NPP)							1				-
	1111111	Evtand	ad miccia	n						10.5	1					

#### 3.3.5 Implementation

The GHGIS space segment will rely on the following architecture:

- 1. Flight systems (satellites)
- 2. Launch systems
- 3. Mission operations and data systems

This section focuses on the flight systems (spacecraft and instruments they host). Launch systems represent critical enablers, but developments in them are ongoing and not discussed further here. The next section will address mission operations and data systems.

The implementation concept for the Phase 2 space segment starts with an assumed international constellation that builds on the current programs of record for NASA, NOAA, European Space Agency (ESA), CNES, JAXA, and other space agencies, and augments it with new satellites (and associated surface validation observations and data systems) to address residual barriers to

meeting GHGIS Phase 2 requirements. The current (FY11) international program of record of satellites through 2020 is summarized in Table 3-6.

An issue with any satellite program is the risk of launch delays and failures in single-string research-class systems that will introduce gaps in key data records. Therefore, one consideration for an operational GHGIS system must be a strategy for sustained satellite observations including designing individual satellites to offer appropriate reliability and redundancy with a robust replacement program. The NASA operational system that monitors ozone is a classic example. The Total Ozone Mapping Spectrometer (TOMS) instrument (first launched on the Nimbus-7 spacecraft in 1978) and its successor, the Ozone Monitoring Instrument (OMI), have provided a near continuous record of ozone concentrations in the atmosphere, as required. However, that program suffered data gaps because of launch delays (because of launch-vehicle failures) and early failures of orbiting assets (the ADEOS spacecraft in 1997). A robust program with suitable redundancy and planned upgrades will be necessary to avoid these in an operational GHGIS.

The loss of the OCO sensor as the result of a launch-vehicle failure (February 2009) and the recent loss of the Glory sensor for the same reason (March 2011) highlight the issue. If the operational nature of GHGIS is accepted, no single critical sensor loss as a result of launch failure, age, or for other reasons, should bring the system down, as is also the case for the operational GPS system, for example.

A consideration for meeting the GHGIS Phase 2 requirements is the availability and capability of planned satellite observations. For example, OCO-2, possible OCO follow-ons, and related future missions, such as MicroCarb, Merlin, and ASCENDS, can offer important additional monitoring information, even though those missions are also principally driven by exploratory-science requirements of their parent programs and will not necessarily observe the areas of interest with an eye to policy support (decision-support data collection is currently a second priority). Also, the indications are that even if all these observations are combined, they will not offer the flux precision, resolution, cloud-free yield, and sample frequency to meet the final GHGIS space segment requirements.

Such issues can best be addressed by assessing all orbit (LEO, MEO, GEO) and passive and active sensor options (VNIR, MWIR, TIR; FTS and grating spectrometers; spatio-temporal resolution; sensed gases; vertical sampling kernels; etc.), and their combinations. It is proposed that these trades, together with more detailed analyses and modeling, be undertaken as part of the Phase 1 effort to enable space segment decisions to be made, in concert with the other GHGIS components.

#### 3.3.6 Satellite Mission Operations and Data Systems

For the planned international program of record satellites, a federation of Mission Operations Centers and Data Pipelines are envisioned (essentially leveraging capabilities provided by carbon-cycle research programs). Typically, each of these program-of-record missions will collect data asynchronously with other satellites, except where common research observational campaigns are planned.<sup>13</sup> Data pipelines unique to each mission typically generate calibrated observables and geolocated retrievals of geophysical parameters. Subsequent processing by data centers in the carbon-science community then generate products inferred from the observations. For GHGIS Phase 2, an augmented constellation of GHG sounders would be controlled by an integrated Mission Operations Center (MOC). The GHGIS MOC could also coordinate observations with the international program-of-record missions (to the extent possible). For GHGIS Phase 2, the Space Data Center will provide the pipeline data processing for the augmented constellation of GHG sounders and may also ingest products from the international program of record. Much of the latter will be available on various Distributed Active Archive Centers (DAACs) building on existing research programs.

Data downlink systems are also part of the infrastructure for every satellite mission but are not described here. Data downlink infrastructure will be in place to support the international program of record for future satellites through 2020. The addition of the augmented GHG sounder constellation may, or may not, significantly stress the planned downlink infrastructure, depending on spatio-temporal resolution requirements, on-board-processing capabilities that may be implemented, and other considerations.

A Space Data Center will coordinate with surface observations (e.g., TCCON) needed for calibration and validation of instrument retrievals and will deliver to the GHGIS Data Center, at appropriate intervals and interfaces, satellite data products including refined, geo-located estimates of GHG mole-fraction retrievals ( $CO_2$  and  $CH_4$ ), both total-column and vertical profile data (where available), estimated concentrations of various combustion and transport tracers, total  $CO_2$  and  $CH_4$  fluxes on a suitable grid with monthly updates, and other intermediate products, as discussed elsewhere in this report.

## 3.4 Risk-Mitigation Strategies and Next Steps

Currently there are no publically discussed plans by any agency or organization to deploy an operational, global carbon-monitoring system. Absent such a program, continued progress towards meeting GHGIS performance goals and requirements will be limited primarily to ongoing carbon-cycle research programs. As discussed above, the planned international program of record will not deliver the observations need to meet GHGIS Phase 2 performance objectives, at least not through the 2020 time frame that is the span of the current planning horizon.

Development and funding of a formal program for an operational GHGIS may require several years yet to materialize, with no provisions for such a program at present. In the meantime, the following less-costly risk-reduction activities could be undertaken during the Phase 1 period. These seek to preserve the opportunity to deploy a GHGIS Phase 2 capability within a decade or so, should such a decision be made. The dates indicated are based on experience in satellite mission development, an assessment of current critical technology, and the state of maturity of GHGIS design analysis.

<sup>&</sup>lt;sup>13</sup> As discussed above, NASA's Earth Observing System A-train constellation of satellites, which currently includes MODIS, AIRS, TES, and other instruments and ultimately OCO-2, enables observations collected within a few minutes of each other.

The risk reduction tasks for the space segment (with relevance to other GHGIS elements) are

- 1. sensor and system design activity,
- 2. improved OSSE capability,
- 3. technology-development tasks, and
- 4. pilot projects.

#### 3.4.1 Sensor and System-Design Activity

To date, detailed sensor-option analysis and system-design considerations for GHGIS have been limited to small, grass-roots activities by individuals or organizations, the JASON (2010) study and the study documented in the present report. Few opportunities have arisen to work with endusers to define well-posed questions that could be answered with GHGIS information products; to synthesize requirements on products responsive to those questions; to derive quantitative error-budgets, uncertainties, and performance specifications on associated observations, models and data systems; and to perform an adequate exploration of the architectural trade space to generate a cost-/risk-/performance-optimized sensor/system design, in concert with other GHGIS components. Such a design activity would require a significant mission- and sensor-design analysis, systems engineering, and science analysis effort spanning 12 to 24 months, or more. Such a study would need to address implementation plans including programmatics, organizational roles and responsibilities, schedules with key milestones, and budget profiles. A conceptual design and implementation plan would need to be prepared, subjected to independent peer review, and iterated before program formulation.

#### 3.4.2 Improved/Flexible OSSE Toolset

OSSE tools can play a critical role in providing quantitative performance estimates for sensor design and optimization, inverse flux modeling, and other GHGIS needs. Given the complex interaction between different observational methods (basic phenomenology, observing strategies, vantage points, and sensor types) and the range of earth-system models involved in inverse modeling, a numerical simulation approach is required (simple calculations and spreadsheet techniques will not suffice). Current OSSE frameworks are typically focused on a given sensor type or observing strategy. They do not yet offer an integrated assessment of the optimal mix of sensor types and vantage points (including different orbits for satellites and/or the relative value of different satellite and surface observation permutations). At present, OSSEs often take weeks to months to set up and evaluate for each permutation. We propose developing a flexible OSSE toolset that allows rapid, iterative evaluation of the observational trade-space for a GHGIS (including different sensor types, orbits, vantage points, etc.). This would involve a 12- to 24-month focused development and test effort by multiple labs. The proposed improved/flexible OSSE toolset would be available to assess space and possibly other GHGIS components and offer critical support to the system design activity. OSSEs provide a particularly general and valuable framework for all of the components of GHGIS and are discussed separately in Chapter 9.

#### 3.4.3 Technology-Development Tasks

The following proposed technology-development program targets the preservation of options for an expedited deployment of new capabilities within a decade.

Some limiting factors with the existing OCO-2 and -3 designs include the narrow (10-km) swath and the lack of a CH<sub>4</sub> channel. A >500-km wide-field OCO (OCO-WF), augmented with CH<sub>4</sub> and CO channels (to assist with anthropogenic attribution), is a possible next option selected by ESA for Phase A study, but not planned for implementation by the NASA program of record. The key technology challenge for the development of this wide-field concept is the development of advanced immersion gratings.

Observing urban dome trends requires modest spatial and high temporal resolution (<10 km and perhaps hourly sampling to capture diurnal peaks), with boundary-layer sensitivity. Placing an instrument in a MEO or GEO orbit with sufficiently high spectral resolution can provide the required capability. Options should be evaluated and compared, including different types of MEO and GEO sensors, with spectral range and resolution to measure atmospheric constituents ranging from CO<sub>2</sub> and CH<sub>4</sub>, to combustion tracers (CO, NO<sub>2</sub>, SO<sub>2</sub>, etc.) and transport tracers (HDO, N<sub>2</sub>O, O<sub>2</sub>, O<sub>4</sub>, etc.), as well as auxiliary measurements such as temperature and (barometric) pressure to facilitate wind-profile/transport modeling and forecasting. Several key technology challenges would need to be addressed, such as the optical design if high horizontal spatial resolution is a driver; spectrometer design for high spectral resolution and stability; shielding, focal planes, and (possibly new) sensor detector technologies and read-out integrated circuits (ROICs) suitable for a high-radiation environment; design for long life, etc.

## 3.5 Summary

An analysis of current and anticipated near-term spaceborne  $CO_2$  and other GHG measurements indicates that spaceborne sensors could be designed and implemented that would have the capability to support GHGIS goals. The strength of satellite observations lies in their ability to provide global coverage (no denied territory), high measurement density, and high precision, and adequate accuracy. However, spaceborne sensor systems are unlikely to meet performance requirements without the integration of airborne and land-based sensor measurements that can augment as well as serve as transfer standards to enable identification of and correction for systematic errors and biases in the data.

Given the times required for development and deployment of new space sensors, Phase 1 capabilities will necessarily rely on the current assets, plus early OCO-2 data, resulting in an improvement in surface-flux uncertainties. During Phase 1, detailed design and trade-off studies could initiate the development of a Phase 2 space capability that will support the GHGIS requirements, as inferred based on reasonable extensions of performance from existing analyses. A comprehensive set of OSSEs will be needed to provide the rigorous support and assurance of the required (new) performance. Design and technology-development work will be required in the near term, if the next-generation spaceborne sensor system is to be designed, built, tested, launched, and validated within the Phase 2 time frame.

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# Chapter 4. Airborne Sensing

## **Chapter Summary**

The objective of the present Greenhouse Gas Information System (GHGIS) scoping study is to describe an integrated system that provides validated greenhouse gas (GHG) emission monitoring at a country level with an appropriate level of confidence to attribute the source of emissions and discriminate natural from anthropogenic. To achieve a GHGIS that meets these goals requires a system of systems that robustly integrates validated and calibrated measurements with sufficient spatial and temporal resolution from available ground-, air-, sea-, and space-based sensing platforms. This chapter discusses potential contributions from airborne-platform options, focusing on in situ measurements,<sup>1</sup> and provides recommendations for developing such a system.

## Findings

- 1. Sufficiently dense ground- and airborne-based<sup>2</sup> in situ observations can facilitate the location of sources, the inference of surface fluxes, and their aggregation to regional and continental scales by inverse and atmospheric transport models.
- 2. Airborne in situ observations enable calibration and validation of ground-based measurements from fixed locations and satellite-based measurements.
- 3. To confidently attribute regional and national emissions it is necessary to better quantify terrestrial-atmosphere exchange fluxes and GHG concentration throughout the atmospheric column, from strategically located in situ ground and airborne campaigns.
- 4. In situ GHG measurements in the planetary boundary layer (PBL) and in the troposphere by aircraft are spatio-temporally sparse.
- 5. A significant number of international research and academic oriented airborne GHG collection programs exist, including Japanese and European commercial airliner based monitoring programs.
- 6. Advanced airborne platforms (unmanned aerial vehicle, high-altitude airship, and ultralong duration balloon) are sufficiently mature to enable operational utilization.
- 7. Airborne platforms are a cost-effective and risk-mitigating approach to developing spacebased instrumentation.
- 8. Commercially available measurement and analyzer technology is very precise, accurate, robust and stable for implementation of operational airborne-based in situ observation of GHGs.

<sup>&</sup>lt;sup>1</sup> Airborne-based remote sensing of total column-sensed sounding (similar to spaceborne, see Appendix H) measurements in the upper troposphere and stratosphere provide the ability to infer surface fluxes, reduce errors in transport and carbon cycle models employed by flux inversion systems, and support attribution of anthropogenic emission.

<sup>&</sup>lt;sup>2</sup> Airborne-based in situ measurements should be conducted primarily in the PBL.

9. The United States can increase its engagement in international airborne-based GHG measurement programs to foster the development of protocols in support of an international monitoring agreement.

### **Recommendations (Phase 1 Development)**

- 1. Initiate development of an operational US government aircraft-based GHG monitoring program sufficiently dense (defined by system study) to support calibration, validation, and national observational needs; to inform and improve models; and that will couple scales to provide global coverage.
- 2. Utilize cavity ring-down spectroscopy (CDRS), or equivalent-quality, current technology analyzers for airborne-based in situ observation of carbon dioxide (CO<sub>2</sub>), methane (CH<sub>4</sub>), and water (H<sub>2</sub>O).
- 3. Support and collaborate in the In-Service Aircraft for the Global Observing System (IAGOS), Comprehensive Observation Network for Trace gases by AirLiner (CONTRAIL), or both international GHG monitoring programs.<sup>3</sup>
- 4. Obtain a legal opinion concerning international law regarding whether or not sampling air is characterized as collecting meteorological data.
- 5. Initiate the development of an operational US government aircraft-based GHG monitoring program and test bed to: build and deploy a GHG monitoring package using commercially available technology; establish protocols for calibration and validation of ground- and space-based instruments; and establish information assurance and chain-of-custody protocols for monitoring equipment.
- 6. Investigate and assess the establishment of a US-based commercial airliner GHG monitoring program flying international routes.

## **Recommendations (Phase 2 Development)**

- 1. Study and design an airborne monitoring program in conjunction with ground-based and satellite-based systems, utilizing systems studies and test beds to: ensure integration of sampling campaigns and appropriate spatio-temporal scales (flight profiles, frequency, and observations); development of calibration and validation protocols for ground-based instruments; quantify the impact of trade-offs between frequency of limited altitude vs. extensive vertical profile aircraft campaigns; and investigate trade-offs between less-frequent more-capable aircraft campaigns versus less-capable aircraft campaigns, as well as against other sensing modalities.
- 2. OSSE of in situ and remote sensing GHG measurements from mid- to high-altitude aircraft (including commercial airliners) for GHGIS.

<sup>&</sup>lt;sup>3</sup> IAGOS and CONTRAIL focus on mid- and upper troposphere altitudes as such, are important in validating existing spaceborne measurements, assessing the Earth's carbon cycle and atmospheric transport and inversion models. Such measurements do not allow inversion of the resulting data to yield surface emission sources using present-day modeling and atmospheric-transport capabilities, as also noted in Chapter 3.
- 3. Study and investigate application of future unmanned aerial vehicle (UAV) and ultralong-duration balloon platforms.
- 4. Develop and test new airborne monitoring instruments and technology.
- 5. Develop internationally transparent interaction and program support with international airborne GHG monitoring activity(ies).

## 4.1 Introduction

To achieve a GHGIS requires a system of systems that robustly integrates and couples calibrated and validated high-precision measurements with sufficient spatial and temporal resolution from ground-, air-, sea-, and space-based observations to provide global coverage. Validating GHG concentrations over scales from point sources, urban areas, regions, and continents can be achieved using ground-<sup>4</sup> and airborne-based direct in situ observations given sufficient density of observations. With sufficiently dense ground- and airborne-based in situ observations it is possible to locate sources, deduce fluxes, and aggregate them to regional and continental scales through assimilation by inverse and atmospheric transport models bridging the range of spatiotemporal scales (Mays et al. 2009). Without sufficiently dense ground- and airborne-based observations, and an inability to achieve the density due to denied access or other reasons, future satellites may prove able to address and mitigate the collection coverage requirements. However, to do so, future satellites must resolve spatio-temporal, cloud, and marine boundary observation gaps (Buchwitz et al. 2005a, 2005b) and the satellite observations must be precise, accurate, and validated (Buchwitz 2005a, 2005b; Barkley 2006; Karion et al. 2010). Satellites provide an inferred observation that results in estimates of GHG concentrations and fluxes that must initially be calibrated (Buchwitz et al. 2005a, 2005b) and then routinely validated by in situ observations (Ohring et al. 2005, GCOS 2006). Space-based observations require both ground- and airbornebased observations for calibration and validation (Ohring et al. 2005, Wunch et al. 2010, Karion et al. 2010).

Understanding the fate of anthropogenic GHG emissions critically depends on observations and analysis of spatial and temporal GHG concentrations. In particular, in situ and other observations can enable flux quantification, inversion modeling, attribution,<sup>5</sup> and satellite calibration and validation. To confidently attribute regional and national emissions it is necessary to better quantify terrestrial-atmosphere exchange fluxes (Buchwitz et al. 2005a, 2005b; Crevoisier et al. 2006) and GHG concentration throughout the atmospheric column, as well as aggregate observations from smaller scales and strategically located in situ ground and airborne campaigns. Large GHGs concentration uncertainties were found when comparing observations with vertical mixing altitudes in models (Gerbig et al. 2008, 2009) and TransCom studies demonstrate similar uncertainties from simulating vertical mixing in transport models when estimating GHG exchange fluxes employing ground-based observations (Law 1996, 2008; Denning 1999). However, based on a very small number of airborne flask observations flux distribution constraints were achieved when comparing vertical profiles with vertical tracer model distributions (Stephens et al. 2007). To further advance transport and flux inversion models, in

<sup>&</sup>lt;sup>4</sup> Ground-based observations include those from towers.

<sup>&</sup>lt;sup>5</sup> Co-emitted pollutant species, trace gases, and isotope composition can be used for attribution of GHG sources by sectors and nations.

situ measurements at the surface-atmosphere boundary (Crevoisier et al. 2006; Gerbig et al. 2008, 2009) and in the lower to upper troposphere or lower stratosphere (UT/LS) of trace gases are necessary to understand and provide strong constraints on transport and troposphere-stratosphere exchange processes (Boering et al. 1996, Shia et al. 2006, Tiwari et al. 2006, Yang et al. 2007, Matsueda et al. 2008, Miyazaki et al. 2008, Chevallier 2010). Increasing the density of airborne vertical profile observations would contribute data that can be used to decrease the uncertainty in vertical transport modeling (Stephens et al. 2007), hence decreasing modeling uncertainty, while the methodology from exploiting variances between model predictions and measurements to improve models is still progressing. Increased airborne observation density is required for ground-based FTS calibration and validation (Washenfelder et al. 2006, Deutscher et al. 2010, Wunch et al. 2010, Karion et al. 2010). Additionally, increased airborne observation density enhances satellite calibration and validation needs (Ohring et al. 2005, GCOS 2006, Karion et al. 2010) by increasing the probability of co-incident spatial and temporal observations (Peylin et al. 2007, Clerbaux et al. 2008), as also discussed in Chapter 3.

In situ GHG measurements in the PBL and in the troposphere by research aircraft are spatiotemporally sparse (Gerbig 2003, Sawa 2004). The cost and sparseness associated with aircraft GHG measurements have prevented a denser characterization of spatial and temporal GHG variability in and above the PBL. Commercial airliner in situ measurements have been routinely made from Europe as part of the Measurement of Ozone and Water Vapor by Airbus In-Service Aircraft (MOZAIC) since 1994 (Marenco et al. 1998) and the Civil Aircraft for the Regular Investigation of the Atmosphere Based on an Instrument Container (CARIBIC) since 1997 (Brenninkmeijer et al. 1999) research projects.<sup>6</sup> The Comprehensive Observation Network for Trace gases by AirLiner (CONTRAIL), an expansion of the Japan Airlines (JAL) project (Machida et al. 2008), has operated since 1993. These regular GHG observations from commercial aircraft provide an important set of data (Machida et al. 2008) for research into GHG transport that include vertical profiles and UT/LS transects. Aircraft measurements from various intensive campaigns have also been used to quantify or constrain GHGs on a continental or regional scale (Sawa et al. 2004, Mays et al. 2009) and profiles are important for validating models (Stephens et al. 2007).

The utility of GHG measurements on airborne platforms for GHGIS is dependent on the altitude of measurement, the measurement methodology, and the manner in which the measurement is employed. There is a need to increase the density of airborne altitude profiles in the PBL in addition to constraining models they provide an indirect and direct method to estimate regional fluxes (Crevoisier et al. 2006, Stephens et al. 2007, Yang et al. 2007). Regular in situ GHG measurements in the boundary layer undertaken by small commuter airlines or UAVs would have significant utility.

The utility of routine GHG measurements on commercial airliners in the boundary layer has not been sufficiently demonstrated for direct GHGIS measurement (Patra et al. 2011) purposes but has been for modeling purposes. Routine GHG measurement on commercial airliners benefit models and constrain flux estimates (Maksyutov et al. 2003, Crevoisier et al. 2006, Matsueda 2008, Gerbig et al. 2009) and have provided a valuable data set (Machida et al. 2008). By supporting the continuation of existing or establishing a US-based long-term commercial aircraft

<sup>&</sup>lt;sup>6</sup> The MOZAIC and CARIBIC projects have merged into the IAGOS program.

GHG measurement project, an internationally transparent contribution would be established. The role of GHG sampling from commercial airliners, which would be relatively inexpensive, merits further study in a system sense using Observation Systems Simulation Experiment (OSSE) tools, as discussed in Chapter 3 and elsewhere in this report.

In situ measurement technologies and instrumentation are mature and can measure GHG concentration with high precision across scales from meters to regions or continents and in vertical profiles, especially in the PBL. When observations include high-resolution meteorological data (e.g., wind vectors) and are coupled with back trajectory modeling and episodic climate patterns (e.g., Asian outflow), attribution of source location is possible (Liu et al. 1995, Jacob et al. 2003, Singh et al. 2006, Streets et al. 2006, Flowers et al. 2010, Tohjima et al. 2010). This chapter provides background discussion and specific recommendations addressing airborne system contribution toward meeting GHGIS goals.

Below, chapter recommendations will be summarized for ease of access. The number in braces is the subsection in which the recommendation originates.

## 4.1.1 Summary of Chapter Recommendations

- 1. Expand airborne measurement programs to a sufficient density in support of calibration, validation, and national observational needs, as determined by systems studies and in concert with the use of data from other sensors and platforms. {4.1.2}
- 2. Utilize cavity ring-down spectroscopy (CDRS), or equivalent-quality, analyzers for airborne-based in situ observation of carbon dioxide (CO<sub>2</sub>), methane (CH<sub>4</sub>), and water (H<sub>2</sub>O).  $\{4.1.3\}$
- 3. Conduct a detailed systems study to define the density of airborne platforms that are needed to ensure calibration and validation of instruments and data, inform and improve models, and couple scales to provide global coverage, assuming high-precision instrumentation is used in the monitoring system. {4.1.3}
- 4. Support and collaborate in the IAGOS or CONTRAIL GHG monitoring programs and assess the utility of such programs for GHGIS purposes. {4.1.3}
- 5. Obtain a legal opinion concerning international law regarding whether or not sampling air is characterized as collecting meteorological data. {4.1.3}
- 6. Investigate and assess the establishment of a US-based commercial airliner GHG monitoring program flying international routes. {4.2.3}
- 7. Initiate the development of an operational US government aircraft-based GHG monitoring program and test bed:
  - a. Build a commercially available aircraft GHG monitoring package using the most accurate and precise instruments available. {4.2.3}
  - b. Deploy the GHG monitoring package to fully characterize it. {4.2.3}
  - c. Establish protocols for calibration and validation of ground-based and satellitebased instruments. {4.2.3}

- d. Investigate and establish information assurance and data chain-of-custody issues related to monitoring equipment. {4.2.3}
- 8. Study and design optimum aircraft monitoring program in conjunction with ground-based and space-based systems, to using system studies and test bed to address:
  - a. Integration of sampling campaigns ensuring appropriate spatio-temporal scales (flight profiles, frequency, and observations). {4.2.3}
  - b. Development of calibration and validation protocols for ground-based instruments. {4.2.3}
  - c. Investigation of trade-offs between frequency of limited altitude vs. extensive vertical profile aircraft campaigns. {4.2.3}
  - d. Investigation of trade-offs between less-frequent more-capable aircraft campaigns versus less-capable aircraft campaigns, as well as against other sensing modalities. {4.2.3}
  - e. OSSE of in situ and remote sensing GHG measurements from high-altitude aircraft (including commercial airliners) for GHGIS. {4.2.3}
- 9. Study and investigate the application of future UAV and ultra-long-duration balloon platforms with due consideration given to the cost, sensing methodology (in situ and remote), and altitude where such platforms will be yielding measurements. {4.3}
- 10. Design an optimum airborne monitoring program in conjunction with ground-based and space-based systems, to include future UAV and long-duration balloons. {4.3}
- 11. Develop and test new monitoring instruments and technology including:
  - a. Sandia National Laboratories micro-analytical sensor systems. {4.3}
  - b. National Oceanic and Atmospheric Administration (NOAA) AirCore whole air sampling system. {4.3}
- 12. Investigate the use of sensing systems on UAV or ultra-long duration balloon platforms for a variety of applications. {4.4}
- 13. Develop internationally transparent interaction and program support with international airborne GHG monitoring activity(ies). {4.5}

In the remainder of the chapter, general and background information and data related to airborne observation platforms, programs, and technology are presented. A general discussion of airborne observations, covering the questions related to what, where, how, and why, is covered in Sec. 4.2.1. This is followed by a detailed description of current in situ instrumentation technology and a summary of US government airborne platforms and research programs and international programs in Sec. 4.3. Next is a discussion of how an operational GHGIS airborne observation system might be implemented in 3 years in Sec. 4.4. Future airborne systems technology advances 10 years out are raised in Sec. 4.5. Section 4.6 discusses airborne remote sensing for atmosphere, land use, and marine/ocean airborne observation. Section 4.7 briefly discusses the importance of international technical interaction and transparency for an operational GHGIS. Section 4.8 provides a summary.

#### 4.1.2 Airborne Systems

Because of their flexibility and diverse capabilities, airborne systems provide the ability to address a wide range of spatial and temporal observation scales. The wide variety of airborne platforms include aircraft from small (ultra-light) to large, and from single-prop to commercial airliner; balloons from small sondes (radio and balloon) to high-altitude and ultra-long-duration; UAVs from small to large in a variety of designs; and sub-orbital reusable vehicles (if deemed applicable for stratospheric applications). Airborne platforms provide diverse capabilities that address observation requirements and constraints such as payload, duration, range, speed, and altitude. Almost all data from airborne systems can contribute to our understanding of Earth's carbon cycle and transport and flux inversion modeling. As noted above and elsewhere in this report, in situ measurements recorded at lower altitudes, directly support the GHGIS purposes. Airborne remote sensing measurements are applicable to GHGIS purposes (in a manner similar to spaceborne sensing; see Chapter 3 and Appendix H), providing the ability to infer surface fluxes, reduce errors in transport and carbon cycle models employed by flux inversion systems, and support attribution of anthropogenic emission. Airborne remote sensing provides these capabilities, at perhaps lower cost compared to spaceborne, but with denied territory access issues and the need to establish routine campaigns to address spatio-temporal sparseness issues.



http://www.esrl.noaa.gov/gmd/ccgg/aircraft/

Figure 4-1. Airborne observation platforms. Map on right shows sampling locations for aircraft measurements. The PFP or 12-pack is on the left and on the right the PCP. At the bottom is the list of active sampling locations.

### 4.1.2.1 Observation Data

Airborne platforms can be used to collect whole-air samples (flask sampling) or to provide highprecision in situ GHG emission measurements. Flask samples enable additional isotopic and trace gas analysis, but are limited in spatial and temporal variability and density as limited by the number of flasks available. The NOAA/Earth System Research Laboratory (ESRL) Carbon Cycle Greenhouse Gases (CCGG) group has a flask package that provides an example of such instrumentation. The CCGG aircraft program collects air samples in vertical profiles over North America to capture trace gas mixing ratios throughout the boundary layer and free troposphere (up to 8 km). As shown in Fig. 4-1, the system consists of a programmable compressor package (PCP) and a programmable flask package (PFP). The PFP, or 12-pack, is composed of 12 glass flasks and a data logging and control system. The PFP and PCP are available commercially from AOS (Atmospheric Observing Systems) Inc., Boulder, Colorado.

Airborne platforms can be utilized for a variety of other analytical techniques and remote sensing technologies (Payan et al. 2005, Laj et al. 2009), including those for land-use and ocean observation. Airborne observations should include location (three-dimensional global position), time and meteorological data (i.e., pressure, temperature, humidity, wind speed, and wind direction) to facilitate data inversions, as well as modeling development and advancements. To decrease program cost and risk and to ensure validation and calibration, airborne platforms should be used to test and prototype technology that is intended for a space platform (NRC 2010).

## 4.1.2.2 Observation Campaigns

Airborne observations can occur below a maximum altitude, within most of the atmosphere, anywhere above the Earth's surface, from roughly 30 m to 50 to 60 km (upper stratosphere). Airborne GHG monitoring consists of conducting a direct real-time in situ analytic measurement of gas concentration, flask capture of whole air sample for later ground-based analysis, or both. Airborne collection campaigns are flexible; they can be routine, defined for mission-specific strategic objectives, focused on critically important terrestrial areas, regions, or altitudes, or some combination of the three (Mays et al. 2009); for example, vertical measurement profiles only within the planetary PBL, measurements only in atmospheric transition zones between boundary layers (PBL–troposphere and troposphere-stratosphere), measurements spanning defined regions or continents, or along coastal zones.

## 4.1.2.3 In Situ Instruments

In situ instrumentation technology is currently commercially available and can provide highprecision measurements from ground- and airborne- based sensing platforms. For more than 10 years, the preferred technique for high accuracy in situ airborne  $CO_2$  measurement has been conducted via non-dispersive infrared spectroscopy (NDIRS). Recently, commercial instruments that rely on laser spectroscopy are best-in-class for trace-gas sensing. These sensors can measure  $CO_2$ ,  $CH_4$ , and  $H_2O$ . The analyzer conducts a time-based measurement utilizing a near-infrared laser to measure the spectral signature of the molecule using cavity ring-down spectroscopy (CRDS) technology. Whole-air sample using flask-capture technology and subsequent accelerator mass spectrometry analysis is the "gold standard" (ground-truth or baseline) measurement. However, accelerator mass-spectrometry-based analysis requires significant infrastructure, time, and fiscal resources and any significant increase in analysis volume requires additional ground infrastructure capacity investment, so such measurements must be viewed as augmenting other high-volume/-density measurements.

#### 4.1.2.4 GHG Concentration Distribution

To accurately understand and attribute the contribution made by an emitter, or an emitting nation, it is necessary to monitor the concentration and distribution of GHGs over a large area, relative to emission and absorption rates over that area. As discussed elsewhere, great interest is focused on  $CO_2$  because it is the most significant GHG, it directly correlates to combustion of fossil fuels and land-use changes, and is exchanged between the atmosphere and both the terrestrial biosphere and oceans. To increase the confidence in anthropogenic GHG discrimination and attribution it is necessary to measure  $CO_2$  frequently, with high accuracy, over a large region, and diurnally and seasonally. To cost-effectively understand the four-dimensional GHG fluctuation, ground-, air-, and space-based measurements must be coupled in a system sense.

Airborne-based observations can play an important role in the development of a cost-effective, integrated GHG monitoring system because of the high-resolution of in situ measurements, campaign design flexibility, boundary accessibility, low relative cost, and platform variability. Airborne measurements can couple and span the ground- (point-source and small region) to space-based (global) scales. If space-based measurements are lost or unavailable (for example, because of satellite loss/failure, cloud coverage, aerosol scattering, nighttime, or orbit re-visit rate), the flexibility and high resolution provided by airborne systems can, with appropriate resources and access, satisfy measurement gaps. This requires defining a collection campaign's vertical and horizontal profiles and its frequency to ensure coverage.

Further, airborne platforms can (also) host remote-sensing instruments, especially if at high altitudes from which most of the atmosphere is below the aircraft, as discussed separately in Appendix H.

## 4.1.3 Currently Available Airborne Technology

GHG analyzer technologies exist to make real-time in situ airborne observations of  $CO_2$ ,  $CH_4$ , and  $H_2O$  with high accuracy, low noise, and high stability (Chen et al. 2009, 2010). These analyzers are now flown on many of the airborne programs platforms in the US government and internationally.

#### 4.1.3.1 In Situ Instrumentation

CRDS-based analyzers have been developed that deliver high precision and low drift to measure the CO<sub>2</sub>, CH<sub>4</sub>, and H<sub>2</sub>O GHGs at the parts-per-billion (ppb) level. The CRDS technique introduces a gas sample into an optical cavity where the optical absorbance of the sample is determined, providing gas concentration or isotopic ratio measurements. The basic components of the 2010 Picarro Model G2301-m CRDS analyzer, by way of example, are a laser, an optical cavity with two or more mirrors, and a photo-detector, as illustrated in Fig. 4-2. Light from the laser is injected into the cavity through one partially reflecting mirror. Inside the cavity over time the light intensity builds up and, using a photo-detector located outside the cavity, is monitored through the second partially reflecting mirror. By rapidly turning off the laser and measuring the light intensity in the cavity as it decays (exponentially), the "ring-down" measurement is made. The light intensity decay depends on the losses due to the cavity mirrors and the absorption and scattering of the sample being measured. An effective path length of tens of kilometers through the sample is produced after shutting off the laser, since most of the light remains trapped within the cavity for a long period of time. The high sensitivity of the CRDS is because of the long effective path length (Crosson 2008).



Figure 4-2. 2010 Picarro Model G2301-m flight measurement CRDS analyzer for CO<sub>2</sub>/CH<sub>4</sub>/H<sub>2</sub>O and a basic block diagram of the components (www.Picarro.com; Crosson 2008).

Current implementations of the CDRS technology are found to be stable, can be flown without drying the air or in-flight calibration, and yield highly accurate airborne measurements of  $CO_2$  and  $CH_4$  (Chen et al. 2009, 2010; Karion et al. 2010). Again returning to the Picarro's Model G2301-m by way of example, it has been flight-tested at NOAA/ESRL to determine its precision (defined as the standard deviation of continuous measurements of a single gas) in flight; it was 0.08 ppm for  $CO_2$  and 1 ppb for  $CH_4$  (Karion et al. 2010). Similar results have been reported by other groups (Chen et al. 2010).

The 2010 G2301-m decreased in power and size by 30% (relative to previous implementations) and has the performance and system specifications shown in Table 4-1.

The best CDRS instruments offer high precision and compare well to results from flask capture analysis (Karion et al. 2010, Chen et al. 2010). A near-term (perhaps long-term) monitoring program will continue to depend on flask capture sampling analysis for calibration and validation requirements, but determining the sampling frequency, measurement impact, and cost require additional study.

**Power dissipation** 

Warm-up time from off

Maximum Aircraft Altitude

Table 4-1. Performance and System Specifications for the 2010 G2301-m.

Performance Specifications, in air						
Parameter		Specification	CH <sub>4</sub> Specification	H <sub>2</sub> O Specification		
Precision (1- $\sigma$ over 30 secs, vibration @ 20 Hz, 1g):	< 200	) ppbv	< 1.5 ppbv	< 100 ppmv		
Drift at STP (Peak to peak of 300 second average):	< 200 hours	) ppbv over 30	< 1.5 ppbv over 30 hours	< 100 ppmv + 5% of reading		
Drift with Changing Temp (30 second peak to peak over 3 hrs; 15°C/hr within range 10-35°C):	< 7.5 ppbv/°C		< 0.05 ppbv/°C	N/A		
Drift with Changing Pressure (30 sec peak to peak over 3 hrs; <1.4 Torr/sec in range 250 – 760 Torr):	< 700	) ppbv	< 7.5 ppbv	N/A		
Operating Range	300 p	opm to 700 ppm	300 ppb to 2,600 ppb	0 – 2.5%		
Measurement Interval (Mode 1)	< 2.5 seconds		< 2.5 seconds	< 1 minute		
Measurement Interval (Mode 2)		econds	< 5 seconds	< 5 seconds		
Rise/Fall time (10-90%/90-10%) <		seconds	< 2.0 seconds	N/A		
System Specifications						
Parameter		Value				
Measurement Technique		CRDS				
Measurement Cell TemperatureControl		Within 0.002 °C				
Measurement Cell Pressure Control		Within 0.003 atm				
Inlet gas temperature		10 °C to 35°C				
Inlet gas pressure		250 - 1000 Torr				
Inlet gas flow rate		0.35 to 0.45 L / min				
Variation in Gas Flow	20% peak to peak (From 250 Torr to 1000 Torr)					
Gas type		oil free ambient air, non-condensing				
Ambient Temperature Range	-	+ 10 °C to + 35°C				
Maximum Rate of Change in Ambient Temperatu	ire	15°C/hr				
Relative humidity	0 % to 100%, non condensing					

 Maximum Rate of Change in Altitude
 1000 meters per minute

 Data from www.Picarro.com and Datasheet for 2010 Picarro Model G2301-m.

#### 4.1.3.2 Summary of US Government Airborne Programs and Platforms

The US Government conducts a number of airborne-based Earth Observation and Climate change research programs at the National Aeronautics and Space Administration (NASA), NOAA, National Science Foundation (NSF), and DOE-SC Atmospheric Radiation Measurement (ARM). As comprehensive review of these programs is not possible, short descriptions of some will be presented. There have been a large number and wide variety of programs both based and undertaken within these agencies and sponsored academic research. One of the first large-scale airborne programs started with the NASA Global Atmospheric Sampling Program (GASP) program in the 1970s, utilizing commercial airliners. Airborne-based observation is a mature observation approach and continues to advance technologically, as evidenced by UAV developments. A broad sampling and description of these programs follows.

< 370 Watts, steady state

< 1 hour @ + 15°C

Altitude @ 250 Torr

#### 4.1.3.2.1 Airborne Programs

#### NASA Programs

*Global Atmospheric Sampling Program (GASP)* – The GASP program began in 1972. It was the first to use commercial airliners in routine service to obtain atmospheric data. The program progressed from design and acquisition of hardware to collecting global data on a daily basis. Fully automated systems were operated on a United Airlines B747, two Pan American World Airways B747s, a Qantas Airways of Australia B747, and the NASA CV-990 research aircraft. Atmospheric trace constituents in the upper troposphere and lower stratosphere were measured from March 1975 through June 1979. In situ measurements of atmospheric ozone, carbon monoxide (CO), clouds, and related meteorological and flight information were obtained.

**Global Tropospheric Experiment (GTE) Expeditions**<sup>7</sup> – GTE was initiated as a series of global airborne measurement campaigns to study the impact humans had on the global troposphere. The map in Fig. 4-3 shows the locations for the GTE campaigns. Short descriptions of the Chemical Instrumentation Test and Evaluation (CITE) experiments, Atmospheric Boundary Layer Experiment (ABLE), Transport and Chemistry near the Equator in the Atlantic (TRACE-A) experiments, and Pacific Exploratory Missions (PEM) A and B are provided below.



Figure 4-3. Map of research flight tracks for Airborne Tropospheric Chemistry Field Campaigns (1983–2006).

**CITE Expeditions** – The CITE-1 mission had two airborne campaigns (1983 and 1984) to evaluate instrumentation for measuring CO, nitric oxide (NO), and the hydroxyl radical (OH). The CITE-2 mission focused on intercomparison of techniques for measuring nitrogen dioxide (NO<sub>2</sub>), nitric acid (HNO<sub>3</sub>), and peroxyacetylnitrate (PAN), as well as a re-evaluation of NO techniques. The CITE-3 mission focused on an intercomparison of techniques to

<sup>&</sup>lt;sup>7</sup> GTE material and figures are courtesy of NASA and were copied from http://www.air.larc.nasa.gov/missions.htm.

measure key sulfate species sulfur dioxide  $(SO_2)$ , dimethylsulfide (DMS), hydrogen sulfide  $(H_2S)$ , carbonyl sulfide (COS), and carbon disulfide  $(CS_2)$ .

**ABLE Expeditions** – The ABLE expeditions focused on the atmospheric boundary layer exchange and the chemistry and transport processes over various different regions. ABLE-1 was conducted in 1984 from Barbados and focused on the chemistry and transport processed over the tropical Atlantic Ocean and the rain forest of French Guyana. ABLE-2 was based in Manaus, Brazil, and focused on the chemistry and transport over the Amazon Rain Forest during the dry season of 1985 (ABLE-2A) and during the wet season of 1987 (ABLE-2B). The ABLE-3 mission was focused on the chemistry in the northern latitude and the Arctic tundra as a source/sink of  $CH_4$ , ozone (O<sub>3</sub>), and CO. The first phase, ABLE-3A, was conducted in 1988 from bases in Point Barrow and Bethel, Alaska. The second phase, ABLE-3B, was conducted in 1990 from sites in Canada.

**PEM-WEST Expeditions** – PEM-West focused on characterizing the impact of the natural and anthropogenic emission from the Asian continent on the chemistry of the troposphere over the northwestern Pacific Ocean. PEM-West encompassed two field campaigns during the two major contrasting meteorological regimes in the northwestern Pacific. The first, PEM-West(A), occurred during minimum outflow from the Asian continent. Illustrated in Fig. 4-4 are the flight paths and predominant wind direction during the outflow. PEM-West(B) was conducted during spring 1994, a period of maximum outflow from the Asian continent (Fig. 4-5).



Figure 4-4. PEM-West(A) study was conducted from September to October 1991. On the left are flight tracks and the right depicts the predominant continental outflow winds.

**TRACE-A and TRACE-P Expeditions** – The TRACE-A experiment was conducted in September and October 1992 to investigate the distribution of atmospheric trace gases over the tropical South Atlantic. This portion of the Atlantic troposphere is coupled by atmospheric transport of emissions from both South America and southern Africa. The experiment was conducted to study the impact of emission from these two continents on a seasonal enhancement of tropospheric O<sub>3</sub> over a large region of the South Atlantic Ocean off the coast of Brazil and southern Africa. The objectives of TRACE-A focused on determining the relative importance of natural versus anthropogenic emission/processes on the formation of this O<sub>3</sub> enhancement. The second experiment, TRACE-P, was conducted in March and April 2001. The TRACE-P objectives were to determine the chemical composition of the

Nominal Flight Tracks for the NASA Aircraft During

Asian outflow over the western Pacific in spring in order to understand and quantify the export of chemically and radiatively important gases and aerosols, and their precursors, from the Asian continent and to determine the chemical evolution of the Asian outflow over the western Pacific in spring and to understand the ensemble of processes that control the evolution. The flight tracks of TRACE-A and TRACE-P are shown in Fig. 4-6.



Figure 4-5. PEM-West(B) study was conducted during the spring (February to March) of 1994. On the left are flight tracks and the right depicts the predominant continental outflow winds.



Figure 4-6. On the left are flight tracks for TRACE-A experiment in the southern Atlantic and on

#### NOAA Programs (http://www.esrl.noaa.gov/gmd/ccgg/)

the right are flight racks for TRACE-P in the western Pacific.

The discussion on NOAA presented here is focused on the CCGG group programs and is not necessarily representative of all of NOAA's activities. Additional discussion is provided in Chapter 5 on ground measurements. The NOAA ESRL CCGG group conducts ongoing discrete measurements from land, sea-surface sites, and aircraft, and continuous measurements from baseline observatories and tall towers. These measurements document the spatial and temporal distributions of carbon-cycle gases and provide essential constraints to our understanding of the

global carbon cycle. It began the cooperative air sampling network effort, represented in Fig. 4-7, in 1967 at Niwot Ridge, Colorado. The network is an international effort that includes regular discrete samples from the four NOAA ESRL/GMD baseline observatories, cooperative fixed sites, and commercial ships. Air samples are collected approximately weekly from a globally distributed network of sites. Samples are analyzed in Boulder by CCGG for CO<sub>2</sub>, CH<sub>4</sub>, CO, molecular hydrogen (H<sub>2</sub>), nitrous oxide (N<sub>2</sub>O), and sulfur hexafluoride (SF<sub>6</sub>). Measurement data are used to identify long-term trends, seasonal variability, and spatial distribution of carbon-cycle gases.



Figure 4-7. NOAA CCGG cooperative measurement program network.

The CCGG aircraft program has been dedicated to collecting air samples in vertical profiles over North America since 1992. The program objective is to capture seasonal and inter-annual changes in trace-gas mixing ratios throughout the boundary layer and free troposphere (up to 8 km). Most aircraft flights collect 12 flask samples at different altitudes; the samples are stored in glass flasks for later analysis of CO<sub>2</sub>, CO, N<sub>2</sub>O, CH<sub>4</sub>, H<sub>2</sub>, and SF<sub>6</sub>, as well as isotopes of CO<sub>2</sub> and CH<sub>4</sub>, and multiple halo- and hydrocarbons. The CCGG also has a number of additional aircraft special projects, which include:

- Indianapolis Flux Experiment (INFLUX) INFLUX is a case study of the greater Indianapolis region contributing toward the atmospheric measurement of CO<sub>2</sub> and CH<sub>4</sub> (along with other related species) as a way to evaluate a first step towards a monitoring, reporting, and verification system that could be deployed across the planet. Through aircraft measurement, instrumented cell towers, and continued improvement of the approach, the goal is increased understanding of the uncertainties. See Appendix G for more details.
- Mid-Continent Intensive (MCI) MCI is a test bed for methodologies used to determine the carbon flux between land surfaces and the atmosphere. The goal is to validate and compare regional carbon flux estimates derived from "top-down" atmospheric budgets

and "bottom-up" ecosystem inventories, facilitating further evaluation and improvement of both approaches.

- US Coast Guard Collaboration: Alaska (ACG) Collaborating with the US Coast Guard in Alaska, where a C-130 aircraft conducts biweekly flights as part of their Arctic Domain Awareness mission, usually flying from Air Station Kodiak up to Barrow and back, the CCGG has installed flask packages, a continuous CO<sub>2</sub>/CH<sub>4</sub>/H<sub>2</sub>O analyzer (Picarro), and a continuous O<sub>3</sub> monitor (2B Systems) on the C-130.
- HIAPER Pole-to-Pole Observations (HIPPO) This is described below in NSF/National Center for Atmospheric Research (NCAR).
- Indianapolis Urban Plume Study
- Sacramento Urban Plume Study
- Martha's Vineyard Tower Project
- AirCore Atmospheric Sampling System

#### **NSF/NCAR HIPPO**

The HIAPER Pole-to-Pole Observations (HIPPO) project is investigating the carbon cycle and GHGs throughout various altitudes of the western hemisphere through the annual cycle. The main goal of this program is to determine the global distribution of  $CO_2$  and other trace atmospheric gases by sampling at various altitudes and latitudes in the Pacific Basin. HIPPO will measure cross sections of atmospheric concentrations approximately pole to pole, from the surface to the tropopause, 4 to 6 times during different seasons over a 2.5- to 3-year period. A comprehensive suite of tracers of the carbon cycle and related species will be measured:  $CO_2$ ,  $O_2$ :N<sub>2</sub> ratio, CH<sub>4</sub>, CO, N<sub>2</sub>O,  $^{13}CO_2$ : $^{12}CO_2$ , H<sub>2</sub>, SF<sub>6</sub>, COS, chlorofluorocarbons (CFCs), hydrofluorocarbons (HFCs), hydrochlorofluorocarbons (HCFCs), and selected hydrocarbons. HIPPO will transect the mid-Pacific Ocean. The program will provide the first comprehensive, global survey of atmospheric trace gases, covering the full troposphere in all seasons and multiple years.

#### Naval Research Laboratory (NRL) Military Support Division (MSD)

The MSD has a Scientific Development Squadron that operates and maintains aircraft that are available as research platforms. These aircraft support a broad range of projects and experiments, including environmental, and have had a wide range of sensor and instrument payloads.

#### DOE-SC Atmospheric Science Program (ASP)

The ASP within the Office of Biological and Environmental Research (BER) addresses scientific uncertainties related to global climate change, with a specific focus on the role of clouds and their influence on the transfer of radiation in the atmosphere. BER has adopted a unique twopronged approach: utilizing the ARM Climate Research Facility (ACRF), a scientific user facility for obtaining long-term measurements of radiative fluxes, cloud and aerosol properties, and related atmospheric characteristics in diverse climate regimes; and establishing a new standard for climate research observations, by deploying a suite of cutting-edge instrumentation for obtaining continuous measurements of cloud and aerosol properties. Observations at fixed and mobile sites are supplemented periodically with observations from aircraft. The DOE Research Aircraft Facility at the Pacific Northwest National Laboratory consists of an advanced sampling platform, the Grumman Gulfstream I (G-1) and associated flight crew, technical and engineering support staff, and state-of-the-art instrumentation, available for support of missions in the DOE ASP.

#### 4.1.3.2.2 Airborne Platforms

A number of research-oriented airborne systems are supported by the US government. The platforms associated with various agencies include aircraft with NASA, NOAA, NSF/NCAR, NRL, and DOE-SC ARM; balloon sondes with NASA, NOAA, NSF, and DOE-SC ARM; and UAVs with NASA, NOAA, and DOE-SC ARM. Some are shown in Fig. 4-8. These airborne platforms are summarized below (not necessarily complete). The aircraft are used in a collaborative manner amongst the agencies exploiting the overlap in research, experiments, and instrumentation interests and needs. There a large number of airborne (aircraft, balloons, and UAVs) research platforms associated with academic institutions. The European research community also has a variety of research platforms.

These aircraft platforms serve a variety of Earth-observation missions but are not dedicated operational GHG monitoring platforms. The military has a large variety of operational-related airborne platforms addressing missions ranging from weather observation to war fighting.



Figure 4-8. Some examples of the US research aircraft.

*NASA Aircraft Overview* – The platforms available as of 2010 are listed in Table 4-2, obtained from the recent NASA publication *NASA Airborne Science Newsletter* (Spring 2010).

Airborne Science Program Resources	Platform Name	Center	Duration (Hours)	Useful Payload (Ibs.)	GTOW (lbs.)	Max Altitude (ft.)	Airspeed (knots)	Range (Nmi)	Internet and Document References
Core Aircraft	ER-2	NASA-DFRC	12	2,900	40,000	>70,000	410	>5,000	http://www.nasa.gov/centers/dryden/ research/AirSci/ER-2/
	WB-57	NASA-JSC	6	6,000	63,000	65,000	410	2,172	http://jsc-aircraft-ops.jsc.nasa. gov/wb57/
	DC-8	NASA-DFRC	12	30,000	340,000	41,000	450	5,400	http:///.nasa.gov/centers/dryden/ research/AirSci/DC-8/
	P-3B	NASA-WFF	12	16,000	135,000	30,000	330	3,800	http://wacop/wff.nasa.gov
	Gulfstream III (G-III) (mil: C-20A)	NASA-DFRC	7	2,610	45,000	45,000	459	3,400	http://airbornescience.nasa.gov/ platforms/aircraft/g3.html
NASA Catalog Aircraft	DHC-6 Twin Otter	NASA-GSFS- WFF	7	5,000	12,000	25,000	160	500	http://www.twinotter.com
	King Air B-200 AND UC-12B	NASA-LARC	6.2	4,100	12,500	35,000	260	1250	http://airbornescience.nasa.gov/ platforms/aircraft/b-200.html
	DHC-6 Twin Otter	NASA-GRC	3.5	3,600	11,000	25,000	140	450	http://www.grc.nasa.gov/WWW/ AircraftOps/
	Learjet 25	NASA-GRC	3	3,200	15,000	45,000	350/.81 Mach	1,200	http://www.grc.nasa.gov/WWW/ AircraftOps/
	S-3B Viking	NASA/GRC	>6	12,000	52,500	40,000	450	2,300	http://www.grc.nasa.gov/WWW/ AircraftOps/
	Ikhana (Predator-B)	NASA-DFRC	30	3,000	10,000	52,000	171	3,500	http://airbornescience.nasa.gov/ platforms/aircraft/predator-b.html
New Technology	Global Hawk	NASA-DFRC	31	1500	25,600	65,000	335	11,000	http://airbornescience.nasa.gov/ platforms/aircraft/globalhawk.html
	SIERRA	NASA-ARC	11	100	445	12,000	60	550	http://airbornescience.nasa.gov/ platforms/aircraft/sierra.html

Table 4-2.	NASA Aircraft	Platforms Available	è
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Data from NASA Airborne Science Newsletter, Spring 2010.

*NOAA Aircraft Overview* – NOAA has 13 research aircraft. As of 2003, the platforms available are listed in Table 4-3, obtained from the NOAA report on Airborne Platform Requirements for the Ten-Year Period from FY2003–FY2012.

Aircraft Type	GIV-SP	WP-3D	CE-550	AC-690A	DHC-6	AC500S	B-212	MD-500	LA-27
Manufacturer	Gulfstream	Lockheed	Cessna	Gulfstream	DeHavilland	Rockwell	Bell	Hughes	Lake
Common Name		P-3	Citation	Turbo Cdr	Twin Otter	Shrike	Helicopter	Helicopter	
Number Owned	1	2	1	1	2	2	1	1	2

Data from Report of NOAA's Airborne Platform Requirements for the Ten-Year Period from FY 2003 – FY2012.

*NSF NCAR Aircraft Overview* – NSF has four research aircraft serving the science community in understanding and predicting the earth system. The Gulfstream V and the C130Q are located in Colorado, the King Air is located in Wyoming, and the Twin Otter is located in Monterey, California. The Gulfstream V supports the HIPPO of Carbon Cycle and Greenhouse Gases Study.

NRL Military Support Division (MSD) – The Scientific Development Squadron operates and maintains three P-3 Orion aircraft that are uniquely configured, two RC-12 aircraft, four Scan

Eagle UAVs, and one MZ-3A airship. The majority of the fleet is stationed at the NAS Patuxent River, Maryland. The squadron is military certified and operated and deployable worldwide.

**DOE ARM Aircraft Overview** – DOE has two primary aircraft and leases additional as needed to support Office of Science and ARM program needs. The two aircraft are the Gulfstream-159 (G-1) and a Cessna Turbo 206. There is also a UAV program that has a number of platforms, in particular the General Atomics Gnat-750, Altus, and Altus-II.

#### 4.1.3.3 International Programs – IAGOS and CONTRAIL

A number of research programs have utilized commercial airliners as an aircraft observation platform to ensure routine atmospheric profiling with vertical PBL profiles and UT/LS transects, resolving spatio-temporal sparseness (Gerbig et al. 2003; Sawa et al. 2004; Machida et al. 2008). These programs have helped characterize the spatio-temporal characterization of GHG distributions above the PBL, where they are generally well-mixed.<sup>8</sup> The IAGOS and the CONTRAIL, both of which are currently active programs, will be discussed.

*IAGOS* – The IAGOS program is a partnership between Airbus Industries, European research institutions and universities, and commercial airlines. The IAGOS objective is to operate a global-scale distributed infrastructure for long-term observations of atmospheric trace gases ( $O_3$ , CO, CO<sub>2</sub>, CH<sub>4</sub>, NO<sub>y</sub>, NO<sub>x</sub>, H<sub>2</sub>O), particulate matter, and cloud particles from long-range inservice commercial airlines flying A340 and A330 aircraft. IAGOS is a program that has resulted from a consolidation of the European-based MOZAIC since 1994 (Marenco et al. 1998) and the CARIBIC since 1997 (Brenninkmeijer et al. 1999) research projects. IAGOS observations include  $O_3$ , CO, relative humidity, and cloud droplet backscatter and an optional package.<sup>9</sup> All instrument packages are commercial off-the-shelf and designed and certified to fly on Airbus A340 and A330 aircraft. Certification is required because installation requires penetration of the Airbus aircraft hull. Air inlet flow is controlled by a flow pump. Observations are recorded on 4-s intervals corresponding to a vertical or horizontal resolution of roughly 20 to 30 m, or 1 km, respectively.

One aircraft over one year of flight can provide ~2.45 million in situ observations with 680 vertical profiles (0 to 12 km), assuming a typical Airbus utilization factor of ~93% and a trans-Atlantic flight time of 8 hours (~7200 in situ observation/flight). Figure 4-9 provides the global flight tracks for the IAGOS program; note the lack of Pacific Ocean transects.

**CONTRAIL** – The CONTRAIL program is an expansion of the JAL project (Machida 2008) and has operated since 1993 using two Classic Boeing 747s. The main objective of CONTRAIL is to measure GHGs. The JAL foundation manages the program and is composed of Tohoku University, the National Institute for Environmental Studies, the Japan Aerospace Exploration Agency (JAXA), the Meteorological Research Institute (MRI), JAL, and JAMCO. From 1993 to 2005, GHG (CO<sub>2</sub>, CH<sub>4</sub>, and CO) concentrations in the upper atmosphere (~10 km) from

<sup>&</sup>lt;sup>8</sup> It is for this reason, that tracing/attributing GHG distributions above the PBL to surface-source behavior presents a serious challenge.

<sup>&</sup>lt;sup>9</sup> The following are options for the second instrument package: (1)  $NO_x$ , (2)  $NO_y$ , (3)  $CO_2$ +CH<sub>4</sub>, or (4) aerosol particle size distribution and composition (can detect soot, volcanic ash, and dust).

Australia to Japan have been observed. Air samples were collected approximately two times per month and the data were analyzed by MRI.



Figure 4-9. Flight tracks flown for IAGOS (MOZAIC and CARIBIC programs).

By 2006, new observation equipment, in situ continuous and flask sampling equipment, was developed, certified, and installed in new Boeing 747-400 and Boeing 777 aircraft. By 2007, five Boeing aircraft had observation equipment certified and installed (three 777s and two 747-400s). JAMCO has obtained approval for supplemental-type certification from the US Federal Aviation Administration and Japan Aviation Authorities to install this equipment on Boeing aircraft. The air is captured without skin penetration by pulling it off the existing aircraft air conditioning, and inlet flow is managed by a pump and flow controller. Figure 4-10 provides a comparison of the global flight tracks for the MOZAIC, CARIBIC, and CONTRAIL programs; note the presence of Pacific Ocean transects.

In situ measurements from commercial airliners significantly increase spatio-temporal density of measurements, addressing sparseness issues in a relatively inexpensive manner. Data from CONTRAIL vertical profiles (takeoff and landing) are being utilized to understand and constrain surface fluxes and atmospheric transport modeling of CO<sub>2</sub> concentrations (Patra et al. 2011). During 2009 there were approximately 27,000 daily commercial airliner flights for the major (top 39) carriers globally; if a fraction of these flights were used for GHG observations, a significant decrease in spatio-temporal data sparseness would be achieved. To understand and illustrate the value of the IAGOS or CONTRAIL programs in terms of addressing spatio-temporal sparseness, a simple calculation is undertaken and the results summarized in graphical form in Fig. 4-11. If five flights a day were instrumented to measure GHGs and the following assumptions held (the utilization of a commercial/cargo airliner is 90% [328.5/365 days of a year]; average duration of international flights is 8 hours/day [~9,460,800 seconds/year]; and an in situ measurement is made every 4 seconds/flight

[~2,365,200 measurements/year]), then 11,826,000 measurements/year and 3,285 vertical-profiles/year would be made during the flight transects.



Figure 4-10. Flight tracks flown for the MOZAIC, CARIBIC, and CONTRAIL programs.

The value and importance of airborne in situ observations has been briefly summarized in discussions in Sec. 4.3.2 and Sec. 4.3.3. As part of any GHGIS system a routine global observation contribution is necessary. Joining an international program provides a technical gain in terms of decreasing observational data sparseness and increasing data for satellite and modeling validation.



Figure 4-11. Number of measurements/year and number of vertical-profiles/year that could be made, for a given number of flights/day that had GHG measurement instrumentation packages.

The IAGOS and CONTRAIL programs conduct in situ measurements. From the literature, it is not clear if there are any legal liabilities associated with these programs. A key issue that should

be addressed is the determination if any international laws or treaties may restrict such sampling. Meteorological sampling and measurement of a variety of environmental parameters is an ongoing activity on all commercial airliners.

## 4.2 Phase 1 (Operational Airborne-Based Observation System)

Validating GHG concentrations over scales from urban areas, to regions, to continents can be achieved with the contribution of airborne-based in situ observations given sufficient density of observations. Such an airborne observation system is achievable in 3 years; the only limiting factor is the availability of resources. The in situ measurement technologies (AOS, Inc.) have GHG analyzers (Picarro, Inc., and LiCor, Inc.) and flask capture technologies (AOS, Inc.) have been commercialized. An operational airborne system would need to be designed with the appropriate mix of aircraft platforms and campaigns to address observation requirements and national needs, in concert with other GHGIS components. As part of GHGIS such an airborne system would need to meet sampling density and location requirements to support aggregation through assimilation by models bridging across this range of spatio-temporal scales, in concert with other GHGIS measurement modalities.

This subsection describes the general characteristics of an airborne-based atmospheric observations system that could be delivered in 3 years. The system coverage and observations would provide input to modeling and analysis components, in concert with other GHGIS sensors, enabling the characterization of GHGs distributions. This discussion assumes the existence (design) of an appropriate ground-based observation network. The basic system relies on complementary routine and concentrated aircraft campaigns that are assumed to be implemented and operational; the locations and profiles require the following additional analysis:

- Routine GHG operational airborne observations in small aircraft generally associated with a ground location to provide observations of sources and sinks over time and supplemented by more sophisticated and greater spatial (vertical and horizontal) jet campaigns.
- Routine frequent commercial airborne GHG measurements hosted by long-haul international carriers that transect in the UT/LS and short-haul carriers that commute primarily in the PBL, if OSSE studies can demonstrate that such measurements are of significant value within a GHGIS.
- Concentrated aircraft campaigns that produce observations to assess the routine GHG operational airborne observations; calibrate/validate ground and space measurements; address tactical and strategic national observation requirements; and further refine modeling and analysis tools.

# 4.2.1 Characteristics of Routine Operational Airborne Observations Associated with a Subset of Ground Sites

The fundamental characteristic of ground-site associated airborne-based observation requires vertical profiles through the PBL and into the middle troposphere using small aircraft with high spatio-temporal resolution. These routine aircraft profiles can be made with CRDS analyzers to measure GHGs. The number of observation locations and aircraft campaigns will be determined

and will likely require small jet aircraft with more sophisticated instrumentation, including flask samples, and acquiring observations over a much greater range and vertical profile.

To account for diurnal and seasonal variations, additional analysis will be needed to determine the number of multi-flights/flight-day required. Flask samples should also be utilized on a subset of flights to facilitate observation aggregation and correlation across different locations, to ensure measurement of other gases and isotopes, and for calibration and validation requirements. No land-use or ocean monitoring has been considered, but could be part of the goals of these observations.

## 4.2.2 Characteristics of Routine Commercial Airborne Observations

The fundamental characteristic of commercial airborne-based observation requires vertical profiles primarily in the PBL using smaller commercial aircraft with high spatio-temporal resolution, or in and through the PBL and into the UT/LS on international commercial airlines. These routine commercial aircraft profiles can be made with the CRDS analyzers to measure GHGs since they have proven to be robust, stable, and accurate. Flask samples on a subset of flights would facilitate aggregation and correlation of observations from different locations and ensure measurement of other tracer gases and isotopes. No land-use or ocean monitoring has been considered, but should be part of these observations.

## 4.2.3 Characteristics of Concentrated Airborne Observational Campaigns

Concentrated aircraft observation campaign design depends on the operational observational need or mission gaps and must ensure tactical and strategic observation requirements are satisfied. A detailed systems analysis is required to quantify and define designs to resolve many of the issues raised in this paragraph. Concentrated aircraft observations should provide spatial and temporal observation coverage of GHG distributions across regional to continental scales and ensure sufficient continental-scale observations, in concert with other GHGIS sensing modalities; sufficient upwind and downwind, perimeter, and coastal observations relative to a region or continent; open ocean and coastal boundary observations designed with in- and outflow boundary conditions resolved; sufficient observations dependent on episodic climate events and associated ground-based observation density; and regional diurnal observations within and above the PBL correlated with high-resolution meteorology. Additionally, concentrated airborne observation campaigns may be necessary to independently assess routine observations associated with a ground site (those discussed in Sec. 4.4.1); for calibration/validation of ground and space measurements with special focus on vertical profiles; and to address appropriate horizontal spatial coverage for trace gas distributions and model refinement advancements.

# 4.3 Phase 2 (Future Airborne Systems Technology Advances)

Measurements from airborne platforms provide a low-cost approach relative to space-based measurements, albeit with much-reduced global coverage, per platform, and are subject to denied-territory limitations. As technology developments continue to decrease the size, weight, and power (SWaP) requirements for instrumentation, airborne costs will continue to decrease as

both platform size and payloads decrease while technical capability increases. The proliferation of UAV production and application reflects technology advancements.

The development and application of UAVs (e.g., AeroVironment, Inc.'s Global Observer<sup>10</sup>) and ultra-long-duration balloon technology for GHG observation will open new possibilities for observing, monitoring, and measuring remote locations of the Earth and atmosphere; for example, persistent dwell opportunities.

The Predator (NASA Global Hawk, see Fig. 4-12) and Global Observer (AeroVironment, Inc., see Fig. 4-13) fly autonomously with long duration and range capabilities while carrying large payloads. This opens new sensing capabilities and possibilities for innovative observation campaigns. UAV technology will increase the value airborne platforms provide relative to risk mitigation, increasing technologic innovation, enhancing calibration and validation processes, and decreasing cost when used to develop and test future space-based instrumentation (NRC 2010). The application of airborne platforms for space instrumentation development has led to most of NASA's significant space program results (NRC 2010).



Figure 4-12. NASA Global Hawk.

General technology advances beneficial to GHGIS will result in the computational hardware and modeling domains, including embedded processing at the sensor. Advances related to instrumentation will result from miniaturization supporting SWaP gains, such as micro-analytical sensor systems (Schubert 2010). Micro-analytical systems based on modular MEMSbased components for gasphase analysis been have in



Figure 4-13. AeroVironment, Inc. Global Observer.

development and could be deployed in the field (Schubert 2010). New technology development as such as the AirCore atmospheric sampling system (Karion et al. 2010) will also benefit SWaP requirements and facilitates balloon or UAV deployment of whole air sampling.

In Fig. 4-14 on the right is the AirCore and on the left is a diagram of the laboratory testing apparatus. The AirCore below is a 150-m-long stainless-steel tube capped at one end and open at the other with a 0.025-cm wall thickness and a 0.64-cm outside diameter. AirCore passively samples the atmosphere relying on positive change in ambient pressure for collection. While

<sup>&</sup>lt;sup>10</sup> Stratospheric global persistent remote sensing capability, targeting payloads up to 400 lb and an endurance up to 1 week, at an altitude of 65,000 feet (www.avinc.com). At this writing, this UAV has successfully conducted some test flights, but its operational capabilities have not been established as yet.

rising to a high altitude (tested to 8 km) the tube empties; as it drops through the atmospheric column the positive pressure change refills the tube with ambient air and the tube is capped on the ground (bottom of profile) until analyzed. A continuous vertical profile is captured with no mixing in the tubing (i.e., convection) due to the slow molecular diffusion of air. AirCore is flexible (i.e., thickness, weight, length, shape, size, etc.) and can be hosted on multiple airborne platforms, including aircraft, balloons, and UAVs. See Karion et al. (2010) for measurement performance relative to repeatability and comparison to aircraft flask data.



Figure 4-14. The AirCore (right) and diagram of laboratory testing apparatus (Karion et al. 2010).

The operational GHGIS will benefit from technological advancements as they are evaluated and approved for utilization in the system.

# 4.4 Airborne Remote Sensing for Atmosphere, Land Use, and Marine/Ocean Observations

As previously discussed, airborne systems can measure GHG concentrations utilizing in situ and flask capture techniques. Such measurement can be achieved over the ocean routinely with no detrimental impact from clouds or marine boundary haze. While this study is mainly focused on obtaining measurements attributable to specific countries and thus over their terrestrial surfaces, airborne systems provide a mechanism to obtain in situ measurements downwind and offshore from where anthropogenic emissions occur. Airborne remote sensing systems with or without in situ capabilities are also applicable to atmosphere, land use, and marine/ocean observations.

In addition to atmospheric in situ and flask-capture techniques, airborne systems are an important element of a national remote sensing system, and a GHGIS in particular, utilizing remotely sensed data for observations of atmosphere, land use, and marine/oceans, supported by ground and space observations, and field studies. Airborne remote sensing is an efficient method for the expeditious collection of data over a specified area and is a cost-effective means of monitoring the atmospheric, terrestrial (land use), and marine/ocean environments. It enables the rapid acquisition of data for sudden or unexpected events, such as forest fires, and provides an intermediary scale with which to validate satellite data (along with in situ measurements), as discussed previously.

Appendix H provides detailed discussion of GHG concentration measurement in the atmosphere via airborne-based remote sensing. Airborne remote sensing of the atmosphere can provide flexible yet targeted observations of specific regions.

Asner (2009) showed how aircraft systems can cover large areas for measurements. In general, the airborne component of a national system will rely on data collected by instruments flown on aircraft providing optical, radar, laser radar (LIDAR), and hyper-spectral data. In airborne remote sensing, downward- or sideward-looking instruments are mounted on an aircraft to obtain images of the Earth's surface. An advantage of airborne-based remote sensing, compared to satellite remote sensing, is the capability of offering very high spatial resolution images (20 cm or less) at lower cost, albeit with a more limited coverage area. Space-based remote sensing has the advantage that it provides a large coverage area but achieving high spatial resolution requires high-cost spacecraft (with large collecting apertures). Space-based remote sensing, unlike airborne-based, must resolve the effects of the ionosphere on signals (attenuation, degradation, errors, etc.), thus some instrumentation may only be technically feasible for airborne systems. Conversely, airborne remote sensors must contend with the turbulent boundary layer on the aircraft hull, aero-optical effects, and, for passive data retrievals, deal with the fact that the contribution from air near the aircraft can be large, even though that may not be of interest.

Newer radar instruments have been employed to collect forest-cover information through clouds (Hoekman and Quinones 2002). Airborne sensors utilizing high-resolution imaging can contribute data related to land-use/land-use-change, such as agricultural production, industrial facilities (especially energy-related nuclear, coal, wind, and photovoltaic plants), and reforestation/afforestation. Since remote sensing technology cannot assess soil and dead wood carbon stock, an indirect method for measuring forest carbon in the Amazon by merging airborne and satellite LIDAR information has been discussed (Asner 2009). Progress is also occurring in the development of technologies and approaches to remotely sense forest carbon stocks using airborne sensors (Drake et al. 2003; Brown et al. 2005).

Rosenqvist (2003) points out that the ability to retrieve biomass is enhanced when airborne sensors with polarimetric synthetic aperture radar (SAR) are utilized (e.g., the Jet Propulsion Laboratory's AIRSAR or DLR's E-SAR). Combining LIDAR with L-Band polarimetric radar using NASA's LVIS and UAVSAR has been effective in validating the Biomass and Vegetation Canopy Structure measurement requirements of NASA's DESDynI mission, scheduled for launch in 2017. If P-band wavelengths are used this can provide better sensitivity in higher woody biomass regions, as measured by NASA's AirMOSS and ONERA's SETHI system, and proposed for the European Space Agency's BIOMASS mission, which may launch in 2016. Airborne VHF-band SAR systems also have some potential for use in higher biomass regimes, as demonstrated by Sweden's CARABAS system (Rosenqvist 2003).

# 4.5 International Transparency

Long-term success and acceptance of a GHGIS will require international contributions. GHGIS as an operational system contributing toward an international agreement will have specific reporting and data chain-of-custody requirements. It will be necessary and beneficial for the United States to quickly leverage international efforts and to initiate transparency-related activity(ies). Recent international treaty/agreements have been strengthened and sustained

through international engagement (e.g., International Atomic Energy Agency nuclear safeguards and Comprehensive Test Ban Treaty). To this end, the United States should actively engage in collaborations and contribute to programs that meet or correspond to our GHG monitoring objectives.

An opportunity to join a global airborne-based monitoring partnership exists that increases routine atmospheric GHG monitoring and appears cost-effective and reliable, when factoring in international interactions. The European IAGOS program has expressed interest in US participation. The Japanese CONTRAIL program may also present a similar collaborative opportunity. Establishing US national laboratory collaborations would support monitoring objectives and transparency needs.

# 4.6 Summary

Airborne-based platforms and measurement technology are mature and can immediately provide direct and indirect contribution to GHGIS monitoring capability. Combining a globally distributed sufficiently dense ground- and airborne-based (transects and profiles in the PBL) in situ measurement system would support discrimination and attribution of sources; the inference of surface fluxes and their aggregation to regional and continental scales by inverse and atmospheric transport models that bridge the spatio-temporal scales; and GHG concentration throughout the atmospheric column in the PBL. However, unencumbered global access is not anticipated, which requires that a monitoring system include space-based capabilities to resolve denied access issues. Airborne in situ observations are required for calibration and validation of ground-based Fourier-transform spectrometer measurements and hence satellite-based measurements. OSSE analysis of a monitoring system that includes ground, airborne, and space capabilities are required to design the most cost-effective capability for the nation.

An important issue that an operational GHGIS will need to address is continuity of monitoring ("measurement chain-of-custody") capability. The unfortunate loss of recent space-based measurement platforms during launch, OCO in 2009 and GLORY in 2011, increase awareness of this issue. When space-based measurements are lost or unavailable (for example, due to launch failure, satellite loss/failure), the flexibility and high resolution provided by airborne systems can, with appropriate resources and access, be applied to satisfy measurement gaps. This will require defining an airborne collection campaign (vertical and horizontal profiles and frequency) to ensure monitoring coverage. A replacement strategy for the space system contribution will need to be addressed to ensure constancy in monitoring with overlapped systems (CCSP 2003; GCOS 2003; Ohring et al. 2005) since gaps are possible with platform loss due to launch, mission life, and hazards of space. For GHGIS, the development of a space system component will need to provide sufficient resources and build gap-filling airborne- and space-based capabilities to support contingency plans for loss mitigation (for example, quick response launch).

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# Chapter 5. Ground-Based Sensing

## **Chapter Summary**

This chapter discusses the contribution that measurements taken from the ground would make to a GHGIS system. A cornerstone component of a top-down greenhouse-gas (GHG) emission verification and validation system, as described in this scoping study, will be atmospheric measurements of spatial and temporal distributions of GHGs and trace-gas species that are direct markers of GHG-emission sources. In general, there is significant overlap between the needs of GHGIS and of the general carbon cycle and atmospheric chemistry communities. This allows GHGIS to leverage ongoing activities, e.g., basic monitoring and field intensives, particularly during the GHGIS developmental phase. An initial basic-science approach of higher density of observations than possibly needed may be indicated for diagnosis of model results and determination of the true level of intensity needed in an operational framework, as is proposed to be determined by system studies. The following findings and recommendations provide a general summary.

## Findings

- 1. Given the dominance of the *amplitude* of terrestrial and oceanic biosphere  $CO_2$  (bidirectional) fluxes over fossil-fuel-generated  $CO_2$  emissions, discrimination and attribution of anthropogenic  $CO_2$  presents a major GHGIS challenge.
- 2. Discrimination will be aided by the detection of relevant fossil-fuel  $CO_2$  tracers such as radiocarbon (e.g.,  ${}^{14}CO_2$ ) and other combustion byproducts.
- 3. Direct observations of tracers with short photochemical lifetimes (e.g., because of atmospheric photochemical reactions) will be useful and perhaps critical in providing a time-stamp from the source; such information could be quantified to assist transport and inversion-model retrievals.
- 4. Sufficient meteorological data are necessary to provide information to the retrieval system and such data need to include the depth of and other information about the planetary boundary layer (PBL).

## **Recommendations (Phase 1 Development)**

- 1. Synthesize and standardize data streams of existing basic carbon cycle, atmospheric chemistry, and environmental pollutants, and develop a coordinated National Atmospheric network as part of an integrated GHGIS that leverages and builds upon existing infrastructure and expertise across all agencies.
- 2. Using the United States as a test bed, leverage and/or augment ongoing activities and field projects of relevance to GHGIS needs, as indicated by system studies.
- 3. In a requirements-based framework, invest in proven and developing technologies to increase automation of analyses and the world-wide capacity of key analyses that we already know GHGIS will need (e.g., <sup>14</sup>CO<sub>2</sub>, AGAGE suite of tracers, chip-based CO<sub>2</sub>, SF<sub>6</sub>, CO sensors, next-generation FTS), as indicated by system studies.

4. Begin the required socialization in the international community for GHGIS research that would transition into operational monitoring. This could leverage activities undertaken by the Integrated Global Carbon Observing System, the World Meteorological Organization, and efforts under the CTBT.

# **Recommendations (Phase 2 Development)**

- 1. In anticipation that treaty needs will likely include net  $CO_2$  (e.g., LULUC/AFOLU) emissions, develop improved analysis of biosphere and fossil-fuel  $CO_2$  tracers and required biophysical modeling that combines and integrates remote sensing and in situ measurements, as discussed elsewhere in this report.
- 2. Co-design of tracer measurement and transport-inverse-modeling strategies to obtain maximum benefit from available and emerging technologies. This includes observations towards better model boundary layer physics and model intercomparison projects (MIPS) and OSSEs, as also discussed elsewhere in this report.
- 3. In a requirements-based framework and as indicated by a systems analysis, invest in new analytical techniques (with longer development times) to measure and monitor combustion trace gases, isotopes, and specific novel tracers.

# 5.1 Introduction

A cornerstone component of a top-down greenhouse gas (GHG) emission verification system will be atmospheric measurements of spatial and temporal distributions of GHGs and trace-gas species that are direct tracers of GHG emission sources. Averaged over the globe,  $8.4 \pm 0.5$  GtC of fossil fuel carbon dioxide (CO<sub>2</sub>) (based on energy statistics) were emitted into the atmosphere in 2009. Land use change contributed an additional  $0.9 \pm 0.7$  GtC. Fossil-fuel CO<sub>2</sub> emissions are smaller compared to annual gross (bidirectional) fluxes between the atmosphere and ocean and terrestrial biosphere of ~100 GtC, with an estimated net uptake of  $2.4 \pm 0.4$  GtC and 3.4 GtC by the ocean and terrestrial biosphere, respectively (GCP 2010). Sources of purely anthropogenic GHGs, i.e., gases with no (or insignificant) natural sources e.g., sulfur hexafluoride (SF<sub>6</sub>), perfluorocarbons (PFCs), and hydrofluorocarbons (HFCs), as discussed in Chapter 1, are easier to identify than anthropogenic sources of CO<sub>2</sub>, especially as natural/biogenic CO<sub>2</sub> sources dominate.

Given the dominance of gross terrestrial and oceanic biosphere  $CO_2$  fluxes over fossil-fuelgenerated  $CO_2$  emissions, discrimination and attribution of anthropogenic  $CO_2$  presents a major GHGIS challenge. It will be aided by the detection of relevant fossil-fuel  $CO_2$  tracers in important ways, such as radiocarbon ( $^{14}CO_2$ ) and combustion byproducts. Further discussion of radiocarbon and other tracers is given below.

Other tracers will likely provide valuable information for inverse models, particularly tracers associated with anthropogenic emissions but not specific to them, such as carbon monoxide (CO), ozone (O<sub>3</sub>), nitrogen and sulfur oxides (NO<sub>x</sub>, SO<sub>x</sub>), volatile organic compounds (VOCs), and secondary organic aerosols (SOAs) (e.g., Bon et al. 2010, Molina et al. 2010 and references therein). Direct observations of tracers with short photochemical lifetimes, e.g., because of atmospheric photochemical reactions, will be useful and perhaps critical in providing time-stamps from sources; such information could be quantified to assist the transport and inversion

model retrieval. Long- and short-lived GHGs that have no natural sources (e.g., SF<sub>6</sub>, PFCs, HFCs) and naturally produced tracers (e.g.,  $^{222}$ Rn) are attractive first-order targets to help train transport models (e.g., Gloor et al. 2007). When combined with vertical profiles (e.g., light or commercial aircraft; sonde/balloon; other novel atmospheric samplers) or transects (e.g., ARCTAS, HIPPO), the same trace species can help elucidate planetary boundary layer (PBL) venting and mixing with the free troposphere.

Assimilation of meteorological data will be required to reduce uncertainty in transport models. Direct observations of the planetary boundary layer height using radiosondes, LIDAR, SODAR, and wind-profiling radar will be important, if not crucial, in defining (and assimilating), or developing, improved parameterizations of the planetary boundary layer height and dynamics that depend on diurnal cycles, isolation, wind profiles, cloud cover, and other phenomena.

Future climate-treaty language will not likely be based solely on direct anthropogenic GHG emissions, but rather on "net" emissions. These will include land-use change and offsets, including terrestrial carbon sequestration in a variety of dynamic ecosystems and biomes (LULUC/AFOLU). These activities will result in changes in above- and below-ground carbon stocks and fluxes of CO<sub>2</sub>, methane (CH<sub>4</sub>), nitrous oxide (N<sub>2</sub>O), and, to a lesser extent, CO. In the United States, above- and below-ground carbon stock data are collected and assessed by the USDA/USFS (Shaw et al. 2005, Riemann et al. 2010) and fluxes assessed via AmeriFlux (e.g., Baldocchi et al. 2001, Xiao et al. 2008) and scaled from plot to region using remote-sensingdriven biogeochemical and biophysical models (e.g., Potter et al. 1993, Baldocchi et al. 2001, Law et al. 2006, Xiao et al. 2008). The ground-based observation component of the GHGIS will need to include assessments of land-use change and offsets, while initially focusing on attribution approaches of direct emissions. Integration between land observations and orbital and sub-orbital platforms will be necessary to scale attribution and carbon-stock assessments. Land observations will also be used to calibrate remote-sensing products (e.g., disturbance including fire, canopy height, NDVI, LAI, fPAR, soil moisture) necessary for the biophysicalbiogeochemistry modeling and carbon allocation to yield biosphere fluxes that can be used as priors within the inversion modeling or as direct biomass estimates (e.g., Frolking et al. 2009, Treuhaft et al. 2003, 2010).

Infrastructure and measurement programs needed for GHGIS are a natural complement to the Integrated Global Carbon Observation System (IGCO), under the Global Earth Observing System Systems (GEOSS). From a pragmatic standpoint, this should allow the GHGIS ground-based observations to leverage and complement fundamental carbon-cycle science research and with dual-use data provide efficiencies and reduce unnecessary duplication (cf. Ciais et al. 2010).

The density and frequency of the observations will ultimately be dependent on the scale and time domain of the region being inverted and the relative importance of other (biospheric) fluxes from which the anthropogenic GHG emissions need to be disentangled. Current top-down methods provide constraints only on emissions over fairly large spatial scales. To increase resolution requires a denser network of observations taken at more frequent time intervals. Different scales will require different logistic and instrumentation needs. For example, tall towers have concentration footprints of  $10^6 \text{ km}^2$  and can provide regional information, whereas eddy-flux covariance towers have local footprints. This adds complexity to synthesizing the data from existing networks. The minimum timescale of observations is defined by synoptic weather

patterns modulated by diurnal variations of the height of the planetary boundary layer. GHGs are generally emitted at the surface and can yield steep concentration gradients in the boundary layer: in urban domes the vertical gradient for  $CO_2$  (surface to top of boundary layer) can be  $\geq 100$  ppm with a comparatively minor increase once above the boundary layer (e.g., Stephens et al. 2007; ARCTAS data courtesy of T. van Curen, California Air Resources Board; C. Sweeney, NOAA/ESRL, personal communication). Direct observations within the boundary layer and in the free troposphere will be required. To move from a scoping to an operational framework will require an iterative process of observations in both background (clean air) and urban settings, and building the knowledge base with focused intensives<sup>1</sup> at the urban and regional scale, including various emission mixtures such as mainly anthropogenic (e.g., Four Corners, urban domes) to "mixed" sources with "simple" (e.g., Great Plains) and complex (e.g., California) terrain, meteorology, and atmospheric transport.

Seasonal variations in background biosphere fluxes can be exploited to test discrimination methodologies and leverage logistics and infrastructure: e.g., during winter biosphere, local fluxes can be at a minimum. An initial basic science approach of higher density of observations than possibly needed is required for diagnosis of model results and determination of the true level of intensity needed in an operational framework.

# 5.2 Currently Available Activities and Infrastructure

Cumulatively, the air quality, carbon cycle, climate, ecosystem, biophysics, radiochemistry, and related communities provide a rich stream of existing data and an infrastructure that could be leveraged under, or augmented and complemented by GHGIS (cf. Table 5-1 and Figure 5-1). Stack monitoring sensors (e.g., CEMs) are used in bottom-up inventories to assess empirical relationships between the amount of fuel burned and emissions. At present, methods for assessing GHG emissions from the land surface consider CEMs to be part of the bottom-up inventory system. In the last decade, there has been an increased and formalized attempt to coordinate global efforts to study the carbon cycle under various phases of the "Earth Observing System," most recently the IGCO system. Individual networks, assets, and activities thereof are funded at the national level. The number of such "networks" comprises a loose confederation of related researchers that are not GHGIS-mission-driven, supported by a single national funding entity, or coordinated by a single agency or program office. An example is the international FLUXNET network, which is a network of networks. These networks comprise individual research sites at which investigators use a similar or common eddy-flux covariance and micrometeorology scheme to determine ecosystem fluxes of CO<sub>2</sub>, moisture, and sometimes CH<sub>4</sub> (cf. Falge et al. 2002a, 2002b; Davis et al. 2003; Law et al. 2002; Miller et al. 2007). In addition to different science focus areas and funding sources (e.g., AMERIFLUX), the requirements are not necessarily the same across observations of the same constituent. Concentration footprints vary widely: ground level samples will have the smallest footprint: eddy flux covariance towers have a concentration footprint of 10s of square km, whereas "tall towers" can have concentration footprints of 106 square km (e.g., Andrews et al. 2005, Baldocchi et al. 2001, Gloor et al. 2001).

<sup>&</sup>lt;sup>1</sup> An intensive in this context is a field campaign which brings together a broad array of investigators and instrumentation to study a well defined scientific aspect of an environmental process. The time duration is limited by funding constraints and/or resource availability. This is in contrast with the long term sustained environmental sampling campaigns that are designed from inception to last multiple decades.

Lagrangian particle trajectory analysis is useful to assess the influence of possible sources and sinks on trace gases from expected emission regions to the actual sensor (whether tower or other) before the actual inversion (e.g., Lin et al. 2003, Miller et al. 2008).

Table 5-1. Existing basic research and monitoring activities that could be leveraged or augmented by GHGIS. Note that the global total of individual sites is far less than the sum due to many different "network" activities being geographically co-located. The table does not include proposed networks such as the US National Ecological Observing Network (NEON), or the ICOS GHG tower network. It does not include stack monitoring by the Environmental Protection Agency (EPA) or Air Resource Boards that feeds into bottom-up estimates. Not included are an indeterminate number of entrepreneurial research activities. In the EU as part of the emissions monitoring network (under ICOS), an additional set of 60 short towers is planned to measure  $CO_2$ , CO, and  $CH_4$ .

Network	Sites	Purpose	Dist.	US	<b>US Funding</b>	
AGAGE	12	F- and long-lived GHGs	Int'l	Yes	NASA	
ARM	10	Atmospheric radiation	Int'l	Yes	DOE	
CTBT rad	79	Nonproliferation, rad-chem	Int'l	Yes	NNSA	
FIA	>1000	Carbon Stock Assessment	US	Yes	USFS	
<b>FLUXNET</b> <sup>a</sup>	403	Ecosystem fluxes – in situ	Int'l	Yes	Various	
GCHN	>7000	Meteorology	Int'l	Yes	NWS	
Cooperative Air <sup>b</sup>	112	Carbon Cycle, Atmos chem.	Int'l	Yes	NOAA	
IAEA-WMO GNIP	873	$\delta$ 18O, $\delta$ D in precipitation	Int'l	Yes	Entrepreneurial	
Scripps <sup>c</sup>	12	Carbon cycle	Int'l	Yes	Various	
TCCON	19	Column profiles – in situ	Int'l	Yes	Various	
EPA	365	Criteria pollutants, HAPs	US	Yes	EPA	
IMPROVE	179	Visibility (aerosols)	US	Yes	Various	
Weatherbug	~8000	Meteorology	Int'l	Yes	Private-Public	
NOAA Climate	150	Climate-change monitoring	US	Yes	NOAA	

<sup>a</sup> Only active FLUXNET sites are counted.

<sup>c</sup> Scripps archives CO<sub>2</sub> from its network for future <sup>14</sup>C analyses.

Non-specific infrastructure that could be utilized includes cellular phone towers and aircraft hazards (often in excess of 200 m). The Mid-Continent Intensive (MCI) and the ongoing Indianapolis Flux (INFLUX) campaigns utilize mid-height (100-200 m) cellular phone towers. See also Appendix E. For regional flux studies, 100-200 m towers are adequate. At the urban scale, physical infrastructure exists (e.g., street and traffic lights, aerials on buildings) that could be leveraged, particularly with inexpensive chip-based sensors, e.g.,  $CO_2$ ,  $SF_6$ , ozone (O<sub>3</sub>), although the precision of those sensors, at present, is insufficient for GHGIS needs.

<sup>&</sup>lt;sup>b</sup> Within the Cooperative Air Sampling Network, a small number of sites currently have <sup>14</sup>CO<sub>2</sub> analyses being made by the National Oceanic and Atmospheric Administration (NOAA), Department of Energy (DOE), academic, and European Union (EU) researchers, but <sup>14</sup>C is not a core measurement. In the United States, NOAA is augmenting short towers with tall towers that have a much larger concentration footprint. Nearly all of the Cooperative Air Sampling Network sites are part of the WMO GAW.



Figure 5-1. Map of (some of) the existing infrastructure and sites where atmospheric chemistry and or carbon cycle observations are made based on Table 5-1 except for GCHN, NOAA climate, GNIP, and Weatherbug. Landmask is 2005 population density (CIESIN data product).

Much available data is reported in standardized notation and (SI) units. Electronic and searchable data archives exist for much of the raw data and more formalized data products. In some cases, latency issues are problematic and exacerbate individual researcher-based quality assurance/quality control (QA/QC) procedures. Flexibility, structure, and available metadata from the various distributed active archive centers (DAACs) are variable. GHGIS should work with the World Meteorological Organization (WMO), which has an established role for facilitating unencumbered access to relevant carbon cycle and atmospheric data across international boundaries through (research-based) cooperative agreements. An example of such an international data partnership is the Global Atmosphere Watch (GAW), which includes the World Data Centre for Greenhouse Gases.

The carbon-cycle community, which has historically focused on clean air and non-urban sites, has gone to great lengths to standardize and inter-calibrate their respective reporting scales in part because the signal of interest (change in mole fraction  $CO_2$ ) is small: ~0.1 ppm out of ~385 ppm (presently), with annual increases of only 1 to 2 ppm (Conway et al. 2010, Keeling and Whorf 2004, Keeling et al. 2010). The WMO facilitates informational exchange at the  $CO_2$  Experts Meeting and the International Conference on Carbon Dioxide (which has expanded to include other GHGs). Across the various activities, there are national-level workshops and national-international scientific meetings to promote standardization and intercomparison. In some cases, and because there are no distributed standards and reference materials for every measurement type, individual researchers use in-house process standards and reference materials. These communities often resort to informal and (financially) unsupported round-robin intercomparisons to confirm that results can be merged with or without bias corrections. Agencies, such as NIST, the IAEA, and the WMO, could and should be proactively engaged to meet expected primary and secondary reference material needs of GHGIS.

The NOAA Earth System Research Laboratory (ESRL) currently processes and measures ~20,000 discrete whole-air samples from individual flasks per year. The analysis includes the suite of MAGICC gases (CO<sub>2</sub>, CH<sub>4</sub>, CO, SF<sub>6</sub>, H<sub>2</sub>, and N<sub>2</sub>O). Carbon-13 (<sup>13</sup>C) and Oxygen-18 (<sup>18</sup>O) of CO<sub>2</sub> analyses, and <sup>13</sup>C and <sup>2</sup>H of CH<sub>4</sub> are made at the University of Colorado (CU) directly on whole-air from flasks. Samples nearly similar in number are analyzed for rare trace gases and halocarbons. Similar activities, albeit not at the same scale, are performed by Carbo-EU, CSIRO, Environment Canada, and various other entrepreneurial research activities. A small number of the NOAA towers have continuous trace-gas analyzers and ceilometers, and approximately a dozen sites in the United States have approximately biweekly light aircraft profiles coordinated in the tower footprint.

Extraction and purification of CO<sub>2</sub> from NOAA flasks designated for <sup>14</sup>C analyses (not the full network) occurs at CU, and expansion may occur at NOAA/ESRL. The flasks are part of a Programmable Flask Package; NOAA and CU researchers have designed an automated extraction system to which the flask packages can be connected and the CO<sub>2</sub> cryogenically trapped and stored in Pyrex ampoules (Turnbull et al. 2010a). Presently, AMS-<sup>14</sup>C analysis on NOAA flask samples occurs at UC Irvine (UCI) and Lawrence Livermore National Laboratory (LLNL). The Scripps (SIO) CO<sub>2</sub>-O<sub>2</sub>/N<sub>2</sub> network uses conventional 5-liter glass flasks used for  $\delta^{13}$ C measurements at SIO and  $\Delta^{14}$ C at LLNL.<sup>2</sup> Internationally,  $\Delta^{14}$ C was measured regularly in the 1950s and 1960s as part of the WMO-IAEA program to assess the distribution of isotopes in the environment, but many of these stations have been dormant for decades. The longestmaintained datasets are those in Germany/Austria (by I. Levin) and New Zealand (by M. Manning). Entrepreneurial activities also occur by researchers in Germany, the Netherlands, Australia, Japan, and elsewhere.

Currently, two AMS laboratories in the United States have documented long-term reproducibility for <sup>14</sup>C measurements at the  $\pm \leq 2\%$  (1 $\sigma$ ) level: the Center for Accelerator Mass Spectrometry at LLNL and the Keck AMS laboratory at UCI (Graven et al. 2009, 2010a, 2010b; Guilderson et al. 2006; Turnbull et al. 2007; Turnbull et al. 2009; and S.J. Lehman and J.B. Miller, personal communication). At present, the facility at UCI, which in addition to being used by UCI faculty provides analytical services to the academic and research community, is at capacity. The Center for AMS, a multi-user multi-rare isotope facility, has an additional annual capacity of nearly 4,000  $\leq 2\%$  analyses. AMS-<sup>14</sup>C analysis requires reduction of CO<sub>2</sub> to graphite before analysis. CAMS capacity accommodates more than 10,000 graphitizations,<sup>3</sup> as required for the AMS-<sup>14</sup>C analyses, per year. INSTAAR-CU, which currently processes the lion's share of NOAA CO<sub>2</sub> samples, will soon have the capacity to accommodate up to 3,000 graphitizations per year.

In the last 5 years, there has been a significant advancement in *in situ* trace-gas and stableisotope measurement technologies. The instrumentation relies on a variety of spectroscopic

<sup>&</sup>lt;sup>2</sup> δ denotes relative enrichment/depletion of a stable isotope (e.g. <sup>13</sup>C or <sup>18</sup>O) in a given material relative to a standard of known composition (expressed in %<sub>0</sub> or per mil). Δ<sup>14</sup>C denotes the relative enrichment/depletion of radiocarbon (<sup>14</sup>C) in a given material relative to a standard of known composition and normalized by δ<sup>13</sup>C to account for natural fractionation.

<sup>&</sup>lt;sup>3</sup> Graphitization is the chemical process of reducing  $CO_2$  to elemental carbon in the presence of a metal catalyst and a stoichiometric excess of hydrogen gas for subsequent AMS analysis using cesium sputter sources. Solid targets are necessary because of the ionization efficiency and the need to deal with the interference caused by the mass ambiguity of <sup>14</sup>N.

technologies (e.g., near infrared, cavity ring down lasers), FTS/FTIR, and gas chromatography coupled with mass spectrometry (e.g., AGAGE's Medussa GCMS) (Miller et al. 2008, Yang et al. 2002, Berden and Engeln 2009). Field-deployable instrumentation includes rack-mounted and "open" sensors used for eddy flux covariance measurements. Chip-based sensors based on NDIR, electro-chemical, and piezoelectric technology (e.g., CO<sub>2</sub>, SF<sub>6</sub>, CO, O<sub>3</sub>) are extensively used in industrial applications (e.g., HVAC for CO<sub>2</sub>), although, as noted above, the precision of chip-based sensors is currently insufficient for GHGIS needs. R&D to translate these "industrial" emission technologies to basic monitoring in ambient concentrations is in progress and utilization of these technologies is currently undergoing rapid expansion.

## 5.2.1 Uncertainties in Data Derived from Current Capabilities

Uncertainties in data derived from current capabilities can be assigned to (1) analytical (e.g., Tables 5-2, 5-3), (2) confounding factors or influences on a specific tracer, and (3) synthesized flux error (e.g., inversions for the biospheric flux component of CO<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>O, CO). At larger scales, uncertainties are not necessarily independent because of partially common history of an air parcel's mixing and transport (Lagrangian) history, or if constituents are co-emitted (see Chapter 6).

Currently, the synthesized model-flux error is significantly larger than propagated confounding factors, direct flux estimates (e.g., eddy fluxes scaled from site to regional scales), and individual analytical (direct) measurements. An example of the model uncertainty is provided by the TransCom 3 project (Gurney et al. 2002, 2003), which used a combination of observations of  $CO_2$  and  $\delta^{13}CO_2$  to invert for terrestrial biogenic fluxes. A boundary condition in this intercomparison was an assumption that fossil-fuel CO<sub>2</sub> emissions were well known. Although this model-intercomparison project is now ~10 years old, the  $\pm 100\%$  (1 $\sigma$ ) uncertainty in the retrieved terrestrial biospheric CO<sub>2</sub> fluxes highlights the scale of the uncertainty in the transport models. There has not been a formal inversion comparison using more advanced tracer-transport models. The full suite of remote-sensing-driven (e.g., MODIS) biophysical-biogeochemistry models has not been directly compared in a formal and structured model intercomparison project. Errors of scaled biogenic fluxes can be small (few to 10s of percent) for site-specific and subannual comparisons with observations at eddy-covariance flux sites (e.g., Hibbard et al. 2005, Richardson 2010), but one may anticipate that the model-to-model uncertainty for net fluxes is an order of magnitude larger (Michalak et al. 2010; Post et al. 2010; see also the North American Carbon Project's Interim Synthesis Activities at http://nacp.ornl.gov/int\_synthesis.shtml).

A recent National Aeronautics and Space Administration (NASA) initiative is attempting to resolve this with an intercomparison of a subset of the available models (*NASA CMS 2010, Pilot Study: Surface Carbon Fluxes*, K. Jucks and D. Wickland points of contact). Top-down estimates of emissions of fluorine species demonstrate significant discrepancies with bottom-up projections from emissions inventories, raising questions about the completeness and methodology (and uncertainty) of the information provided by inventories. Global emissions estimates using inversions or scaling arguments of direct observations of long-lived trace gases measured by the AGAGE and similar networks cannot be readily resolved with bottom-up inventories (Levin et al. 2009; Mühle et al. 2010a, 2010b; Rigby et al. 2010). See Table 5-3.

NOAA/ESRL MAGICC Gases					
Trace Gas	Uncertainty				
CO <sub>2</sub> (ppm)	0.03				
CH <sub>4</sub> (ppb)	1.2				
CO (ppb)	0.3				
SF <sub>6</sub> (ppt)	0.03				
H <sub>2</sub> (ppb)	0.4				
N <sub>2</sub> O (ppb)	0.4				

Table 5-2. Analytical uncertainty of flask-collected, laboratory-based measurements of (MAGICC) trace gases (www.esrl.noaa.gov/gmd/ccgg/aircraft/qc.html). The precisions listed are comparable across the majority of the GAW network.

In situ observations of a number of trace-gas species (e.g., CO, CO<sub>2</sub>, CH<sub>4</sub>) and isotopes (e.g.,  $\delta^{13}$ CO<sub>2</sub>) have recently become nearly as precise and accurate as the most reliable laboratory-based analyses. For example, laboratory analyses of  $\delta^{13}$ CO<sub>2</sub> provide a precision of  $\leq 0.03\%$  using isotope ratio mass spectrometry (IRMS) (e.g., Allison and Francey 1995, Masarie et al. 2001) whereas in situ laser-based techniques (e.g., direct absorption) have demonstrated a precision of  $\leq 0.03\%$  in the field (Nelson et al. 2008; Bambha, personal communication). Spectroscopic techniques are continuing to be refined in part due to the finding of unanticipated isotopologue interferences from peaks not adequately resolved in the HITRAN database. Frequent use of reference gases, even for field-deployed instruments, similar to the procedure used in the ICP community (e.g., Schrag 1999), correct for small drifts and reduce the overall uncertainty.

The discrimination of fossil-fuel CO<sub>2</sub> emissions from natural exchanges of CO<sub>2</sub> (terrestrial and oceanic) is significantly aided by isotopic measurements of atmospheric CO<sub>2</sub> and measurements of other combustion tracers (e.g., CO, acetylene, benzene, n-pentanes, propane). Fossil-fuel carbon is devoid of <sup>14</sup>C (and also has a smaller <sup>13</sup>C/<sup>12</sup>C ratio than atmospheric CO<sub>2</sub>), which makes the <sup>14</sup>C content of atmospheric CO<sub>2</sub> susceptible to the influence of CO<sub>2,ff</sub> (fossil-fuel CO<sub>2</sub>). Between the beginning of the industrial revolution and atmospheric nuclear-weapons testing (which produced <sup>14</sup>C via n-p reactions), the  $\Delta^{14}$ C, i.e., the ratio of <sup>14</sup>C to <sup>12</sup>C, includes a correction for mass-dependent fractionation (Stuiver and Polach 1977) of atmospheric CO<sub>2</sub> decreased to the point where the atmosphere "looked" 200 years old (cf., Suess 1955, Tans et al. 1979, Keeling 1979, Stuiver and Quay 1982). See Figure 5-2. The decrease in the <sup>14</sup>C/<sup>12</sup>C and <sup>13</sup>C/<sup>12</sup>C ratio of atmospheric CO<sub>2</sub>, referred to as the Suess Effect, can help discriminate sources of CO<sub>2</sub> (e.g., Graven et al. 2009, Levin et al. 2003, Turnbull et al. 2006, 2008, 2010b; Vogel et al. 2010). Before the nuclear-testing moratorium, atmospheric weapons testing nearly doubled the amount of <sup>14</sup>C in the atmosphere.

Table 5-3. Analytical uncertainty of trace species measured via the AGAGE network (Prinn et al. 2000) and representative northern hemisphere concentrations in 2005. Conversion of percent uncertainty into concentration is approximated via simple multiplication [http://agage.eas.gatech.edu/instruments-overview.htm]. Laboratory-based measurements of a similar suite of trace species are made on whole air collected via flasks by the NOAA Halocarbon and other Atmospheric Trace Species (HATS) group as part of Chlorofluorocarbon Alternatives Monitoring Project (CAMP) [www.esrl.noaa.gov/gmd/hats/].

Compound	~NH (2005) (ppt)	Typical Precision (%)	Compound	~NH (2005) (ppt)	Typical Precision (%)	
CF <sub>4</sub>	74	0.15	H1301	3.1	1.5	
$C_2F_6$	3.5	0.9	H1211	4.5	0.5	
$C_3F_8$	0.5	3	H2402	>0.5	2	
SF <sub>6</sub>	5.3	0.4	CH <sub>3</sub> Cl	570	0.2	
$SO_2F_2$	1	1.6	CH <sub>3</sub> Br	10	0.5	
HFC23	25	0.7	CH <sub>3</sub> I	1	2	
HFC32	~1	5	$CH_2Cl_2$	36	0.8	
HFC134a	29	0.4	CHCl <sub>3</sub>	11	0.6	
HFC152a	4.2	1.2	CHBr <sub>3</sub>	~3	0.6	
HFC125	2.9	1	$CCl_4$	95	1	
HFC143a	6.5	1.2	CH <sub>3</sub> CCl <sub>3</sub>	28	0.7	
HFC365mfc	<1	10	CHClCCl <sub>2</sub>	0.8	2.5	
HCFC22	170	0.3	$CCl_2CCl_2$	5.5	0.5	
HCFC141b	19	0.4	$C_2H_2$	10-200	0.5	
HCFC142b	15	0.6	$C_2H_4$	50-500	2	
HCFC124	1.6	2	$C_2H_6$	500	0.3	
CFC11	257	0.15	$C_6H_6$	10-100	0.3	
CFC12	546	0.05	$C_7H_8$	<1-10	0.6	
CFC13	-	2	GC-MD only*		7*	
CFC113	80	0.2	$CH_4$	1850 (ppb)	0.05	
CFC114	16.5	0.3	N <sub>2</sub> O	320 (ppb)	0.05	
CFC115	8.4	0.8	СО	130 (ppb)	0.2	
			$H_2$	500 (ppb)	0.6	

Air-sea CO<sub>2</sub> exchange and the uptake and respiration of terrestrial carbon has drawn down the <sup>14</sup>C/<sup>12</sup>C ratio in the atmosphere from a bomb peak of ~1000% to ~45% today (e.g., Levin et al. 2010, Graven et al. 2010a, Turnbull et al. 2010b). The tracer aspect of bomb-<sup>14</sup>C makes it a useful multi-decadal carbon cycle tracer: carbon that was photosynthetically fixed in the 1960s and 1970s and that is in multidecadal soil carbon pools is now being heterotrophically respired (cf. Gaudinski et al. 2000, Harden et al. 2002, Trumbore 2000, Swanston et al. 2005, among many). While other tracers, such as O<sub>2</sub>/N<sub>2</sub> and <sup>13</sup>C:<sup>12</sup>C ( $\delta^{13}$ C), are useful for distinguishing land versus oceanic components of the CO<sub>2</sub> variations, these tracers provide less useful information for distinguishing between land biospheric and fossil-fuel components. To separate land exchanges into fossil-fuel and land biospheric components, using inverse techniques based on
$O_2/N_2$  or  ${}^{13}C/{}^{12}C$  data, it is necessary to apply corrections (assumed true and based on inventory products) for the effects from fossil-fuel CO<sub>2</sub> (e.g., Battle et al. 2000, Francey et al. 1995, Gurney et al. 2003, Patra et al. 2008, Rayner et al. 2002). A strong corollary exists: if one can uniquely and independently define the fossil-fuel component in a parcel of air, and using the aforementioned tracers, one can better determine the land biosphere flux. However, also noted here is that volcanic CO<sub>2</sub> typically derives from "old" carbon and contributes to emissions one would consider natural, i.e., non-anthropogenic. Such emissions can be characterized by C-isotope ratios not easily distinguishable from fossil-fuel CO<sub>2</sub> (CO<sub>2,ff</sub>). Further, nuclear reactors, whether for power-production or medical-isotope production, also emit carbon isotopes that can confuse the emissions attribution based on carbon isotope ratios, as discussed further below.



Figure 5-2. (Left) The influence of fossil-fuel  $CO_2$  on atmospheric  $CO_2$  and carbon isotopes. Post-1958  $CO_2$  data from Mauna Loa (Keeling and Whorf 2004, Keeling et al. 2010, Conway et al. 2010) and pre-1958 from air samples from Siple and Law Domes Antarctica (Etheridge et al. 1996, Francey et al. 1999, Friedli et al. 1986). Note that the Suess effect has a larger and faster impact on  $\Delta^{14C}$  than  $\Delta^{13}C$ . (Right) The "post-bomb" <sup>14</sup>C history in the atmosphere and surface ocean (data of Stuiver and Quay 1982; Levin et al. 2010; Manning and Meluish 1994; Graven et al. 2010a; Guilderson et al. 2000; and Guilderson, unpublished). Atmospheric  $\Delta^{14}C$  is an integration of unidirectional carbon (isotopic) fluxes between the atmosphere, ocean, and terrestrial biosphere, natural production in the stratosphere, and dilution due to the release of fossil fuel  $CO_2$ .

 $\Delta^{14}$ C at clean air (background) sites is decreasing at an observed rate of ~5.5%/yr (Levin et al. 2010, Graven et al. 2010a, Turnbull et al. 2009). Box and global transport model based trend analysis implies that the release of fossil fuel CO<sub>2</sub>, if unbuffered by other processes, would decrease  $\Delta^{14}$ C by ~10-15%/yr (Figure 5-3). Although carbon fluxes between the ocean and terrestrial biosphere are larger than those of fossil-fuel CO<sub>2</sub> emissions, the <sup>14</sup>C-isotopic signature yields gradients in excess of 15%/ downwind of sources (Figure 5-4). These gradients have been qualitatively reconstructed in the carbon fixed by annual plants (e.g., Hsueh et al. 2007, Riley et al. 2008) and also via atmospheric transects (e.g., Turnbull et al. 2008).



Figure 5-3. Box model based trend analysis on the influence of natural <sup>14</sup>C production, isotopic exchange and  $CO_2$  fluxes between the atmosphere, ocean, and terrestrial biosphere, and the influence of the combustion of fossil fuel  $CO_2$  (modified from Graven et al. 2010a, courtesy of H. Graven).



Figure 5-4. Simulated distribution of  $\triangle^{14}C$  (‰) relative to the global mean in an ad-hoc, offline coupled carbon climate model including 2000 fossil fuel emissions (Randerson et al. 2002). Image courtesy of JTR.

For illustrative purposes and ignoring complications to the interpretation of atmospheric  $\Delta^{14}CO_2$  values, one can estimate the abundance of fossil-fuel CO<sub>2</sub> (CO<sub>2,ff</sub>) in an air mass from measured values of CO<sub>2</sub> abundance (CO<sub>2,m</sub>) and  $\Delta^{14}C$  ( $\Delta^{14}C_m$ ) using a simplified two-end-member mixing model approach (e.g., Levin et al. 2003). Assuming clean-air or free-tropospheric air measured abundances for background values ( $\Delta^{14}C_{bkg}$ , CO<sub>2,bkg</sub>) and a value of -1000‰ for the fossil-fuel <sup>14</sup>C ratio ( $\Delta^{14}C_{ff}$ ), one can construct two equations for mass and isotope balance with the additional assumption that the rapid turnover portion of the terrestrial biosphere  $\Delta^{14}C_{bio}$  is equivalent to  $\Delta^{14}C_{bkg}$ , i.e.,

$$CO_{2,m} = CO_{2,bkg} + CO_{2,ff}$$

$$(5-1)$$

$$CO_{2,m} (\Delta^{14}C + 1000)_{m} = CO_{2,bkg} (\Delta^{14}C + 1000)_{bkg} + CO_{2,ff} (\Delta^{14}C + 1000)_{ff}$$
(5-2)

These can be combined and rearranged to solve for  $CO_{2,ff}$ :

$$CO_{2,ff} = CO_{2,m} \left( \Delta^{14} C_{bkg} - \Delta^{14} C_m \right) / \left( \Delta^{14} C_{bkg} + 1000 \right).$$
(5-3)

Good high-precision conventional counting laboratories and accelerator mass spectrometry facilities can achieve long-term reproducibility (precision and accuracy) of the  $\Delta^{14}$ C ratio to  $\leq 2\%$  (Graven et al. 2007, 2009, 2010a,b; Levin and Kromer 1997; Stuiver and Quay 1982; Tans et al. 1979; Turnbull et al. 2006, 2008, 2009). Propagating this uncertainty for both the "unknown" and background <sup>14</sup>CO<sub>2</sub> measurement yields a discrimination of CO<sub>2,ff</sub> of  $\leq \pm 1.5$  ppm (1 $\sigma$ ), or  $\leq \pm 3$  ppm (2 $\sigma$ ), on one-time discretely sampled air parcels.

Logistic and resource limitations have required the use of tracer-tracer relationships such as via <sup>14</sup>C-based estimates of CO<sub>2,ff</sub>:CO (Levin et al. 2003, Turnbull et al. 2010b, Vogel et al. 2010) to infer local to regional fossil-fuel CO<sub>2</sub> emissions. Although useful, CO:CO<sub>2</sub>,ff relationships vary in both space and time (Table 5-4). Because of this variability, it is estimated, through CO:CO<sub>2,ff</sub> comparisons and scaling arguments, that city or regional emissions can only be estimated to within  $\pm 25\%$  using continuous CO measurements and 2-3‰  $\Delta^{14}$ C analyses to convert CO to CO<sub>2,ff</sub> (Vogel et al. 2010).

Date and time	Location	$CO:CO_{2,ff}(\times 10^{3})$	Reference
2001 Average	DOE Inventory	32	Blasing 2004
August 2000	North American Survey	$33 \pm 10$	Gerbig 2003
2004 Average	EPA Inventory	23	EPA 2006
2002 Average	Vulcan Product (US)	19	Gurney 2008
May 1994 - 1996 avg	Harvard Forest, MA	$22 \pm 2$	Postnak 1999
July 1994-1996 avg	Harvard Forest, MA	$29 \pm 5$	Postnak 1999
20 May 2004, 7 am	Kremmling, CO	18±10	Graven et al. 2009
20 May 2004, 2pm	Denver, CO	$20 \pm 2$	Graven et al. 2009
28 May 2004, 2 pm	Denver, CO	$27 \pm 8$	Graven et al. 2009
20 July 2004, 10am	Denver, CO	$14 \pm 2$	Graven et al. 2009
26 July 2004, 2pm	Denver, CO	$14 \pm 3$	Graven et al. 2009
20 January 2004	Niwot Ridge, CO	$7 \pm 2$	Turnbull et al. 2006
2 March 2004	Niwot Ridge, CO	$12 \pm 6$	Turnbull et al. 2006
27 Feb & 6 Mar 2009	Sacramento intensive	$14 \pm 2$	Turnbull et al. 2010b
2002-2009	Heidelberg, DE	$15.5 \pm 5.6$	Vogel et al. 2010

Table 5-4. CO:CO<sub>2,ff</sub> relationships used in inventories, and those derived from  $^{14}CO_2$  measurements. Adapted from Graven et al. (2009).

There are additional complications in estimating atmospheric  $\Delta^{14}$ C values because of biospheric fluxes, stratospheric exchange (<sup>14</sup>C is naturally produced in the stratosphere), and other sources, such as the nuclear power industry and reprocessing (Levin and Hesshaimer 2000, Levin et al. 2010, Graven and Gruber 2010, Turnbull et al. 2009), volcanic carbon/CO<sub>2</sub> emissions, out-of-control coal-mine fires that may not be counted as an anthropogenic source in future treaties, etc. In Western Europe, reprocessing may impart a bias of up to 10 ppm CO<sub>2</sub> if the nuclear derived

<sup>14</sup>C is not accounted for (Graven and Gruber 2010). Natural fluxes from geothermal sources contribute to a background flux of CO<sub>2</sub> devoid of <sup>14</sup>C. Tracer-tracer relationships can be used to help clarify the (generally minor, but not always) complications of other sources of <sup>14</sup>C. More importantly, these relationships could be used to assist in forensic fingerprinting of emission sources based on relationships between <sup>14</sup>C-derived CO<sub>2,ff</sub> and other combustion products, such as acetylene, benzene, propanes (Figure 5-5), and a subset of the fluorinated gases (Turnbull et al. 2010b, LaFranchi et al. 2010, Miller et al. 2011). *With respect to biomass burning and forest-fire emissions, a similar corollary in tracer-tracer and* CO-CO<sub>2</sub> discrimination spaces exists (cf., Mühle et al. 2002, and van der Werf et al. 2010 and references therein).



Figure 5-5. An example of combustion product and <sup>14</sup>C-based estimates of fossilfuel  $CO_2$  relationships (aka "tracer-tracer") during an intensive near Sacramento, CA (from Turnbull et al. 2010).

Research is necessary to (1) elucidate potential confounding effects in tracer-tracer space and (2) ascertain the level of sectorial granularity these multi-tracer relationships (may) provide.  $\delta^{13}C$  (and  $\delta^{18}O$ ) of CO<sub>2</sub> will be very useful in urban areas with minimal biospheric fluxes because biospheric CO<sub>2</sub> emissions, including heterotrophic respiration of below-ground carbon, have  $\delta^{13}C$  values similar to many fossil-fuel combustion materials (cf. Pataki et al. 2003, and Newman et al. 2008 and references therein). An additional requirement when using  $\delta^{13}C$  is to understand the partitioning among combustion sources (e.g., LNG/CH<sub>4</sub>, vs. diesel, vs. gasoline, vs. coal) that can influence the interpretation of  $\delta^{13}C$ -CO<sub>2</sub> space (Figure 5-6). An additional possible confounding

effect on  $\delta^{13}$ CO<sub>2</sub> in high-population-density urban regions is the influence of human respiration, which is similar to that of combusted gasoline (e.g., Newman et al. 2008 and references therein).



Figure 5-6. Keeling plot of  $\delta^{13}$ C endmembers of various emission sources and (CO<sub>2</sub>) with observed data from Pasadena (Los Angeles air basin) for 1972-1973 and 2002-2003. Modified from Newman et al. (2008, Figure 5, courtesy of S. Newman.)

### 5.3 Phase 1

#### 5.3.1 What Could Be Delivered with No Augmentation

Without investments in additional infrastructure and instrumentation but with continued programmatic funding, it would be possible to:

- 1. increase  $\Delta^{14}$ C analyses from established whole-air collection sites;
- 2. archive  $CO_2$  and whole air from extant collections to be analyzed later;
- 3. coordinate short-term intensives to explore tracer-tracer space and quantify tracer fingerprints of important GHGs and their sources;
- 4. reconcile and integrate data from existing ground sites;
- 5. intercompare instrumentation and methodologies of rapidly changing technologies (e.g., quantum-cascade laser-based systems);
- 6. develop whole-air trace-gas and isotopic standards for field and lab measurements; utilize biological surrogates (e.g., annual grasses) to qualitatively describe ground-level <sup>14</sup>CO<sub>2</sub> gradients; and
- 7. standardize protocols, QA/QC procedures, and chain-of-custody issues.

#### 5.3.2 Existing Technologies and Methodologies That Could Be Deployed

As noted in many contexts throughout this report, significant research is required to transition from a research-mode network to one that supports an operational activity. It is difficult to assess whether the diplomatic necessities for "monitoring" will have been completed in an operational sense, with open and transparent access to international locations within three years. One of the primary needs within Phase 1 is the continued socialization with international partners to build a research-based GHGIS cooperation. This effort could proceed within the framework of the GAW and evolve into a formal operational monitoring program. The needs of a GHG monitoring network are not equivalent to those required by the scientific carbon-cycle community. Based on initial idealized tracer and transport inversions, there is an estimated factor-of-two decrease in uncertainty between a notional network using GLOBALVIEW versus one that uses the Comprehensive Test Ban Treaty (CTBT) network as the initial backbone. At some level, this is not surprising: GLOBALVIEW sites tend to be sited away from emission sources and either in "clean-air" locations or dominated by natural (ocean and terrestrial) fluxes. The site multiplier (number of extra sites required for redundancy, overlap, and handling biases and errors in collected observations) is conservatively estimated at 3 (i.e., approaching 300 sites). This is similar to the nearly 200 sites used by Rayner et al. (2010), which, assuming a perfect transport model and an idealized <sup>14</sup>C tracer, inferred a 70% reduction in uncertainty for national fossil-fuel CO<sub>2</sub> emissions from the largest emitters. This level of planning is similar to the Integrated Global Carbon Observation system, which anticipates 1,000 sites globally for fundamental carbon-cycle observations. It is anticipated that as methodologies are refined and new purpose-built sensors and systems are brought on line that the physical requirements and sampling density will decrease. GHGIS could leverage the EU's investment in Integrated Carbon Observation System (ICOS). Countries with which the US research community has established relationships include but are not exclusive to: Australia, Brazil, Canada, Japan, Mexico, New Zealand, and countries within the EU, particularly England, France, and Germany.

A concerted effort using the United States as a test bed is an attractive prelude to the international framework. With an initial domestic focus, key scientific and operational questions (unknowns) can be addressed in developing meteorological, trace-gas, and tracer data for inversions at the urban and regional/continental scale. This database will require instrumentation and measurements at a combination of background, mixed, and urban settings. Intensives provide high-density observations that can be explored in finer detail. Intensives take significant planning and in Phase 1 it would be expedient and cost-effective to leverage ongoing intensives (e.g., INFLUX), pending activities (e.g., follow-on to the Mid-Continent Intensive), or recently completed intensives (e.g., CALNEX-CARES, HIPPO, MILAGRO). A related goal of GHGIS observational data is sectorial partitioning and attribution - information that in combination with bottom-up inventories could be tested at Four Corners (see Appendix F) or where there is sufficient bottom-up partitioning. Real-world tracer-tracer relationships often provide scalars that are different than "tunnel" or exhaust experiments (e.g., Gertler and Pierson 1996, Hwa et al. 2002), and GHGIS should not solely rely on idealized tunnel experiments or the scalars from bottom-up inventories. The initial learning phase assessment and quantification of tracer-tracer data in sector emission space requires a good bottom-up inventory and understanding of the partitioning of the source of emissions. The a priori sectorial partition information is then used in multi-parametric tracer-tracer space (e.g., principal component analysis) in addition to simple linear combinations of tracer relationships to explore the granularity of emission space that could be reconstructed.

It is the consensus that existing meteorological observations (ground and particularly air, e.g., sondes and profilers) are insufficient to meet the "nudging" requirements of the tracer transport inversion model (urban, regional, and global). GHGIS needs augmentation of existing networks with more sondes, SODAR, and wind profilers: the benefit of characterizing and quantifying the Planetary Boundary Layer (PBL) is of extremely high value. Given similar requirements for GHGIS and the National Weather Service (NWS), many existing resources could be leveraged and new GHGIS resources exploited to facilitate short-term weather forecasts (cf. National Research Council [NRC] report on regional weather forecasting and prediction needs) and emergency response to large fires or industrial accidents. LLNL and the National Atmospheric Release Advisory Center (NARAC) recently signed an agreement for access to meteorological data from *Weatherbug's* ~ 8000 sites. GHGIS should be able to leverage this activity, particularly during test-bed activities.

The recommendation is for the formalization of an integrated and nested atmospheric measurement network in the US and US possessions. This network could accelerate implementation of NOAA's tall-tower network, augmentation (expansion) of "Tier-1" AMERIFLUX sites, and upgrades to air quality/pollution observation platforms. A challenge to leveraging air quality sites is that existing measurements tend to be made close to the ground. In addition to significant horizontal and vertical gradients in, for example, CO<sub>2</sub>, CO, O<sub>3</sub>, N<sub>2</sub>O, and CH<sub>4</sub> that make interpreting concentrations in the context of emissions challenging, one of the weaker components of transport models is adequately characterizing near-ground physical processes. Deliberate tracer release experiments (e.g., SF<sub>6</sub>) or utilization of mobile sensor packages in urban environments could be used to assess siting requirements with due care in selecting sites that meet the most pressing GHGIS needs. Additional instrumentation could include use of off-the-shelf continuous in situ analyzers (e.g., CO<sub>2</sub>, CO, CH<sub>4</sub>, N<sub>2</sub>O, H<sub>2</sub>O,  $\delta C^{18}O_2$ ,  $\delta^{13}$ CO<sub>2</sub>), PBL defining instrumentation (e.g., SODAR, LIDAR, wind profilers, sondes), micrometeorology packages, and automated programmable flask packages for collection of whole air to be analyzed for halocarbons, biosphere compounds (e.g., COS, isoprenes/terprenes), and isotopes (e.g.,  $\Delta^{14}$ C,  $\delta^{18}$ O<sub>2</sub>,  $\Delta^{17}$ O, and other species). Implicitly, requirements for measurements include formal standardization to internationally distributed and accepted standards, QA/QC analysis, and development of procedural protocols that can be easily adapted and utilized for audit-driven aspects within international treaties.

A smaller number of in situ instruments would be deployed for fluorinated trace gases (e.g., Medusa-GCMS analyzers) and VOCs (PTR-MS or GC-FID systems). FTS/FTIR technology to estimate column profiles of  $X_{CO2}$ ,  $X_{CO}$ ,  $X_{CH4}$ ,  $X_{N2O}$  provides a direct bridge between the ground-based, orbital, and sub-orbital platforms (e.g., Yang et al. 2002; Macatangay et al. 2008; and Wunch et al. 2009, 2010. See also Chapters 3 and 4). These instruments could be deployed to expand the background monitoring network and used in urban environments where high-frequency analysis coupled with independent  $CO_{2,ff}$  estimates can be used to document and understand the tracer-tracer relationships of primarily anthropogenic emissions. TCCON, a self-organized group of international researchers who use the same protocols and data reduction for FTS/FTIR column estimates, will be used as part of the ground-truthing of OCO-2 and very likely other remote-sensing and airborne platforms (Wunch et al. 2010, see also Chapter 3). To

maintain high-quality column-profile estimates, regular aircraft and/or sonde profiles are necessary (as frequently as every 2 weeks). The FTS/FTIR technology is attractive over other column averaging instrumentation because of its ability to estimate column profiles nearly continuously during daylight hours, even in cloudy conditions.

No formal dedicated network design OSSEs specific to North America or globally have been performed as part of this study, or other studies we are aware of. Entrepreneurial activities have been performed for regional networks in California (Lucas et al. 2010) and elsewhere. In the NRC (2010a) report, Miller documents the use of a first-order equidistant tall-tower network for the United States. Ideally, one wants concentration footprints to overlap for redundancy and to allow the exploration of biases and variable uncertainty for observations, the transport model, and priors (including terrestrial and oceanic fluxes). Major instrumentation delivery times and the formalization of paperwork (rent/lease) for physical access to towers and/or land to site a new instrument would allow a small number of OSSEs to be performed for more optimal site selection. In terms of locating FTS/FTIR and more novel trace-gas analyzers (for halocarbons, fluorinated gases, aerosols), an initial focus on urban locations is likely to yield tracer-tracer relevant information much more rapidly than at background or mixed-source locations. In urban domes, although horizontal and vertical gradients are large, there is an added benefit of a large signal-to-noise ratio. For example, the Los Angeles air basin, one of the more polluted regions in the United States, exhibits maximum diel (diurnal, i.e., over a 24-hour period) CO<sub>2</sub> concentrations as much as 100 ppm higher than surrounding "clean air" (Newman et al. 2008, ARCTAS data courtesy of CARB, Newman unpublished CALNEX data), although concentrations above the boundary layer are near background (Figure 5-7). Ground-based surveys in metropolitan Boston and elsewhere document large variance in CO<sub>2</sub> concentrations. As a consequence, careful siting of sensors is required so that mean (concentrations) fluxes are estimated in lieu of variance (Wofsy et al. 2010). Local Air-Resources Boards can provide invaluable assistance in pre-planning of urban site selection, particularly given the complex micrometeorology within an urban and high-rise dominated environment and preponderance of local sources (e.g., traffic). In addition to GHG instrumentation it will also be necessary to deploy instruments to determine the height of the PBL in order to estimate the volume into which the emissions are being emitted. Expansion of the volume of the mixed layer and leakage out of the boundary layer can lead to unanticipated concentration changes. On short (diel) timescales, unless atmospheric conditions are set up for an inversion, the boundary layer height will, as a result of cooling, collapse at night and rise during the day. On longer timescales (and relevant for baseline studies), the urban heat island effect can be important in driving boundary layer height and changes in concentration. For example, in Los Angeles between 1972-1973 and 2002-2003, average ground-level concentrations increased by ~30 ppm, whereas background "clean-air" CO<sub>2</sub> increased by nearly 50 ppm. Either significant biosphere uptake occurred or (more likely) the volume into which the emissions were released increased because of (local, micro-climate) warming (Newman et al. 2008) deepening the boundary layer and increasing the urban dome surrounding Los Angeles.

To exploit the unique fossil-fuel tracer aspect and to assess other sources of  ${}^{14}\text{CO}_2$  and transport uncertainties, measurement precision and accuracy for  $\Delta^{14}\text{CO}_2$  need to be lower than 2‰. As discussed above, current state-of-the-art AMS systems are capable of  $\leq 2\%_0$  reproducibility and precision (Guilderson et al. 2006; Graven et al. 2007, 2009, 2010a, 2010b; Turnbull et al. 2006, 2008, 2009). Such reproducibility (~±1.8‰) is quite respectable for systems that were not specifically designed for <2%<sup>14</sup>C-AMS analyses. Empirical evidence shows that individual highprecision analytical runs can nearly equal 1‰ counting statistics (e.g., Guilderson et al. 2006; and Guilderson and Graven, work in progress). Additional uncertainty comes mainly from sample preparation, the behavior of samples in the ion source, irregularities imposed during tuning, and in several cases fundamental design of the spectrometer or fabrication of key components.



Figure 5-7. (top)  $CO_2$  concentration over and around Los Angeles during the ARCTAS intensive. Ground-level  $CO_2$  is as high as 516 ppm whereas outside of the city and just above the boundary layer  $CO_2$  is near background at 386 ppm (symbol size scales between these endpoints). Thin yellow line shows the flight path. Courtesy of Tony VanCuren (CARB). (bottom) Hourly surface  $CO_2$  concentration at a coastal Los Angeles basin site (Palos Verdes [blue] and Pasadena [red]). Diel variations can be ~100 ppm in addition to ~10s of ppm baseline difference between cleaner and more urban air. Data courtesy of S. Newman (Caltech).

Idealized synthetic inversions using <sup>14</sup>C as an idealized fossil-fuel CO<sub>2</sub> tracer and the United States as a test bed indicate that we will need ~10,000 unknowns/year (30 tall towers and daily samples) to ~  $\pm 1\%$  precision/accuracy, or 50 towers and samples every 3 days (NRC 2010a) to meet the first-order requirements in testing and designing a formal GHGIS system. Dedicated instruments need to be characterized by high throughput and also ideally capable of 1‰ long-term reproducibility. Historically, commercial AMS systems have been designed in a cost-conscious and not performance-based environment. An effort will be needed to combine the best of commercial systems with the more nimble research and development accelerator-based

systems. It is anticipated that, through Phase 2 of the proposed GHGIS development, an operational system with sub-country and perhaps individual major urban-dome resolution would require several dedicated instruments per continent. This is regardless of the hoped-for success of in situ <sup>14</sup>C analyzers: there will be a significant physical replication and direct comparison of results until newer technologies are accepted let alone widely deployed.

## 5.4 Phase 2 Science and Technical Gaps, and Opportunities

The direct estimation of fossil-fuel  $CO_2$  "loading" requires discrimination from background  $CO_2$  and other sources of  $CO_2$ . This is a tractable, albeit challenging problem that is mainly limited by logistics (e.g., <sup>14</sup>CO<sub>2</sub> samples collected around every 3 days at several hundred locations) and knowledge and interpretation of tracer-tracer relationships and isolation of potentially confounding factors. Efforts in the Phase 1 and Phase 2 periods should be directed at providing measurements that reduce the uncertainty in  $CO_2$  flux estimates, both biogenic and fossil fuel, and improve the spatial resolution of estimates for different sources, in concert with air and space sensors.

A great deal of uncertainty remains regarding the degree to which the errors in transport modeling can be reduced in the next decade given current and projected measurements and modeling of meteorological information. A suite of tracers is necessary because no single tracer by itself is completely immune to confounding factors. Therefore tracer measurements will likely be important, if not essential, for attributing air masses to source locations in addition to enhancements in meteorological measurements, data assimilation, and reanalysis. Improved analysis of biosphere tracers such as  $\delta^{18}O_2$ , isoprenes, terpenes, and COS, and derived quantities, such as atmospheric potential oxygen (APO) (Manning and Keeling 2006), should also be pursued. Research and development investments into new and existing analytical techniques for combustion trace gases, isotopes, and specific novel tracers, such as fluorinated gases, halocarbons, VOCs, and aerosols, are a key component of a Phase 2 GHGIS effort. Development of spectroscopic techniques for <sup>14</sup>C/1<sup>2</sup>C, which gestated at the same time as accelerator mass spectrometry (Labrie and Reid 1981), have yet to provide a field-deployable in situ instrument, but these efforts should continue.

Although substantial work has been conducted on atmospheric tracers of combustion and biospheric processes, these studies have not typically been directed at the GHG source attribution problem and, hence, available data are not necessarily well suited to meet the GHGIS needs. Investigations into the use of short-lived species and tracer-tracer relationships for inferring sources and sinks of GHGs will be of great importance. Co-design of tracer measurement and inverse-modeling strategies should be conducted to obtain maximum benefit from available and emerging technologies.

Cost tradeoffs for in situ measurement techniques typically exist between more-frequent but lessprecise analyses versus less-frequent, higher-precision analyses. Such tradeoffs are not necessarily required for whole-air samples brought back into the laboratory for subsequent analyses. Collection, replication, extraction or archival, and QA/QC requirements will likely continue to dominate the cost for many physical based measurements. Thus laboratory-based measurements should endeavor to obtain the highest precision and, implicitly, also accuracy. In situ (continuous and discrete) analyses open up new avenues for GHGIS but also bring challenges for quality assurance, quality control, and ultimately, in the context of international agreements, "chain of custody" of remotely or automatically accessed data streams.



Figure 5-8. Hypothetical timeline of land observation activities in Phase 1 and Phase 2.

Biosphere models are the source of prior estimates for many flux inversion models, and therefore the availability of accurate biospheric models will likely be important to a future GHGIS. The accuracy of various biospheric models and their application in  $CO_2$  attribution remains a matter of ongoing research. Ground-based measurements are a key component of the development and validation of biospheric models. Thus, enhanced measurements to support biospheric modeling will likely be needed for future refinement of GHGIS flux estimates. Additionally, the ability of biospheric models to produce reliable estimates of fluxes of tracers of biogenic activity (e.g.,  $\delta^{13}C$  and VOCs) would be extremely valuable.

In the broader context of net  $CO_2$  emissions including LULUC/AFOLU, GHGIS land observation and remote-sensing assets will need to work closely together and beyond initial ground-truth comparisons (see Figure 5-8). During Phase 2, current civilian imagery (e.g., LANDSAT) and remote sensing platforms (e.g., MODIS on AQUA) will be augmented by NASA's planned DESDynI mission. If implemented, DESDynI will provide observations that will support improved estimates for carbon stocks and their changes. Beyond the initial groundtruth phase, these products will need to be continuously assessed and validated, which will require direct (physical) observations utilizing low technology but person-intensive analyses (e.g., tree diameter at breast height measurements, soil carbon inventories) and autonomous/continuous measurements (e.g., eddy-flux covariance). [This page intentionally left blank.]

# Chapter 6. Measurement Data and Uncertainty Quantification

## **Chapter Summary**

Measurement data and uncertainty quantification (UQ) entails two basic tasks. The first is combining data of different sensing modalities and spatial and temporal support to produce integrated observations with attached quantified uncertainties traceable to a common methodology. The second is to carry out local, data-driven analyses of large emission sources to identify trends, changes and anomalies, in concert with the Greenhouse Gas Information System (GHGIS) modeling components, described in Chapter 7, as part of the GHGIS Missions

# Findings

- 1. Although there is some cross-calibration across networks and sensing modalities, as described in Chapters 3 and 5, for example, there is no coordinated effort to combine and cross-calibrate all measurement data sources, certainly not for the purposes of an operational GHGIS.
- 2. There is opportunity to detect changes and trends in greenhouse gas (GHG) emissions in urban domes and industrial sites using data-driven analyses based on sensor observations.
- 3. Within high-emission locations (urban domes, industrial sites), the large amount of spatio-temporal variation in GHG concentration makes interpolation uncertainty the dominant source of data uncertainty.
- 4. The high data volume required to support a GHGIS will lead to computational challenges in implementing methods for Data UQ.

## **Recommendations (Phase 1 Development)**

- 1. Begin an effort to collect, combine, and cross-calibrate available data sources monitoring GHGs. It will be important to include all available sensing modalities since their combination can be expected to reduce uncertainties. With this combined data source, produce grid-level data suitable for model-based inversions and attribution to anthropogenic GHG sources.
- 2. Use available urban and industrial test bed data (e.g., from Four Corners, see Appendix F) to begin developing and testing approaches for making data-driven inferences for large GHG emission sources. Also use such test bed data to better understand local spatio-temporal variations in GHG concentrations.
- 3. Develop disciplined statistical spatio-temporal models for combining disparate data sources and producing appropriate estimates and uncertainties for interpolation.
- 4. Develop framework, methods, and statistical representations of uncertainty that can accommodate the high volume of data required for GHGIS, and can leverage the available computing resources for GHGIS.

5. Develop physical-statistical modeling methods that can accommodate a high volume of data (GHG concentrations, fluxes, winds, etc.) and produce estimates of GHG emissions while accounting for the most important sources of uncertainty.

### **Recommendations (Phase 2 Development)**

- 1. Continue to develop, refine and advance UQ approaches found to be effective in Phase 1.
- 2. Develop UQ capability to make efficient use of new and future sensing networks, modalities and platforms for inferring trends in GHG emissions, exploiting advanced computing and data streaming systems.

### 6.1 Introduction

Operationally, measurement data and UQ entail two basic tasks. The first is combining data from different sensing modalities with spatial and temporal support to produce integrated observations with attached quantified uncertainties traceable to a common methodology. The second is to carry out local, data-driven analyses of large anthropogenic GHG emission sources to identify trends, changes, and anomalies. Data UQ tasks and their place within the larger GHGIS Missions Operations Center (GMOC, see Chapter 8) are depicted in Fig. 6-1. Data UQ consists of the development of framework, methods, and algorithms to carry out these two basic tasks.



Figure 6-1. Measurement data uncertainty quantification within the GHGIS Mission Operations Center (GMOC). Once sensor information is communicated to the GMOC, the data UQ task converts raw data to concentrations with uncertainties. Sensor-specific analyses produce observed concentrations and their uncertainties. These multiple data sources are then combined to produce integrated, updated observations with a common description of their uncertainty. This common uncertainty description accounts for dependencies within sensing modalities, biases, outliers, and possibly other influences. Integrated observations with uncertainties can be adapted to the modeling resolution required for inversion-based analyses for anthropogenic surface fluxes. These data can also be used to perform data-driven analyses for trends, changes, and anomalies.

The vision is for a methodological and algorithmic development in support of these tasks that will evolve as part of a continuous process. An initial collection of algorithms, code, and analyses will be assembled, developed, verified, and brought into production mode within the GMOC. Over time, new algorithms and methods will be developed, tested, verified, validated, and added to the GMOC. Some of these additions will supplement existing capabilities. Others might replace outdated, less efficient and less adequate algorithms. The GMOC is envisioned as hosting the ability to reprocess archived, raw data to produce updated data products for the past as well as forecasts for the future, to enable the tracking of trends and their changes.

While it may be easy to state what is desired for data UQ, exactly how to implement the process that will produce it is less clear. This chapter will describe promising approaches for carrying out the two main tasks: combining data from multiple, heterogeneous sensing modalities and making data-driven inferences, particularly on large emission sources. While the suggested approaches have been used in a variety of environmental monitoring applications, the scale of GHGIS makes adaptation of these approaches challenging. From a Data UQ perspective, the data volume and rate will pose computational challenges that will need to be addressed. Also, the relative value of different sensing modalities is unclear at the outset, so the criteria and methodology for how best to carry out top-down monitoring of GHGs will need to evolve with time and as experience is gained. To this end, much of the early work in Data UQ will focus on the development of approaches in the context of test beds, both real and simulation-based.

# 6.2 Sources of Uncertainty

Each individual observation comes with its own uncertainty that is a mix of both random and systematic effects. As stated in discussions in this report in more than one context, uncertainties associated with data that are the product of current sensors and capabilities can be assigned to sensor properties, analytical issues, and confounding factors or influences on specific tracers. Much of this uncertainty is systematic—it cannot be overcome by replication. Also, these uncertainties are not necessarily independent since a single sensor type or network may have common biases from their common calibration, or be influenced by common extraneous factors that can complicate data analysis and inversion. At larger scales, dependence may be the result of partial common (Lagrangian) history of an air parcel's mixing and transport, or if constituents are co-emitted.

While individual sensors can give accuracies of carbon dioxide (CO<sub>2</sub>) concentration of under 1 ppm, the local variation in concentration over space and time is likely to be the dominant source of uncertainty for making any kind of inferences about changes and trends in concentrations and emissions. Figure 5-7 (taken from Chapter 5) reproduces a time trace of hourly sensor measurements at an urban site (Pasadena, CA) and at a cleaner coastal site (Palos Verdes, CA). The former is an inland urban environment, whereas the latter is near the seashore, with prevailing on-shore winds for much of the diurnal and seasonal cycles. The daily fluctuations can be seen to be as large as 100 ppm for the urban site and as large as 10 ppm for the cleaner site. This variation is important for any basic inferences that can be made from  $CO_2$  and other GHG concentrations and their attribution to anthropogenic sources.



Figure 6-2. Hourly surface  $CO_2$  concentration at Los Angeles basin sites (Palos Verdes [blue] and Pasadena [red]). Daily variations can be ~100 ppm for the urban site; ~10s of ppm for cleaner (coastal) site. Here the temporal variation in concentration dominates uncertainty in the observations. Data from Chapter 5 (courtesy S. Newman, Caltech).

The concentration of CO<sub>2</sub> over space s and time t can be represented as an unknown, continuous field denoted by c(s,t). The quantity c(s,t) can represent a vector, whose components denote the multivariate concentration field of multiple species of interest, including CO<sub>2</sub>., i.e.,  $c(s,t) = [c_1(s,t), c_2(s,t), \dots c_N(s,t)]$ , for *N* species. Generally, any physical measurement, whether it is a flask capture, an in situ measurement, or a remotely sensed column, can be represented mathematically as an integral over the space-time concentration field,

$$X = \int_{(s,t)\in F} c(s,t) \, ds \, dt \quad , \tag{6-1}$$

where X = [Xi, i = 1, ..., N] denotes the corresponding vector, and *F* denotes the space-time domain (footprint) over which the (measurement) average is taken. In the case of a slowly filling flask measurement, *F* corresponds to a single spatial location that can reach back in time for up to an hour. For a column measurement, *F* may have a well-resolved time window, will average vertically according to a particular averaging kernel (see Chapter 3 and Appendix E, for example), and may cover spatial region from 10 to 1000 km<sup>2</sup>. Many sensing modalities can estimate their particular *X* to within a few ppm. Satellite retrievals (Chapter 3 and Appendix E) produce estimates of *X* aggregated over vertical columns described by different *F*s. Such "raw" measurements can be useful in their own right and can facilitate the inference, if not quantification, of *changes* over time in local or regional surface GHG emissions.

In considering an equation like the one above, one also acknowledges that the measurement process can introduce systematic (bias/epistemic) errors that can only be removed by validation and calibration, and not removable by averaging, and random (aleatoric, unbiased) errors than can be driven to zero by averaging, i.e.,

$$X_{\rm m} = X + \varepsilon \quad , \tag{6-2}$$

where  $X_m$  denotes the measurement of X and  $\varepsilon$  denotes the difference between (the desired) quantity X and its measurement  $X_m$ . If  $\varepsilon$  is uncorrelated with the measured X components, standard techniques can assess and quantify the variance,  $\varepsilon$ , that is part of the uncertainty in inferring X from  $X_m$ . If the components of  $\varepsilon$  are correlated with the measured quantities, suitable

approaches can also be employed, but may require independent input to provide, rather than deduce, the relevant correlations.

Inferences about  $CO_2$  concentration over a space-time footprint of interest G are needed for other types of direct inferences, as well as to feed model-based inversions (Chapter 7). For example, it may be desired to infer how much the concentration over Los Angeles, within the boundary layer (BL), averaged over a year, has grown from one year to the next. This corresponds to a very specific footprint G. This is also a complicated quantity that can be represented mathematically by (ignoring the corresponding  $\varepsilon$  for simplicity),

$$Y = \int_{(s,t)\in G} c(s,t) \, ds \, dt \,. \tag{6-3}$$

Therefore uncertainties in the underlying concentration field, c(s,t), and its spatial and temporal evolution, determine the uncertainty in the aggregated quantity Y. So even if a flask-capture measurement X has an uncertainty that is less than 0.5 ppm, the accuracy for the average concentration over small space-time volume G covering the location and time of the capture Y can be substantially larger, if random errors dominate uncertainties. The lack of knowledge about the past wind field, coupled with the fact that footprint for the flask capture covers a single spatial point, implies that the relevant domain of c(s,t) is uncertain. For this reason, additional data sources that allow for a more accurate reconstruction of c(s,t) will reduce uncertainties regarding the G-footprint-averaged concentration estimates Y. It will also be necessary to understand the space-time correlation structure in the concentration fields so that information from point and aggregate measurements can be realistically attributed to the rest of c(s,t).

The extent to which a single measurement at a point in space and time informs about Y depends on the spatio-temporal properties of c(s,t). The data in Fig. 6-2, as well as results from other studies (e.g., Idso et al. 1998, 2001; Widory and Javoy 2003), suggest spatio-temporal variations in urban environments that are substantial. Therefore, accuracy beyond 1 ppm may prove unhelpful in inverting in situ measurements in such environments, the main issue associated with the sampling of a field with large gradients and amplitude fluctuations, rather than the accuracy with which concentrations from a single-point sample can be determined. More measurements or additional measurements with footprints closer to the G footprint of interest are needed. For this reason, ground-based Fourier-transform spectrometers (FTSs) that produce observations over a 10- to 100-km<sup>2</sup> spatial footprint over continuous time (when the sun is out) could prove very useful. This also highlights a difficulty with sun-synchronous low Earth orbit (LEO) satellite observations discussed in Chapter 3. These produce a column measurement at a single (solar) time of day at each location: measurements at noon in an urban area are known to yield quite different results than early-morning measurements. As discussed in Chapter 3 and Appendix E, sampling kernels of satellite measurements determine the profile within the vertical extent of F; and it is desired for F to average over the BL, while not integrating nonlocal effects above the BL that are only loosely coupled to surface behavior and in a manner that is not easily quantifiable or can be modeled today. More details regarding uncertainties in remotely sensed data can be found in the report by the National Research Council (NRC 2010).

Data UQ is also tasked with producing data products suitable for incorporating in the inversion analyses described in Chapter 7. Here, multiple measurements over space and time with differing supports need to be combined to inform about concentrations at the modeling grid cell level.

Each data source  $X_i$  has its own associated "footprint" Fi; these data can provide information about the continuous field aggregated over grid cells that have a footprint  $G_j$ , as shown in Fig. 6-3.



Figure 6-3. Principled accounting of uncertainties requires an explicit accounting of the spatio-temporal support/footprint of the various sensor observations  $F_1, ..., F_N$  as well as meteorological data sources. It also requires accounting for the spatio-temporal support of the model grid used for the inversion  $G_1, ..., G_M$ . Here uncertainties can be described by probability distributions that account for data interdependencies.

Here, the dependence from overlapping footprints must be accounted for. In addition, modeling approaches can also be devised to account for possible bias, aberrant observations, or other possible extraneous factors. In principle, uncertainty regarding the data footprints can be accounted for as can uncertainties introduced by interpolation over space and time. This will also require data inputs to modeling, including uncertainty quantification for wind fields, and possibly other meteorological and environmental processes (rain, haze, photochemical smog, etc.).

A dominant contribution to uncertainty in the aggregated concentrations over the grid cells  $Y_1, \ldots, Y_M$  is likely to be traceable to interpolation over space and time. Data from Idso et al. (2001) suggest that a single near-surface point-measurement gives the average CO<sub>2</sub> concentration over a 1-km<sup>2</sup> area only to within 20 to 80 ppm. Additional observations will help reduce the uncertainty for this aggregated cell. More elevated, tower-based observations can be expected to be less variable (Bakwin et al. 1998). Point measurements are likely to be more valuable at rural locations where variations are smaller. More aggregated data sources (e.g., column measurements) will likely be required to deal with high variations present in urban locations. Quantitative statements to this effect await additional test bed investigations.

The aggregation of physical observations over space and time must be carried out in a statistically principled manner to avoid the introduction of systematic errors and to account for extraneous spatio-temporal dependencies. Exactly how this aggregation is to be performed remains to be developed and will benefit from work with and data from well-instrumented test

beds. Also noted is that a practical computational approach that can deal with the high data volume and can properly integrate the various sources of uncertainty remains to be developed.

## 6.3 Combining Information

### 6.3.1 Combining Data from Multiple Sensing Modalities

Different measurement modalities report CO<sub>2</sub> (and other GHG) concentrations at various levels of geographical resolution and aggregation. For example, some spaceborne sensors measure the total CO<sub>2</sub> in two (near-) vertical columns, passive-infrared (IR) spaceborne sensors and FTSs measure the total CO<sub>2</sub> within a single vertical column, flask measurements collect air over time periods up to an hour at a single point in space, and in situ measurements from towers or aircraft provide CO<sub>2</sub> measurements at a point in space and time, sampling over the air volume convected past the measurement point over the sensor integration time and, as a consequence, is a function of the wind vector field. The constantly changing sampling locations associated with aircraft samples lead to additional computational challenges. Within a given geographical area, measurements from different modalities are related as they sample a common underlying CO<sub>2</sub> concentration landscape – denoted by c(s,t).

At a larger scale, time-series plots of  $CO_2$  concentration measurements from multiple locations show similar diurnal and seasonal (or anti-seasonal for stations in the southern hemisphere) cycles, enabling one to quickly identify gross outliers and gross instrument errors. These seasonal variations need to be accounted for to infer any changes or trends over time.

Combining measurements from different modalities is currently relied upon to calibrate FTS and satellite measurements with the aid of aircraft flask data (Box 6-1). This is achieved by exploiting a sophisticated physics model that accounts for roughness of the terrain, the height of the BL, and the air pressure, to estimate the profile of  $CO_2$  concentrations vs. altitude. Using that profile, one estimates a calibration factor to ensure consistency between the two measurement modalities. One can replace the physics model with a reference concentration profile and use the observations to adjust the latter empirically to estimate the calibration factor.

In addition, land-based sensing networks must also be harmonized or cross-calibrated to improve the consistency of measurements (see Chapter 5). These examples show the usefulness of exploiting time-coincident data from multiple sources. Developing a principled framework for data integration is desirable as this enables an objective methodology for automatic and ongoing instrument calibration—by modeling systematic instrument biases and detecting outliers, aberrant observations, and coherent  $CO_2$  concentration estimates, together with measurement uncertainties – that is suitable for further analysis and feeding inversion models.

Statistical spatial-temporal models present an attractive approach for combining and interpolating sensor information over different scales and support. Such models can take the same exogenous input variables, and exploit the correlation of measured concentrations from different modalities and of various GHGs, together with spatial and temporal correlations to interpolate the  $CO_2$  concentration field with an estimated continuous space-time resolution. This statistical approach has emerged from geo-statistics and over the last 20+ years has been successfully applied in a

variety of applications in the environmental sciences. Examples include modeling of the spatialtemporal diffusion of ozone (McMillan et al. 2005) and predicting urban air quality (Liu et al. 2008; Riccio et al. 2006). Evidence that this approach can accommodate multiple measurement modalities in a related context is given in Isaacson and Zimmerman (2000).



Although these models are statistical, they have the potential to seamlessly integrate data collected at varying levels of aggregation in both space and time (known as *the change of support problem* (Stein 1999; Gelfand et al. 2001; Banerjee et al. 2004). Combining data through the statistical model can identify ongoing systematic departures of an individual sensor symptomatic of instrument drift and departures for entire groups of sensors, leading to real-time calibration. Such integration can also reveal other issues with data quality, such as aberrant observations and outliers. But most importantly, it produces a coherent aggregated description of  $CO_2$  concentrations, together with their uncertainties. These products are suitable for further analysis and can be adapted to the grid resolution required for inputs to models and inversion-based inferences.

Using a principled statistical modeling framework is essential to ensure appropriate aggregation and transparency in the data-processing methodology. While there are many statistical methodologies in the literature for the change of support and predictive spatial-temporal aggregation, the most successful approach assumes that the concentration field is the realization of a stochastic spatial-temporal process to develop a Bayesian hierarchical model for the observables (Berliner 2000, Arab et al. 2007). There are numerous advantages to the hierarchical Bayesian formulation: First, uncertainties in both the model and the data are combined to quantify the uncertainty in predicted aggregated  $CO_2$  concentrations. That uncertainty will be larger in areas of sparse data coverage, so that a map of the uncertainty as a function of position can help inform placement of future sensors.

Second, the statistical model can account for metrological effects and instrument properties. Third, the Bayesian method can integrate new data sequentially as they become available instead of starting the analysis *de novo*, as more data continuously become available.

Prior information about the possible magnitude of  $CO_2$  sources and sinks, e.g., from an inventory of oil tankers, ore railroad cars, and other energy consumption indicators, such as urban calorimetric measurements, can also be incorporated as data in models. Using the Bayesian paradigm, it is conceptually possible to estimate a posterior distribution for the magnitude of the various sources and sinks, given the  $CO_2$  measurements.

The downside of a Bayesian hierarchical approach is computational: predictive inferences currently rely on Monte-Carlo Markov chains to draw samples from the predictive distribution conditionally on the data. Fortunately, the computations are parallelizable, making them suitable for cluster computing. Meeting GHGIS goals will also likely require (and offer opportunities to develop) more efficient computational approaches.

In summary, we advocate Bayesian hierarchical models as a principled and transparent framework for integrating data from multiple sensing modalities to make aggregated coherent  $CO_2$  concentration predictions, together with their uncertainty, and to produce inferences on the magnitude of (anthropogenic)  $CO_2$  sources and sinks.

While no such model currently exists for  $CO_2$  concentrations, past experience and successes in modeling airborne pollutants make it plausible that a working model can be developed within the Phase 1 period. It is also noted that although most of this section's focus was on  $CO_2$ , these approaches are appropriate for any tracer gas.



## 6.3.2 Using Tracer Gases to Reduce GHG Concentration Uncertainties

Ideally, any data combination framework should accommodate time series data from multiple measurement modalities and locations and from different GHGs and co-emitted gasses (e.g., nitrogen oxide [NO<sub>x</sub>], carbon monoxide [CO], sulfur dioxide [SO<sub>2</sub>], aerosols, <sup>14</sup>CO<sub>2</sub>) (see Box 6-2). This will be pursued from an inversion perspective in Chapter 7. From a data-driven

perspective, such tracers have proven useful in reducing uncertainty in measurement concentration of  $CO_2$  near large emitters.

Such tracers could include, for example, sulfur hexafluoride (SF<sub>6</sub>) and <sup>14</sup>C, as discussed in the Turnbull et al. (2006, 2007, and 2009) studies, or CO as a combustion and transport tracer (Palmer et al. 2006, Wang et al. 2009, Box 6-3), or methanol, formic acid, or formaldehyde as biogenic tracers (e.g., Beer et al. 2008, Millet et al. 2008, Razavi et al. 2010). Nitrogen dioxide (NO<sub>2</sub>) and SO<sub>2</sub> are also useful tracers for combustion or coal burning (see Boxes 6-2 and 6-3, or Lin et al. 2010; Li et al. 2010, for example). However, care must be taken in reliance on tracers for information on CO<sub>2</sub> because the ratio of these species to CO<sub>2</sub> depends on changes in combustion-system exhaust. Hence, the use of such tracers to reduce uncertainty regarding fossil-fuel CO<sub>2</sub> concentrations will likely require analyses and calibrations specific to each emission source and/or location.



Left: In situ NO<sub>x</sub> and SO<sub>2</sub> measurements correlate with CO<sub>2</sub> measured 6 km from the Parish power plant. The relationship between these two tracers and CO<sub>2</sub> is consistent a stack plant near Houston as well as the CEMS emissions. Right: In situ measurements of CO and CO<sub>2</sub> in air above Houston. The joint observations can separate urban from industrial emissions. Also, for purely urban data, the CO concentrations are very informative about the CO<sub>2</sub> concentrations. However, slope of the fitted relationship differs from other urban areas. Hence, the use of tracers to decrease fossil-fuel CO<sub>2</sub> uncertainties will have to be tailored for specific locations/sources (Data courtesy NOAA-ESRL).

# 6.4 Approaches for Data-Driven Inference

Model-based inversions described in the next chapter will give estimates of fluxes over a large scale by assimilating a variety of data sources. However, it will be useful to develop more empirical or data-driven analysis approaches to provide direct information about changes in GHG emissions. The trade-off is between greater reliance on modeling to invert a particular data set, or lesser reliance on modeling in favor of richer/denser data sets. To the extent that model uncertainties are likely to dominate, one gravitates towards reliance on more data, albeit at cost. The National Research Council study of Pacala et al. (NRC 2010a) suggested an effort to monitor large emission sources such as urban areas and power plants to detect changes in

emissions without making use of large-scale transport models. Concentrating on large emission sources has two key advantages:

- the CO<sub>2</sub> signal is dominated by fossil-fuel emissions (see Barford et al. [2001] for assessments in the Los Angeles area);
- the relatively strong signal leads to local increases in CO<sub>2</sub> concentrations that are easy to detect against the background (increases from 3 ppm to 100 ppm have been observed depending on proximity to local sources and weather conditions). See Idso et al. (2001), Widory and Javoy (2003), Velasco et al. (2005), and Mays et al. (2009) for some examples, and Fig. 6-2.

Such analyses have the potential to detect local changes in GHG emissions on their own using carefully selected data sources that are strategically placed/sampled in space and time. Such observations could be combined with inventory-based estimates to improve or validate reported emission estimates.



Figure 6-4. CO<sub>2</sub> concentration (dry-air mole fraction, XCO<sub>2</sub>) FTS measurements at three different locations: JPL; Lauder, New Zealand; and Darwin, Australia. As expected, the northern hemisphere site shows higher concentration. Also, the urban site (JPL) shows a very different daily signature compared to the two rural sites. The FTS instrument measures the CO<sub>2</sub> concentration in a column extending from the instrument to the sun. Here, a 21-day measurement set is shown. Data source: TCCON wiki (tccon-wiki.caltech.edu).

### 6.4.1 An Illustrative Example

First, consider an illustrative example that makes use of the FTS that gives  $CO_2$  (and other GHG) concentrations in a column over a 10- to 100-km<sup>2</sup> spatial footprint. Figure 6-4 shows FTS measured concentrations over the same 3-week period at three different locations; concentrations are recorded as often as every 30 s (Wunch et al. 2009, 2010). The FTS at the Jet Propulsion Laboratory (JPL) shows how  $CO_2$  concentration varies over the course of a day in the Los Angeles area— $CO_2$  concentration increases by about 5 ppm until about midday and then decreases. This is attributable to a combination of BL fluctuations,  $CO_2$  emissions, winds, and area topography. Daily  $CO_2$  variation over this urban area is markedly different than other rural regions. This variation also illustrates the challenge discussed in Chapter 3 of the reliance on sun-synchronous LEO satellite measurements that

sample at a fixed solar time over a given location. While these daily variations tend to make inferences more difficult using data that are averaged over space and time, they can enhance the ability to detect *changes* in  $CO_2$  emissions using direct, localized, empirical analyses.

Consider now an additional FTS control site that might be set up upwind from the JPL site (perhaps on one of the Channel Islands). Each day, the difference between the measurements at JPL and the upwind control site would provide a measure of  $CO_2$  produced in (added by) the Los Angeles area that day. By looking at this difference, one removes a number of common effects in the measurement that are not directly attributable to  $CO_2$  production – tropospheric  $CO_2$ , the variable (increasing) global mean  $CO_2$  concentration, seasonal (and other temporal) variations, spatial variations, as well as other common environmental effects. Not to oversimplify the case, of course, winds are not always on-shore and from the same direction in Southern California, so the utility and exploitation of such a data-set pair would be conditional on a suitable wind field.

Assuming such sampling complexities can be overcome and do not lead to systematic, conditional biases, one could assess  $CO_2$  production in the Los Angeles area by considering the time series of differences. If this difference grows – on average – by, say, 10% from one year to another, it indicates that the net emissions of the Los Angeles area have grown by 10% over this time. Of course and as noted above, such a time series will be noisy because of seasonal or environmental fluctuations such as changes in wind direction or heat waves. Hence, a statistical assessment will be required to quantify the uncertainty and significance of this assessment. Still, this approach has the potential to detect rather small relative changes in GHG emissions over a specific spatial region. The accuracy of current in situ sensors (<1 ppm) is likely to prove sufficient to detect changes of 10%, perhaps less, per year. The more difficult piece of this type of study is to ensure coverage of the area over space and time so that one can be assured the difference is attributable to changing emissions, and not seasonal or daily variations.

In summary, such data-driven monitoring and analyses offer a number of advantages over morecomplicated, inversion-based analyses:

- They yield transparent, simple inferences;
- They exploit high-resolution data over space and time;
- They make use of thoughtful data collection and differencing to estimate trends and changes over time; and
- Analyses from many different urban areas, power plant locations, etc., could be combined to infer about larger regions, possibly a country.

Of course, such empirical approaches also have drawbacks:

- They do not give direct inference about anthropogenic  $CO_2$  emissions only changes in local  $CO_2$  concentrations. The actual causes of this change could have a variety of origins. Additional work would need to be done to infer and attribute  $CO_2$  surface emissions.
- Inferences will be less precise in areas of high meteorological variability.
- It is not obvious how to choose a control site for the FTS or other instruments.

• It is still an open question how much instrumentation is required to characterize an urban area such as Los Angeles.

More generally, this simple example highlights some basic principles in tailoring sensor placement and data collection to carry out more direct and transparent analyses. By thoughtfully exploiting the strengths of available sensing modalities it may be possible to cancel out features of  $CO_2$  concentrations that make inferring emissions difficult. An example using remotely sensed  $NO_2$  concentrations is given in Box 6-4. Some obvious directions for further assessment are given below.

- Inclusion of other tracer species such as  $NO_x$ , <sup>14</sup>C, CO, or SO<sub>2</sub> to sharpen inferences about anthropogenic GHG emissions using statistical techniques such as principal components and multivariate analysis (Box 6-3).
- Analyses that consider more than a single urban center or power plant.
- Choosing from multiple control sites depending on wind measurements to optimize local inferences.



If this local, inversion-free approach to assessing changes in anthropogenic GHG emissions proves viable, it provides an alternative to defining nationwide emission baselines for the purpose of emissions monitoring and treaty verification. Instead, one could use a year-long sequence of measurements at major emission sources in each country, and look for changes relative to those concentration measurements, without directly specifying actual emissions.

#### 6.4.2 Combining Observations of Large Emission Sources with Inventory-Based Emission Estimates

In addition to observations of large emission sources on their own, observations (top-down measurements) can be combined with inventory-based emission estimates (such as those from

Vulcan or EDGAR) to cross-validate the two types of data sources. This will require some form of local transport modeling since the observations will be  $CO_2$  or other GHG and coemitted gas concentrations while the emission estimates will be (surface) fluxes.



Figure 6-5. Observed (black) and  $1.66 \times$  simulated column  $CO_2$  changes relative to 8 am for 5 days. The 66% difference between observed concentrations and those inferred from bottom-up inventories suggest calibration and bias issues, or other errors, may exist in inventory-based emission estimates.

One example of this sort of effort comes from Dubey et al. (2009) who compared FTS data at JPL with the spatio-temporally resolved  $CO_2$  inventory from Vulcan (Gurney et al. 2009). Specifically, hourly inventories over a  $10 \times 10$  km<sup>2</sup> grid over the Los Angeles area are used. FTS observations give a time series of column-integrated 10- to 100-km-resolution concentrations over the Los Angeles urban area. A nested grid Weather Research Model was used to simulate the atmospheric dynamics and the Vulcan  $CO_2$  emissions were specified at the surface. The forward model predicted column  $CO_2$  changes (increase over early morning values) that were compared with the FTS data as shown in Fig. 6-5 (15-min. averages). The modeled values had to be scaled by a factor of 1.66 to be brought in qualitative agreement with observations. This suggests that emission estimates for the area are 1.66 times larger than the original (Vulcan) estimate. Though no formal UQ was carried out in this study, the estimated scaling factor of 1.66 has itself a fair bit of uncertainty associated with it. More detailed examination of the differences could suggest alternatives to a simple multiplicative scaling adjustment to match observed concentrations relative to those deduced from the inventory-based emission estimates.

Such analyses could include a variety of other sensor observations. One could also consider carrying out such analyses for multiple cities and power plants. These could then be combined to give a more accurate estimate of total emissions, with associated uncertainty estimates. The resulting uncertainty estimates will depend on the consistency of the comparison. If inventory-based estimates are consistently 20% low, then the resulting uncertainty for the total emissions will be affected only by the estimate of this multiplicative factor. If differences between

observations and inventory-based estimates vary substantially between urban domes and power plants, then uncertainties in the adjusted emission estimates will be (substantially) larger.

#### 6.4.3 Steps Toward Operational Inversion-Free Inferences

While the above ideas suggest promise, they are largely untested. The merit of these inversionfree approaches needs to be demonstrated. The accuracy of such approaches along with the required sensor deployment must be assessed. This can be done over Phase 1 of the proposed GHGIS development, using existing data sources, augmenting current, ongoing studies with additional sensors and analysis, and developing a high-fidelity simulation-based test bed capability to test out potential sensor deployment and analysis strategies, as well as assessing the relative merits of data-rich estimates, with little or no reliance on modeling, or modeling-rich (inversion) estimate bases.

While the simple examples above discussed using a pair of FTS instruments, there are a wide variety of sensor options that range from inexpensive small sensor networks to airborne-based platforms. Exploring suitable allocations of sensors for sampling urban centers, power plants, or even denied territory in select countries for an operational system could be carried out with the help of synthetic and real test beds. The remote-sensing community recommends that simulation-based test-bed data should be compared to Observation Systems Simulation Experiments (OSSEs), as also discussed in Chapters 3 and 9 in this report.

An efficient way to help assess and decide on sensing strategies is to develop a flexible, multiuse, realistic simulation-based test bed capability, in concert with an OSSE. This should be done for localized sampling frameworks, such as urban centers and power plants. This will speed up assessment of local sensing strategies since it will likely require at least 2 years of data before first inferences can be made. This will likely need to be done at a higher fidelity than typical transport models used for inversions, as a benchmark, so that it may also assess the relative merits of measurement precision/accuracy vs. cost and number of sensors. It will also be important to build in sufficient usability and flexibility so that a common OSSE can be used for a variety of related studies related to sensor allocation and placement.

To explore the relative merits of the other limit, a simulation-based test bed offers a practical approach for developing surveillance strategies for denied territory. Questions include, what level of sensing effort is required to assess emissions within a denied country of interest? What accuracy can be obtained? Tohjima et al. (2010) suggest some inferences can be made using downwind sensors. More detailed simulation-based studies about the feasibility of such approaches are necessary to better understand the limitations in such country- and perhaps subcountry-level inferences.

Simultaneously, real test beds within the United States and abroad can be exploited to assess the feasibility of detecting emission-source changes in urban centers and power plants. In particular, it will be important to establish the efficacy of combining urban and companion control sites for assessing changes in GHG concentrations at key locations. Ongoing studies, such as the HESTIA project's assessment of Indianapolis and the Four Corners study in New Mexico, can potentially be exploited to assess the value of different sensing strategies. In particular, it will be necessary to determine the minimum sufficient sampling required to assess emission changes. These real

test beds can also be used to understand and help quantify the connection between changes in GHG concentrations and changes in GHG emissions.

#### 6.4.4 Building Up to Large-Scale Quantification of Changes in GHG Emissions

Separate, local estimates of changes within a region or country could be rolled up to infer cumulative changes over the entire region. For most of the top emitting countries, the majority of fossil-fuel GHG emissions come from urban centers and large power plants (for the United States, this is about 75%). This argues for using available instrumentation to characterize changes in these two major sources of anthropogenic GHGs. Since the number of sources and their relative contribution to emissions is fairly well known for these top emitters, a sampling-based approach may be feasible for making inferences about the total contribution from these sources at a country-level aggregation. Of course, this will require access to samples at these sites in top-emitting countries.

Finally, we note that FTS measurements can be linked to emissions as demonstrated in Dubey et al. (2009). In that paper, concentration measurements are compared to concentrations constructed by combining bottom-up emission estimates with a transport model. Such approaches have the potential to estimate bias in bottom-up data. This suggests approaches for combining sensor measurements with bottom-up emission estimates to give improved estimates of country-wide emissions. Sampling-based approaches may be adequate, so a representative set of measurements of urban centers, power plants, etc., may be sufficient for assessing or adjusting bottom-up, consumption-based emission estimates. A combined sensing/bottom-up effort is currently under way as part of the HESTIA project at Purdue University (Zhou and Gurney 2009).

#### 6.4.5 Physical-Statistical Modeling to Account for Model Uncertainties in GHG Emissions Inferences

Finally, an alternative inference strategy to inverse modeling using a computationally demanding forward model is to develop a physical-statistical model for simultaneously estimating wind fields, GHG concentrations over space and time, and surface flux (Berliner 2000, 2003; Wikle et al. 2001, 2003; Wikle and Hooten 2010). This class of models replaces the computational transport model with a statistical model that embeds much of the physics within the formulation. The key feature of this physical-statistical formulation is that uncertainties regarding wind field, concentration field, and emissions are all incorporated into the analysis in a unified manner. The analysis also accounts for uncertainty attributable to measurement sparseness, while allowing prior emissions information to be included. The more inclusive treatment of uncertainties under this approach often leads to more realistic uncertainty estimates as compared to those obtained under more standard inversion methodologies such as the ensemble Kalman filter (Evensen 2009) or variational approaches (Rabier et al. 2000, Lorenc 2003).

Below is a simple example demonstrating how one might use a physical-statistical modeling formulation to simultaneously estimate a wind field and concentration field from sparse sensor observations.

Consider a process motivated by advection-diffusion dynamics approximated by onedimensional dynamics described by the equation

$$\frac{\partial c}{\partial t} = u(s,t)\frac{\partial c}{\partial s} + \frac{\partial}{\partial s} \left( b(s)\frac{\partial c}{\partial s} \right) \quad , \tag{6-4}$$

where s indexes space, t indexes time, c(s,t) is the concentration field, u(s,t) is a spatio-temporal advection parameter (i.e., wind), and b(s) is a spatially dependent diffusion/dispersion parameter.



Figure 6-6. Reconstruction of concentration and wind velocity using a physical-statistical modeling approach. By encoding wind dynamics (advection-diffusion) and boundary conditions into a statistical model, the resulting concentration and wind fields can be estimated with their uncertainty. The physical dynamics are also updated given the concentration and wind observations. This basic approach can be used to estimate emissions as well.

The basic physical-statistical modeling approach discretizes the above equation and embeds it within a statistical model. Uncertainties are allowed at each discrete time step in this statistical formulation, accounting for differences between model and reality. The physical observations of concentration and wind speed at 10 locations over this one-dimensional space help constrain the uncertainty in the discrepancy between model and reality. As observations become denser, it is quite likely that the dominant uncertainty will be the link between model and reality, and, not least, the approximation of the convection process as one-dimensional. An approach like this has the potential to quantify this form of uncertainty. See Fig. 6-6 for an example. A challenge will be to develop computational approaches to handle the large scales of such problems, and the large volume of heterogeneous data.

### 6.5 Surveillance for Early Warnings of Potential Extreme Climate Events

In addition to surveillance of expected, incremental changes, GHG monitoring should also look to detect precursors to sudden, extreme events that could alter global climate. As a first step, we should list potential mechanisms for such extreme events, and list possible approaches for their early detection. While this may not be in the purview of UQ, it is nonetheless of importance in considering where and how to focus GHG sensing efforts. Possible extreme changes include:

- Abrupt land-cover changes, possibly induced by drought or fire;
- Sudden change in methane (CH<sub>4</sub>) emissions in the Arctic;
- Changes in CO<sub>2</sub> uptake in the oceans; and
- Abrupt changes in global ice coverage.

A careful elicitation of potential mechanisms that could lead to abrupt climate change, along with approaches to detect their precursors, should be carried out.

## 6.6 Conclusion

This chapter concludes by listing key points and future directions for measurement of UQ, and then points out what work should be done in the near term.

#### 6.6.1 Key Findings

- For urban and industrial locations, the dominant uncertainty is due to interpolation over space and time. This sparsity can be mitigated with additional sensors, or by more-integrated measurement modalities, such as ground-based FTS. Improving the accuracy of in situ measurements without addressing sparsity in coverage is unlikely to improve inferences of emissions.
- In order to see changes and trends in GHG emissions over urban domes or power plants, two or more years of continuous (or at least semi-continuous) monitoring is required. The sooner dedicated, operational monitoring of these high-emission sources can be established, the more likely it is that we will be able to infer changes in GHG emissions.
- The development of targeted test bed studies, both real and simulation-based, in anthropogenic-emissions-dominated regions with multiple sensors and modalities and multiscale and multispecies modeling for formal data UQ is crucial. Pilot US test beds like Four Corners, Los Angeles, Salt Lake City, and Indianapolis need to be harnessed for UQ study. Opportunities also exist in international areas like Mexico City, Canada (downwind of the United States), Jeju, Korea (downwind of China), New Delhi, and Beijing.
- TCCON FTS networks offer high precision in column, are less sensitive to BL variability in models, and capture large emissions footprints (100 km). They should be expanded for power plant and urban monitoring. We should also be considering the use of "control" sites to measure pristine air near urban domes and industrial emitters.

- Distributed CO<sub>2</sub> sensor networks (100s) may offer inexpensive opportunities if they can be combined with more precise sensors and sufficient precision (<3 to 5 ppm) so they can provide relevant information and not more noise.
- Multispecies measurements help attribute concentrations to emissions sources and provide tests of inventories, especially ratios. These already exist for air-quality applications and have immediate potential for an operational system.

### 6.6.2 Proposed Activities for Phases 1 and 2

Rather than specify activities in Phases 1 and 2, as the sensing modality chapters have, here we note the tasks that are required for data UQ. They likely can be accomplished within 3 years, i.e., within Phase 1 of the development of a GHGIS, and will be refined as sensing networks grow and develop in Phase 2. The data UQ activities focus on developing capabilities and making them operational. Initial activity will be developing and refining methodology for

- combining information across different sensing modalities, and
- producing data products for model-based inversion analyses with appropriate uncertainties at the model grid level of aggregation.

The methodologies used will need to accommodate large amounts of data that will be required for a GHGIS – a challenge in its own right – and will need to be sufficiently reliable and stable to support the operational nature of the proposed GHGIS.

Current experience is rather limited when it comes to UQ for GHG measurements in urban or industrial settings. Therefore the development of targeted test bed studies, both real and simulation-based, in anthropogenic-emissions-dominated regions, with multiple sensors and multispecies modeling for formal data UQ is crucial.

These real test beds will allow us to better understand and quantify systematic variations in emissions (hourly, daily, seasonally, yearly, and over space). Their dependence on local and regional conditions (wind, BL, temperature, humidity/rain, topography, etc.) obtained from far-field atmospheric observations can be compared with in-stack measurements and bottom-up inventories. This focused high-fidelity analysis is crucial since daily fluctuations in  $CO_2$  concentration are larger than the annual global change (see Figs. 6-2 and 6-4).

Specifically, the test bed development will help to

- quantify and achieve the best possible accuracy by developing a UQ-based signature science that combines information from multispecies observing systems, at different spatial and temporal support;
- develop statistical space-time modeling, gap filling/interpolation approaches for combining information from and cross-calibration of various sensing modalities;
- develop computationally efficient ways to represent uncertainty and dependencies for large concentration fields distributed over space and time;

- determine which statistical modeling approaches will be most effective for localized inferences such as the detection of trends, changes, and hypothesis testing;
- determine the appropriate amount, combination, and accuracy of different sensing modalities required to feed inversion analyses, as well as to detect trends and changes in emissions given their uncertainties; and
- determine the feasibility of larger-scale inferences such as combining space-based sensing with strategically placed land sensors to infer emissions from a denied country.

# Chapter 7. Modeling and Modeling Uncertainty Quantification

# **Chapter Summary**

The role of modeling, simulation, and modeling uncertainty quantification in GHGIS is to provide inversions of observational data, including from space, air, and surface measurements, into estimates of regional emissions of anthropogenic GHGs with quantified uncertainties. Careful adherence to model calibration, verification, and validation is required as modeling may be a substantial source of uncertainty within the overall GHGIS system. This chapter discusses the contributions from modeling, simulation, and modeling uncertainty quantification and provides recommendations toward developing such a system. The following is a general summary of our findings and recommendations:

# Findings

- 1. Model-retrieval systems are important tools to infer emissions from measurements of atmospheric composition, and improvements can increase greenhouse-gas information system (GHGIS) accuracy and/or reduce observational costs.
- 2. Uncertainty in greenhouse-gas (GHG) emission retrievals will be dominated by four main sources of bias, rather than unbiased noise (in the absence of any biases, accurate emission estimates could be achieved with an observation network similar to the current  $CO_2$  network, even with considerable levels of unbiased noise):
  - a. emission-representation errors,
  - b. model errors,
  - c. observation-model grid mismatch errors, and
  - d. observational errors.
- 3. Models would likely contribute the biggest source of bias and uncertainty if a GHGIS were to be implemented today.
- 4. No comprehensive analysis and quantification methodology currently exists to estimate model biases, as they would apply to GHGIS.
- 5. At present, atmospheric models are *calibrated*,<sup>1</sup> or *tuned*, by selecting parameterization constants and functional forms to fit a specific set of observational data. In principle, this calibration needs to be carried out for each spatial/temporal (grid) resolution at which the model will be used, because some parameterizations in current models do not correctly account for changes in the scales over which they model the dynamics.
- 6. GHGIS will need a formally documented *calibration, verification*, and *validation* process for its models. Research has been carried out by the scientific community on verification and validation of atmospheric models, even though based on somewhat different definitions of these terms compared to ones adopted in this report.<sup>1</sup> Delivery of robust

<sup>&</sup>lt;sup>1</sup> See discussion in Chapter 1 and Appendix C for definitions and discussion of *calibration*, *verification*, and *validation*, as applied to modeling and in other contexts.

GHGIS products will demand atmospheric model retrievals that meet the required uncertainty specifications; hence model verification and validation will be required for GHGIS, as discussed in the Introduction, with special focus on those aspects of models responsible for most of the uncertainty in retrieved emissions.

### **Recommendations (Phase 1 Development)**

- 1. Create a next-generation ensemble modeling-retrieval system using:
  - a. existing carbon dioxide  $(CO_2)$  inversion models enhanced to include multiple sensor modalities, both fossil-fuel and natural/biospheric  $CO_2$ , and coemitted tracers such as CO and NO<sub>x</sub>, atmospheric chemistry, and
  - b. a multimodel assimilation and uncertainty quantification (UQ) framework.
- 2. Create a program to develop next-generation atmospheric-transport models that can be verified and validated in the sense of their definitions and discussion in the Introduction in Chapter 1 and Appendix C, and, for example, demonstrate grid-convergence that can be characterized by quantified uncertainties in their results.

### **Recommendations (Phase 2 Development)**

- 1. Implement observational test beds to improve and validate model-retrieval systems.
- 2. Enhance the GHGIS modeling-retrieval component to include:
  - a. improved atmospheric chemical transport models and biospheric models,
  - b. multiple/alternative parameterizations for physical processes within each model,
  - c. assimilation of observations of physical processes and other chemicals to assess and constrain model errors,
  - d. more comprehensive UQ, including bias detection and correction, and
  - e. higher, or variable, grid resolution.
- 3. During Phase 2 of a GHGIS development project, implement next-generation atmospheric-transport models, as they become available, whose development was initiated during Phase 1 development.
- 4. Use GHGIS modeling-retrieval system for Observation Systems Simulation Experiments (OSSEs) to help optimize the GHGIS observational network.

## 7.1 Introduction

Atmospheric models would be used in GHGIS to calculate solutions of equations that simulate the effect of emissions (most of which come from ground-level) on atmospheric concentrations of emitted chemicals, and their chemical reactions and products in the atmosphere. Such models provide a relationship between emissions at any point in time and space (mostly on the surface) with measurements of concentrations at any time and space in the atmosphere. These relationships can be used to mathematically "retrieve" the most-probable emissions distributions to have produced the observed concentrations. Such model-retrieval systems and models are important tools by which concentration observations downwind of several regions can mathematically constrain emissions in upwind regions consistent with the simulation of the dynamics described by physical laws in the codes, as also discussed in Chapters 1 and 6, and Appendix B.

This chapter discusses a model-retrieval system for GHGIS and the work that will be required to advance it. Model-retrieval capabilities available now are described, along with their sources of error, what could be delivered by the end of Phase 1 and Phase 2 of a GHGIS development project, as well as network design, the value of tracking multiple chemical species, and potential benefits to other science fields.

#### 7.1.1 Overview of How Atmospheric Models and Retrieval Theory Can Estimate Emissions

An atmospheric model is, in essence, a code to solve the equations of physics that control the state of the atmosphere (including winds, temperatures, and chemical concentrations), given an initial state and appropriate boundary conditions. Because of the importance of weather to human society, considerable resources have been devoted, over many decades, into developing models that can solve this multiphysics, multiscale problem whose dynamics reside on scales ranging from molecular diffusion to the size of the planet, and whose equations are famously chaotic. These models have developed to the point where they can forecast temporal variations in the atmospheric state, such as passage of temperature fronts over a given location, to an accuracy of a few hours in many cases. Nonetheless, many challenges remain, and different types of models have been developed to answer different questions.

The emission of chemicals (such as  $CO_2$ ) is usually handled as a boundary condition to atmospheric models and is typically given in units such as molecules (or grams) per unit area, per unit time. The models then solve the equations of motion and calculate the concentration of chemical species throughout the atmosphere as a function of time. Thus, the framework of atmospheric models is well suited to the problem of connecting emissions to chemical-species concentrations downwind, which is what is usually and most easily measured. Models, however, generally run forward in time and, as a result, calculate concentrations as a function of emissions, whereas GHGIS needs to know the reverse. Hence, various techniques have been developed to invert this relationship and retrieve emission source magnitudes and locations, given measurements of concentrations. These techniques are variously known as inverse, retrieval, or assimilation methods.

As discussed in Chapters 1 and 6, and Appendix B, the use of concentration measurements in time and space, along with winds provided to the simulation, to retrieve emissions at locations far from the measurement locations, offers a way to reduce measurement density and accuracy that would be required without a model-retrieval system. A model-retrieval system also provides a way to combine information from multiple measurement times and locations (that may not be regular), and multiple measurement modalities (including ground, air, and space). The relative importance and reliance on modeling, vs. increased observational data (spatial) density, was discussed in Chapters 1, 3 and 6, and Appendix B, and represents a main GHGIS challenge. If model uncertainties are high, or difficult to quantify, then a heavier burden must be placed on measurements, with attendant costs. If models prove reliable, with quantifiable uncertainties,

then fewer observational data, i.e., at lower density, etc., will be required. It is not possible to state a priori, certainly not at this writing, where the optimum along this dimension lies. Careful future experimentation and test-bed experience can help explore the balance.

### 7.1.2 Inverse/Retrieval/Assimilation Techniques Currently Available

Inversion techniques have been developed to assimilate  $CO_2$  concentration measurements and estimate  $CO_2$  emissions/sources in a spatiotemporally resolved manner. Reviews of such methods can be found in the NRC Report (2010a) and Ciais et al. (2010). All inversion methods solve some variant of the Bayesian inverse problem for the  $CO_2$  source strengths, obtained by minimizing the cost function,

$$J = [d - H(s)]^{\mathrm{T}} R^{-1} [d - H(s)] + [s - s_{\mathrm{pr}}]^{\mathrm{T}} Q^{-1} [s - s_{\mathrm{pr}}] .$$
(7-1)

Here *d* and H(s) are vectors of measured and simulated concentrations, respectively, the latter derived using a transport model that translates CO<sub>2</sub> emissions to time-varying CO<sub>2</sub> concentrations at "sensor" locations where d is measured. The  $s_{pr}$  is a prior belief/guess of what the source strengths should be. *R* is a covariance matrix that represents/estimates measurement errors, or, how closely model predictions should resemble observations, while *Q* is a covariance matrix that represents (provided weights on) how closely the final estimates should adhere to the priors.

Typically, Earth's (or a region's) surface is divided into regions and an unknown CO<sub>2</sub> source (positive or negative, e.g., a sink), is assigned to each. These sources are then estimated from the data by minimizing the cost function in Eq. 7-1 above, i.e., the suitably weighted difference between the prediction of concentrations from the priors and the measurements. If H(s) is linear (approximately true for CO<sub>2</sub>), the distribution of *s* can be solved analytically as a multivariate Gaussian. To date, biospheric/natural CO<sub>2</sub> fluxes have been the primary focus, but a few studies have also tried to account for and discriminate anthropogenic vs. biospheric/natural emissions. Observations from in situ ground sensors, aircraft, and satellites have been used. The main classes of inversion methods are reviewed below – the differences between them mainly involve whether uncertainty in the inferences is calculated and how the data is handled (i.e., whether incremental updates to the inferences are possible with streaming data).

#### Bayesian "Batch" Inversion Methods

Bayesian "batch" methods have gained prominence in the last decade once estimates for terrestrial and oceanic CO<sub>2</sub> fluxes were developed based on bottom-up methods. These "batch" methods require that all the data to be used in the inference are available at the time of the inversion and all the fluxes, over the entire duration of interest, are inferred simultaneously. These methods provide estimates for  $s_{pr}$  and are updated using atmospheric CO<sub>2</sub> measurements (e.g., Houwelling et al. 2003, Rodenbeck et al. 2003). The choice of  $s_{pr}$  influences the inferred fluxes. In contrast, Michalak et al. (2004) modeled  $s_{pr}$  as a multi-Gaussian, whose mean could only assume two values (terrestrial and oceanic), and modeled spatial correlations in Q using an exponential covariance. In Mueller et al. (2008), this method was used with measurements from the NOAA/ESRL network to infer *s* on a mesh that is four times denser than the ones used in Houwelling et al. (2003) and Rodenbeck et al. (2003). Gourdji et al. (2008, 2010) incorporated
additional variables (leaf-area-index [LAI], fraction of photosynthetically active radiation [fPAR], GDP and population density, among others) as predictors/surrogates of  $CO_2$  fluxes, while inferring *s*. Figure 7-1 shows the distribution of biospheric fluxes derived from the two predictors and compares them with the optimized fluxes. In their study, GDP and population density accounted for 75% of the variation attributable to anthropogenic emissions. More recently, they extended their method to reduce the dimensionality of the inversion (Gokede et al. 2010).



Figure 7-1. Top: Biospheric fluxes of  $CO_2$  predicted by LAI and fPAR indices. Bottom: Final (optimized)  $CO_2$  fluxes. The left column figures are for May 2000, and the right column figures are for July 2000. The spatial patterns are qualitatively captured by the auxiliary-variable-based prior model. Figure from Gourdji et al. (2008).

#### Variational Methods

Bayesian "batch" inversion methods described above are often formulated using matrices and performed in one pass. If used with high-resolution satellite measurements, large matrices result, leading to unwieldy computations. Variational formulations (e.g., Chevalier et al. 2005, Baker et al. 2006) overcome this difficultly through iterative, gradient-based optimization. Chevalier et al. (2005) developed a variational formulation to arrive at an optimal *s* iteratively within the context of a minimization procedure. H(s) was a three-dimensional transport model. Executing it repeatedly in a minimization loop posed the biggest challenge. Recent assimilations of Atmospheric Infra-Red Sounder (AIRS) data by the same group (Engelen et al. 2009, Chevalier et al. 2009) achieved resolutions of  $100 \times 100 \text{ km}^2$ , matching that of the reported AIRS data product (Chapter 3 and Appendix E). The technique employed is a "two-step" procedure in which meteorological observations are assimilated first to provide a better estimate of the atmospheric conditions during a CO<sub>2</sub> measurement campaign, followed by the flux-inversion scheme. Variational methods show potential for CO<sub>2</sub> flux estimation (through the assimilation of different types of measurements), as well as scalability to fine resolutions. However, in these studies, only a point estimate of CO<sub>2</sub> fluxes was calculated. No effort was made to quantify

uncertainty in the estimated fluxes because of the computational challenge of inverting a large Hessian matrix.

#### Sequential Data-Assimilation Methods

These methods, unlike the "batch" methods described above, allow the incremental estimation of  $CO_2$  fluxes as time-varying measurements become available. Thus they can produce provisional, if somewhat less accurate, results if some measurements are unavailable. Since it can take up to 8 months for emissions to "go around the globe" and affect all measurement locations, this can be very helpful. Bruhwiler et al. (2005) devised a Kalman smoother to estimate monthly fluxes. They used  $s_{pr}$  derived from models of terrestrial and oceanic fluxes. Michalak (2008) developed a geostatistical counterpart that replaced the dependence on model-based priors to the simple multi-Gaussian model (with two discrete means) used in Michalak et al. (2004). Peters et al. (2005) developed an Ensemble Square Root Filter to estimate  $CO_2$  sources at a weekly temporal resolution on a 9°×6° grid. The ensemble method allows the use of a black-box H(s) (TM5 in this case) and forms the core of CarbonTracker (Peters et al. 2007), as also discussed in Chapter 3. *A priori fluxes* are obtained from terrestrial and oceanic models. Synthetic satellite (OCO) measurements have also been assimilated using an ensemble transform Kalman filter (Feng et al. 2009) at a regional scale (1000×1000 km<sup>2</sup>). Joint assimilation of meteorological and  $CO_2$  measurements have also been studied (Liu et al. 2009, Kang 2009).

#### Sampling-Based Inversion Methods

Sampling-based methods that were computationally demanding in the past are now within computational reach and commonly applied to geophysical inversion problems (Sambridge and Mosegaard 2002). These include the use of Monte Carlo and Markov chain Monte Carlo sampling techniques. Sampling-based methods approximate the *a posteriori* emission distributions using ensembles of simulations. Ensemble members are generated from distributions of prior model assumptions and weighted by the likelihood that they agree with observations. The search for model configurations with high likelihoods can be accelerated using genetic algorithms and simulated annealing. Sampling-based methods are attractive because they can incorporate many types of model uncertainties, handle non-Gaussian distributions, and work well with nonlinear models. Applications to emissions inversions are described in Kasibhatla (2004), Ricciuto et al. (2005), and Deguillaume et al. (2007).

## 7.1.3 Model Types and Capabilities Currently Available

#### Climate Models (GCMs)

GCMs solve the fundamental equations of hydrodynamics, thermodynamics, and radiation balance of the coupled atmospheric, ocean, sea ice, and land systems over the entire globe (they are often referred to as coupled ocean-atmosphere models). Spatial resolution is typically 100-200 km for current models, so GCMs require modeling and parameterizations to represent the complex subgrid-scale physics of processes such as clouds, boundary-layer turbulence, and surface interactions. Even if GCMs were free of understood deficiencies, they could not be

expected to forecast detailed weather beyond the 1 to 2 week reach of weather forecasts, but they can forecast changes in climate statistics, e.g., mean temperature, length of heat waves.

GCMs form the basis for the models described below. They are based on physical laws and are generally best at conserving physical quantities and relationships, with the exception of embedded parameterizations that nonetheless attempt to conserve the necessary quantities.<sup>2</sup> GCMs provide important means for understanding changes in climate attributable to climate-forcing effects, such as increased trapping of heat by GHGs.

GCMs have been developed by several institutions in the USA and elsewhere, including NCAR/DOE (CESM), NOAA-GFDL, NASA-GISS, and UKMO (HadCM). See the most recent assessment of the Intergovernmental Panel on Climate Change for details (Randall et al. 2007).

#### Weather Forecast Models

Weather forecast models use observations of meteorological variables (winds, temperature, pressure, and humidity) to constrain the state of a GCM to create the best possible estimate of the current state of the atmosphere (a process known as data assimilation). The GCM is then run forward for a week or two to forecast the weather. A related use is to run the weather model over historical periods and use weather observations to provide an improved estimate of weather that has actually occurred (producing what are known as "reanalysis data").

In order to generate improved forecasts that accommodate uncertainty in initial conditions, weather-forecast systems run an ensemble of different simulations as a surrogate for the distribution of different possible outcomes. This provides improved estimates, as well as an estimation methodology of possible errors/uncertainties. Of course, implicit in this approach is acceptance that the variance of the results of simulations, which may be in doubt, provides a valid surrogate for the (true) uncertainty in each forecast. Nonetheless, when the ensemble spread of weather forecasts is compared to actual forecast error, i.e., the difference between the prediction and the weather that eventually occurs, it is found to be similar (Buizza et al. 2005). The comparison was even closer for the UKMO model when stochastic terms were incorporated into its parameterizations (Slingo et al. 2010).

An issue with weather-forecast models is that assimilating observations and introducing the necessary adjustments to bring about a better agreement with observations, can/will force the model state into states that no longer adhere to the evolution of the physical laws simulated. For example, if observations of pressure and wind are such that the wind is inconsistent with the observed pressure gradient, e.g., because of measurement error, or sparsity of observations, or for some other reason, then changing the state of the model to match observations produces a non-physical, or inconsistent, forcing and state in the model. Continuing to run the weather model with this new state results in "assimilation shock" because the new state of the model is (physically) unbalanced/inconsistent. Fortunately, "assimilation shocks" usually dissipate as the GCM continues to run, but if this is done repeatedly, to force the model to track observations, there is a cumulative effect that persists and is difficult to quantify. Weather forecast models include elaborate initialization techniques to minimize these problems.

<sup>&</sup>lt;sup>2</sup> See related discussions in Chapter 1 and Appendix B.

Weather models have been developed by ECMWF, NASA-GMAO, NOAA-NWS, UKMO, and the US Navy, among others.

#### **Regional Climate Models**

Regional climate models are similar to GCMs, with the key difference being that they simulate only a small part of the globe (from a major metropolitan area and sub-country areas up to, at most, a continent). Simulating a smaller region makes it computationally feasible to run at higher resolution (such as on a 10 km grid, or even smaller). However, regional models must be provided with boundary/inflow conditions (e.g., winds and chemical concentrations) at the edges of their region (computational domain). This information is usually supplied by a global GCM or weather model, so a regional model can be used to calculate the local impact of a global model at a high regional resolution. The need for increased accuracy is most evident in regions with strong local forcings of the meteorology, such as around mountains and valleys, and around point-emission sources, such as power plants.

With small regions, air parcels will often be blown out of the region quickly. This means that even a perfect regional model may not be able to remove biases present in the boundary conditions. It also means that regional models are not as sensitive to conservation errors, since such errors are lost (advected away) from the region. Nonetheless, regional models have been improving their ability to conserve mass and energy in recent years. For example, one of the advection schemes available in the Weather Research and Forecasting (WRF) model does conserve tracer mass (Skamarock et al. 2008).

Regional climate models currently available in the United States include MM5, NOGAPS, RAMS, and WRF.

#### Atmospheric Chemical Transport Models (CTMs)

CTMs solve the equations for chemical reactions between reacting species in the atmosphere (such as CO or hydrocarbons that are oxidized to  $CO_2$ ), as well as of the physical-chemistry equations for the growth of aerosols and their interactions with clouds. CTMs do not try to solve the equations for winds and temperatures. Instead, CTMs rely on meteorological variables provided by a separate file that was produced by either a GCM or a weather model.

Reading meteorological variables from a file is more computationally efficient than calculating them within the model, but does not allow couplings, such as the effects of chemicals and aerosols, to affect the meteorology. The chemical and aerosol capabilities of CTMs are being added to GCMs and regional climate models to develop Earth system models (ESMs), so that the coupling between meteorology, chemical kinetics, and aerosol-processes can be captured.

Examples of CTMs include GEOS-Chem, IMPACT, MATCH, MOZART, and TM5.

#### Earth System Models (ESMs)

ESMs are extensions of GCMs and regional climate models that include the effects of atmospheric chemistry, aerosols, and the biosphere. They are based on fundamental chemical and physical laws to

the extent feasible. However, simplified models are often used because of the complexity of the processes modeled/simulated, especially for the biosphere where the number of interacting organisms and processes is very high, and often unknown.

Examples of ESMs include the NCAR/DOE-CESM and the GFDL-ESM models.

#### Back-Trajectory Models

Back-trajectory models use winds from a GCM or weather model to track the movement of an air-parcel backwards in time. This can be useful when an observation is made and one wants to know where the air parcel has been previously. Back-trajectory models are fast but pose their own challenges, e.g., two nearby starting points can produce wildly different back-trajectories. Back-trajectories also propagate backwards forever and it is not possible to know when a chemical was added to the air parcel along the trajectory, which is essential for attribution in the context of GHGIS.

Examples of back-trajectory models include HYSPLIT and STILT.

## **Biosphere Modeling**

The biosphere is a large and highly variable source and sink of  $CO_2$  through photosynthesis and respiration (cf. Fig. B-2 in Appendix B), and important to GHGIS. Biosphere models calculate carbon fluxes exchanged between different pools (aka reservoirs) within the biosphere (e.g., leaves and soil on land, and different plankton types in the ocean), as well as carbon exchange with the atmosphere.

Examples of biosphere models include CASA, CN, ORCHIDEE, and SiB.

## 7.1.4 Existing Model-Retrieval Capabilities

It is beyond the scope of this report to list and cite the many model-retrieval studies that have been carried out. A few examples are included to illustrate what is currently possible. The TransCom 3 study is symbolic of the many model-retrieval studies focused on biospheric  $CO_2$  fluxes. The Algeciras study shows that model-retrieval techniques can also be applied to non- $CO_2$  sources, and can be particularly effective if the source is known, or can be assumed, to be a point source.

## TransCom 3

TransCom 3 was a landmark study that used an ensemble of 17 different  $CO_2$  atmospheric models, operating under a carefully designed model-retrieval protocol, to retrieve the net biospheric  $CO_2$  emissions from each of 22 regions covering the globe (Gurney et al. 2002, 2003, 2004; Law et al. 2003; Baker et al. 2006). The 22 regions and the observation locations are shown in Fig. 7-2.



Figure 7-2. The 22 TransCom 3 regions (11 land, 11 ocean) along with their a priori net annual biospheric  $CO_2$  fluxes to the atmosphere in GtC/yr, along with associated a priori uncertainties. Circles mark the observation locations. Open circles indicate sites with multiple datasets. From Gurney et al. (2002).

The retrieved emission estimates are summarized in Fig. 7-3. Several points are worth noting. First, the model-retrieval system was able to reduce the uncertainty in biospheric CO<sub>2</sub> emissions over the land regions. Second, the typical uncertainty from a single model (1 $\sigma$ ) was typically of similar magnitude to the annual emission for each region (±200% error at the 2 $\sigma$  level). Third, the uncertainty in the results estimated by the TransCom 3 direct Bayesian retrieval algorithm was usually similar to the variance of results from the ensemble of models.

If each of the 17 individual model-retrieval estimates was independent *and* all errors could be attributed to random causes, then the error in the ensemble mean estimate could be estimated by the ensemble standard-deviation in each region, divided by the square root of 17, which would make the mean estimate for most of the regions statistically significant at the  $2\sigma$  level. However, it is difficult to prove the premise. By way of example, all models are subject to similar systematic errors, especially considering the similarity in their parameterizations, as well as other common-mode issues, so averaging need not reduce the error/uncertainty of the mean as rapidly as  $\sqrt{N}$ , where *N* is the number of members in the ensemble.



Figure 7-3. Retrieved annual net biospheric  $CO_2$  emissions in each TransCom 3 region. Boxes show the a priori emission mean and uncertainty. The symbols on the left and right within each region show the a posteriori results with and without using a background seasonal biosphere flux. The crosses show the mean fluxes. The mean estimated uncertainty across all the models is indicated by the circles. The standard deviation of the models' estimated fluxes is shown by the error bars. Positive values are a source to the atmosphere (Gurney et al. 2003).

#### Algeciras Radioactivity Release

On May 30, 1998, a piece of medical equipment containing cesium-137 (<sup>137</sup>Cs) was accidentally melted in one of the furnaces at the Acerinox stainless-steel production plant near Algeciras, Spain. The accident remained undetected until June 1 and 2, when radioactivity in the plume was detected by distant sensors downwind in France and Italy.

A model-retrieval system developed at the DOE National Atmospheric Release Advisory Center (NARAC) was successfully used to confirm that the emission location was in the neighborhood of Algeciras (Delle Monache et al. 2008). The NARAC model-retrieval system used a sampling-based inversion method (Markov Chain Monte Carlo sampling) coupled to their Lagrangian

atmospheric-transport model. Results of their model-retrieval system are depicted in Figs. 7-4 and 7-5.

However, as mentioned above, a key a priori assumption for this model-retrieval system was that the release was attributable to a single point source, which, while true for some GHG sources (e.g., for emissions from power plants), is not true for others (e.g., for emissions from the transportation sector).



Figure 7-4. The result of the NARAC model-retrieval for the Algeciras radioactivity release. White circles indicate the location of the radiation sensors that detected elevated radioactivity. The large rectangle was the initial search region (prevailing upwind direction). Gray dots mark the initial random guesses (priors) for the location at the start of the stochastic inversion. Black dots mark the estimated release location after the model-retrieval analysis. The white square marks the actual release location (Delle Monache et al. 2008).



Figure 7-5. The four panels show the behavior of the Algeciras radioactive plume over time, as modeled by the NARAC atmospheric transport model (Delle Monache et al. 2008).

# 7.2 Uncertainties of Current Modeling Capabilities

## 7.2.1 Total System Errors

The only large intercomparison of model-retrieval systems with real data is known as TransCom 3. It was carried out around 10 years ago (see Sec. 7.1.4). This intercomparison provided estimates of biogenic emissions from 22 regions around the world, at a scale of approximately 2 regions per continent. The observations consisted mostly of  $CO_2$  measured from fixed flask sampling sites. The participation of a large number of model-retrieval systems under a controlled protocol allowed the TransCom 3 program to provide the best estimates of uncertainty to date from model-retrieval systems.

The uncertainty in annual biogenic CO<sub>2</sub> fluxes from each of the TransCom 3 regions was typically  $\pm 200\%$ , at the  $2\sigma$  level, so a single model-retrieval system would be unable to provide statistically significant results. However, it was found that using an ensemble of model-retrieval systems led to results that were statistically different from a priori estimates (see Sec. 7.1.2).

Ten years of research and development have followed TransCom 3, with improvements in atmospheric models and retrieval algorithms that can be expected to result in overall improvements. For example, model (grid) resolution has generally increased by a factor of  $\sim 2$  since TransCom 3, which can reduce biases from model-observation scale mismatch, as found in the TransCom 4 synoptic intercomparison (Patra et al. 2008). However, no intercomparison like

TransCom 3 has taken place that would allow a quantitative assessment of improvements in retrieval estimates.

The TransCom 3 study used real data, so the  $\pm 200\%$   $2\sigma$ -uncertainty estimate reflects the combined (cumulative) effect of all errors in the models, observations, and other data used in TransCom 3, around 10 years ago.

In Sec. 7.5.1, we show that a TransCom 3-style inversion would have produced accurate emission estimates, with uncertainties of just a few percent, *if* errors in the problem were unbiased. This implies that an important challenge for GHGIS is to reduce the impact of biases on the GHGIS product through some combination of observational constraints and improved model-retrieval systems.

There are four parts of GHGIS that are a source of bias (and noise):

- 1. emission-representation errors, discussed in Sec. 7.2.2;
- 2. model-retrieval errors, discussed in Sec. 7.2.3;
- 3. observation-model gridbox mismatch errors, discussed in Chapter 5; and
- 4. observational errors, discussed in Chapters 3 through 6.

Of these, models are likely to be responsible for the biggest source of biases in current systems. For example, uncertainties in a single parameterization (the atmospheric boundary layer) for a synthetic experiment studying possible fossil-fuel monitoring networks for California, produced errors in retrieved emissions of  $\pm 30\%$  at the  $2\sigma$  level (Cameron-Smith et al. 2009). The need for accuracy in a GHGIS system is so great that improvements from present-day capabilities in all four sources of bias will be required to meet the GHGIS requirements, as described in Chapter 2.

## 7.2.2 Emission Representation Errors

#### Uncertainties Arising from Priors

Inferred  $CO_2$  fluxes represent a compromise between assumed priors and constraints imposed by observations. However, because of the sparseness of observations, priors are informative, i.e., inferences are not totally data-driven. Typically, priors are prescribed using models for vegetation and oceanic fluxes (e.g., Randerson 2001, Takahashi et al. 1997). Houwelling et al. (2003) studied the effects of different prior models on  $CO_2$  flux inferences drawn from synthetic satellite soundings. They showed that using prior fluxes with spatial and temporal correlations provided a maximum reduction in a posteriori uncertainties, with differences between inferences drawn from different prior fluxes on emissions retrievals in TransCom 3. The study indicated that transport-model errors would dominate if the prior constraint was relaxed, in keeping with the general observation that measurements are woefully scarce. The geostatistical inversion method (GIM) by Michalak et al. (2004) reduced the impact of informative priors by limiting them to two discrete values (land and ocean are treated as hyperparameters) and imposing spatiotemporal correlations. GIM was tested on synthetic data and applied to real data in a number of studies (Mueller et al. 2008, Gourdji et al. 2008, Gokede et al. 2010). An algorithmic extension to GIM,

to enable the incorporation of auxiliary, easily observed variables e.g., leaf-area index (that impact the spatial distribution of  $CO_2$  sources) was demonstrated by Gourdji et al. (2008, 2010).

#### Non-Gaussian Prior Distributions

Researchers have probed the effects of different prior flux models on retrieved fluxes, but have generally retained the Gaussian form of the priors. That assumption may be doubtful. Chevallier et al. (2006) tested the assumption of Gaussian priors by comparing  $CO_2$  fluxes predicted using the ORCHIDEE biospheric model (Krinner et al. 2005) with direct (tall-tower) eddy-covariance flux measurements. Discrepancies between model predictions and observations were not Gaussian at most locations. Errors were better approximated using a Cauchy distribution (Fig. 7-6). Further, the temporal correlation was linear (beyond a lag of 2 days) and no particular spatial correlation was observed. The use of non-Gaussian priors is a research area that merits further investigation.



Figure 7-6. Distribution of the departures between observed  $CO_2$  fluxes from tall-towers and those predicted by ORCHIDEE, a biospheric model. The distribution is Cauchy-like and fat-tailed; yet inversions use an equivalent Gaussian distribution (heavy dotted line). Taken from Chevallier et al. (2006).

#### 7.2.3 Model Verification and Validation

Current models rely on parameterizations to incorporate and represent subgrid-scale physical processes. Changing resolution means that the scales that must be parameterized should also change, yet most current parameterizations are usually developed (and tuned) for a limited resolution range. Hence, increasing resolution of most atmospheric models will not bring convergence to the "true" answer, if it converges at all.

Considering that an increase of a factor of 2 in resolution produces an increase of a factor of 16 in computational effort, as discussed in Chapter 1, it is also difficult to explore grid resolution behavior over too large a range. There is discussion in the atmospheric model-development

community of creating scale-aware parameterizations, but this effort is in its infancy at this writing. Nonetheless, individual components of atmospheric models, most notably the dynamical cores that solve the dynamical equations for winds and temperature resolved by the grid, are generally verified before their inclusion in an atmospheric model.

Formally, validation of atmospheric and biospheric models cannot be undertaken prior to model verification. Nevertheless, attempts at validation activities are continually ongoing within the scientific community. It has primarily been performed through two methodologies that complement each other.

The first methodology is direct comparison of physical quantities calculated within models against available observations from satellites, surface, and airborne platforms. Satellite data provide global coverage and, at least to date, usually target larger areas, but as discussed in Chapter 3, are typically too infrequent today to enable the identification of diurnal cycles, and not all quantities are amenable to measurement from space. In contrast, surface measurements can provide more time-resolved information for a large number of possible quantities, but at a limited number of locations that are at, or near, the surface. Aircraft can provide high time-resolution observations along a flight track anywhere within the troposphere and lower stratosphere, but operationally typically sample above the planetary boundary layer (PBL), except during take-offs and landings, and are expensive to operate. With sufficiently long observational time series from multiple sources, coupled with appropriate model simulations, the behavior of the model under different weather regimes and forcing conditions can be assessed and calibrated/tuned.

The second methodology is to intercompare ensembles of model runs against data and each other under controlled conditions, e.g., AMIP & CMIP by PCMDI, TransCom, ACCMIP, CCMVal, C-LAMP. This is best described as an attempt to combine verification and validation. It can also provide the sensitivity of the models to varying parameters and forcings. Traditionally, the meteorology and climate communities use ensembles based on

- 1. perturbations of model initial conditions,
- 2. varying parameterizations used within a single model, and
- 3. models developed by different scientific groups.

Ensembles of the results also provide estimates of uncertainty, or spread/variance, in model output.

In the past few years, a third methodology has begun to be applied to climate models: automated Uncertainty Quantification (UQ), based on mathematical methods. Traditionally, attempts at verification and validation (V&V) described above have been handled directly by scientists. However, the size of the V&V task is growing very rapidly with the growing complexity and scope of state-of-the-art models. As a consequence, automated methods are now applied to the two methodologies described above, and promise faster, more complete, and improved V&V than before, subject to model limitations, as well as the capability to provide sensitivity-analysis information.

A more complete discussion of UQ methods, and the ways it can benefit GHGIS, is given in Sec. 7.2.4.

#### Parameterizations

Many processes captured in atmospheric models are described via "parameterizations." These are representations of specific (often subgrid-scale) processes within the larger framework of the conservation equations of motion (Peters et al. 1995). Parameterizations implemented in atmospheric models are based on theoretical and statistical relationships between measured quantities. Unfortunately, parameterizations for some atmospheric processes are highly uncertain because of a poor understanding of the process, lack of key measurements to calibrate constants, or even because the basis of a parameterization may not be physically valid. Parameterizations with significant uncertainties relevant to GHGIS include:

- vertical mixing and the exchange of material between the planetary boundary layer and the free atmosphere; and
- the representation of clouds that act as a conduit for transporting trace gases in the atmosphere.

Planetary Boundary Layer (PBL) parameterizations and the description of turbulence affect the simulation of winds, mixed-layer depth, temperature, and humidity. These are important to the prediction of the exchange of near-surface GHGs with the free atmosphere, as briefly also discussed in Chapters 1 and 4, and Appendix B. A variety of PBL parameterizations exist because no single scheme outperforms all other schemes, in all situations.

The sensitivities and uncertainties in simulating GHGs can be assessed by comparing multiple PBL schemes within a single modeling system; PBL schemes within WRF include Hong and Pan (1996), Hong et al. (2006), Janic (2002), Mellor and Yamada (1982), Pleim (2007), and Park and Bretherton (2009). Each of these has its own advantages and disadvantages and has been tested with specific datasets.

Clouds and precipitation are important for lofting gases to high altitudes and raining out anything soluble. Predictions of clouds and precipitation have improved over time, but significant uncertainties remain in simulating deep convection, the spatial extent of clouds, mixing within clouds, and the location and amount of precipitation. Deep convection can rapidly transport trace gases vertically (e.g., Barth et al. 2007). However, until recently, measurements to verify deep convective transport of carbon monoxide (CO) and CO<sub>2</sub> have been lacking. Co-located cloud and trace-gas measurements from satellites and aircraft provide information on the extent to which trace gases are lofted into the free troposphere. Coupling surface and satellite measurements can provide a means to calibrate vertical transport and mixing of CO<sub>2</sub> in models. Until calibration studies are conducted for specific cloud systems, the sensitivities and uncertainties associated with clouds and deep convection can be assessed by evaluating these processes using model ensembles with alternative parameterizations for each process. Comparisons with very high resolution simulations, such as can be realized in large eddy simulations (LES), also provide a viable route for parameterization improvement at the coarser scales. However, the caveat of the validity of the physical basis of a particular parameterization scheme remains. An example of a parameterization, referred to as gradient-transport modeling, is discussed in Appendix B.

#### Ecosystem Models

Attributing and quantifying the anthropogenic emissions of  $CO_2$  requires an understanding of biogenic  $CO_2$  emissions (although this is less important when <sup>14</sup>CO<sub>2</sub> is measured, see Sec. 7.5.2). While not a focus of this report, it is important to consider the biosphere and discriminate against its contributions for GHGIS purposes.

Many older model-retrieval studies, such as TransCom 3, used predetermined climatologically averaged distributions of biospheric  $CO_2$  emissions for their regional basis functions. The problem with using temporally averaged emissions is that biospheric emissions are actually highly variable on hourly to yearly timescales. This means that temporally averaged biospheric emissions will introduce large emission representation errors into the model-retrieval system (see Sec. 7.2.2). Some newer model-retrieval systems use terrestrial biosphere models to generate  $CO_2$  emission distributions at high time and space resolutions based on observed meteorological data such as temperature and precipitation (e.g., Peters et al. 2007). Unfortunately, there are fundamental issues with biospheric models (e.g., modeling or diagnosing phenology and adequately parameterizing respiration under different temperature and moisture regimes) that need further research and development.

Many major anthropogenic sources are also on coasts situated upwind of major marine current and ecological systems; compare WRI (2010) to Longhurst (2007). Hence, oceanic emissions are also important, but their variability is driven largely by fixation or remineralization of inorganic carbon in the upper water column (Sarmiento and Gruber 2006). Indeed, it has been shown that constraints on terrestrial carbon cycling can be narrowed through ocean interior inversions (Jacobson et al. 2007a, 2007b; Gruber et al. 2009). An added source of uncertainty for ocean emissions is that the flux (also) depends on the partial pressure of  $CO_2$  just above and below the ocean interface, plus a transfer coefficient coupling the two (Liss and Merlivat 1986, Wanninkhof 1992, Watson and Orr 2003).

Uncertainty in ocean inorganic and biospheric emissions could potentially be constrained in the GHGIS model-retrieval system through satellite observations of wind speed and ocean color, as well as ship-based experiments elucidating carbon flow (e.g., McClain et al. 1998, Boyd et al. 2000).

Multi-model intercomparison and validation studies have already been carried out for biospheric models, e.g., C<sup>4</sup>MIP and C-LAMP for terrestrial biospheric models.

## 7.2.4 Model Uncertainty Quantification

As discussed in Chapter 6 and elsewhere in this report, uncertainty quantification (UQ) methods represent an integral part of the envisioned GHGIS, given the many sources of uncertainties present in atmospheric and biospheric models. Model UQ activities include sensitivity analysis, surrogate model construction, forward uncertainty propagation, model calibration, and assessments of structural uncertainties (model discrepancies), risk, and issues with model coupling. Many of these methods are implemented in existing toolkits (e.g., DAKOTA, Adams et al. 2010) and can be applied to atmospheric models used for GHGIS.

Several approaches are available for sensitivity analysis (SA), surrogate modeling, and forward uncertainty propagation. SA methods identify and rank influential parameters in the models, and quantify those that have the most influence on output variability. This information is useful for enhanced understanding of model response and for down-selecting the important variables. Down-selection reduces the dimensionality of the input space, which facilitates subsequent UQ analysis. Of specific interest to GHGIS are global SA methods that measure parameter effects over the whole input uncertainty space (e.g., Saltelli et al. 2000, Morris 1991, Reagan et al. 2005, Lin and Karniadakis 2009).

Surrogate models (also known as response surfaces or emulators) represent the relationship between input parameters and model output quantities of interest. They are often used to approximate expensive models when large ensembles are needed (e.g., the sampling-based methods discussed in Sec. 7.1.2). Several approaches for surrogate modeling exist. They can be constructed using spline-based methods (Friedman 1991), stochastic expansion methods (Ghanem and Spanos 1991, Le Maitre and Knio 2010), and spatially correlated Gaussian process models (Sacks et al. 1989, O'Hagan et al. 1999, Rasmussen and Williams 2006, Gramacy and Lee 2008).

Forward UQ refers to propagating uncertainties in model inputs, such as initial and boundary conditions and model parameters, through the simulation model to assess the effect of those uncertainties on the model predictions. Nonintrusive, sampling-based approaches for forward UQ can be applied without major modifications to atmospheric models. Random and deterministic sampling methods are both used. Random sampling methods produce space-filling designs given a limited number of samples of the model inputs. Commonly used random sampling approaches are Monte Carlo, Latin Hypercube sampling, importance sampling, and classical experimental designs (McKay et al. 1979, Iman and Conover 1982, Morokoff and Caflisch 1995). Random sampling methods are relatively insensitive to dimensionality and do not rely on smoothness of the system response.

Deterministic sampling methods, in contrast, sample the system at predetermined locations (e.g., quadrature points) in the input space. They are commonly used in spectral projection (Ghanem and Spanos 1991, Xiu and Karniadakis 2003, Le Maitre and Knio 2010) and stochastic collocation (Nobile et al. 2008a, 2008b). By taking advantage of smoothness in the system output, deterministic sampling methods can achieve fast convergence of the functional representation with generally fewer samples than required in random sampling methods for problems with moderate dimensionality. The main drawback with deterministic sampling methods is the exponential increase in the number of samples required as the number of uncertain inputs increases. This issue may be mitigated with sparse quadrature methods (Smoljak 1963) or dimensional reduction (Rabitz and Alis 1999, Ma and Zabaras 2010, Nouy 2007, Coifman and Lafon 2006, Ganapathysubramanian and Zabaras 2008). Strong nonlinearities and discontinuities in uncertain quantities can also present a challenge to spectral projection and collocation methods, which can be addressed using domain or data decomposition (Le Maitre et al. 2007, Sargsyan et al. 2009, Sargsyan et al. 2010, Wan and Karniadakis 2005). Research and development of Model-UQ methods will likely be needed to handle uncertainties in GHG models with realistic complexities, with adaptive methods showing promise at this writing (Gramacy and Lee 2008, Bichon et al. 2008, Swiler and West 2010).

#### Model Uncertainty

Confidence in inferred GHG fluxes based on concentration measurements depends on the accuracy of the concentration measurements and the accuracy of the transport models. If the models have been calibrated against observational data, a joint density of forward model parameter values can be inferred using Bayesian statistical techniques that can account for data uncertainties/noise. The a posteriori density on parameters allows for the prediction of quantities of interest. The posterior predictive density of an observable can then be used to assess goodness of fit. The posterior predictive density can match observations well if the forward model family provides a good fit (Lynch and Western 2004).

If the family of forward models is inadequate, model-data residuals will exhibit a correlation structure on top of any uncorrelated measurement noise. This situation arises if significant model uncertainties are because of gaps in our understanding of atmospheric processes. We must account for these structural uncertainties or model discrepancies. Adding new physics to the forward models or more terms to the surrogate models may provide flexibility in fitting the data, but runs the risk of over-fitting the data and decreasing the models' predictive value, i.e., their ability to add information content. An improved approach is to consider model discrepancy as a sample path of a stochastic process, such as a mean-reverting Gaussian process. Such a model is of the form,

$$y = f(x,\theta) + \varepsilon_{\rm m} + \varepsilon_{\rm d}$$
, (7-2)

where f is the forward model,  $\varepsilon_m$  represents the model discrepancy, and  $\varepsilon_d$  represents the data noise. Model discrepancy provides a formal means to account for structural uncertainties in transport models.

The specific transport or meteorological model used in the transport simulations is critical. If a number of atmospheric models are used in an ensemble, the plausibility (given the observational data) of each transport model can be assessed to determine which is/are most suitable. Within a class of competing models, the degree to which the data provide evidence for each model in the class can be assessed in the context of Bayesian statistics. Given the data and a prior plausibility (e.g., from expert opinion), the marginal likelihood for each model provides an estimate of model plausibility and Bayes Factors (Kass and Raftery 1995, Berger and Pericchi 1996). These quantities are used for model comparison and selection (Clyde and George 2004, Beck and Yuen 2004, Muto and Beck 2008).

If a single model does not emerge as superior, predictions may be improved by averaging over multiple models. The Bayesian Model Averaging (BMA) method can be used to predict a quantity of interest by drawing from the (posterior) distribution of model plausibility (Raftery et al. 2005, Min et al. 2007). BMA has been used to combine predictions from multiple climate models, with appropriate weighting by model plausibility, to arrive at reliable predictions with quantified uncertainty (Giorgi and Mearns 2002, 2003; Tebaldi et al. 2004, 2005; Greene et al. 2006; Furrer et al. 2007; Tebaldi and Knutti 2007; Smith et al. 2009; Tebaldi and Sanso 2009). BMA is analogous to a posteriori predictive density, where the marginalization is instead over the class of competing models.

#### Model UQ and Risk Analysis

It is important to assess the risk that models may fail to accurately assess GHG emissions, or that a country has emitted more than its stated amount given the GHGIS estimates and uncertainties. Risk management is more a process than a product. The objective of risk analysis is to identify the requirements and processes to secure the confidence of assessing GHG emissions.

Probabilistic risk analysis is driven by UQ with a close interface between the two. Risk analysis will define decision criteria, utility functions, and risk-trade objectives in support of decisionmaking strategies. UQ will define the format and mechanisms for propagating uncertainties, including the identification of rational accumulation and resampling points between the coupled analyses, and a taxonomy of aleatory (random/stochastic) and epistemic (systematic, bias, and state-of-knowledge) variances and uncertainties needed to assign statistical confidence intervals to performance probability measures. Recall also discussion of these two types of uncertainties in Chapters 3 and 6.

As also discussed in Chapter 6, a key challenge with risk analysis of GHGIS products is the incorporation and propagation of uncertainties from the data definition and input phase, through numerical simulations, to final estimations of cost and performance. While UQ can help address the definition and manipulation of uncertainty through intermediate performance metrics, risk analysis can help define integral decision criteria and provide a context needed to inform decision process models. A statistical framework will need to be developed by considering both UQ and risk analysis that is both applicable to GHGIS and directly useable by the decision analysis model. This statistical framework should delineate both aleatoric and epistemic uncertainties so that confidence levels can be estimated for the probabilities of performance and cost metrics.

# 7.3 Phase 1

As elsewhere in this report, the Phase 1 GHGIS period is assumed to extend 3 years from the beginning of the GHGIS development project.

# 7.3.1 Modeling Products

The output from a GHGIS model-retrieval system would produce several types of output relevant to policy makers. Specifically, for each chemical species whose emissions are retrieved for (primarily fossil and total  $CO_2$ ), the model-retrieval system could provide

- 1. total emissions for each country,
- 2. global emission maps,
- 3. trends over time for country totals and maps,
- 4. quantities expressed "per GDP" or "per capita" (using GDP and population data from other sources), and
- 5. uncertainty quantification (including standard deviations, covariances, and variability) in each of the above.

Other GHGIS products will be of interest to Earth scientists in various disciplines, such as the distribution and variability of ecosystem parameters and atmospheric chemicals and aerosols. These data would be of value to fields as diverse as farming, forestry, climate change, air quality, and economic activity analysis and forecasting.

## 7.3.2 Phase 1 GHGIS Model-Retrieval System

As discussed in Sec. 7.2, the quality of  $CO_2$  emission estimates that can currently be derived from existing observation networks and model-retrieval capabilities for anthropogenic fluxes is very poor when compared to the requirements needed to support GHGIS (see Chapter 2).

In the course of the Phase 1 effort, the situation can be improved in several ways. First, the observation network could be improved through expanded observational coverage of <sup>14</sup>C and other chemical tracers, global satellite coverage of columns of  $CO_2$  and other GHGs, and additional meteorological observations (Chapters 3, 4, 5, and 6). Second, a model-retrieval system could be developed for GHGIS that is designed to discriminate anthropogenic from natural  $CO_2$  emissions and attribute to anthropogenic sources.

However, no model-retrieval system exists anywhere, today, with all the capabilities needed for GHGIS. But the main capabilities do exist within different models, which could be combined to construct a prototype system. Further, it is recommended that a basic-research effort be initiated to provide the atmospheric and biospheric model-retrieval capabilities needed for GHGIS, with formally documented verification and validation.

It will be important to develop a model-retrieval system based on an ensemble of models. Even with a basic ensemble, the average of the models in the ensemble generally provides a better match to reality than any single model (Potempski and Galmarini 2009, Berner et al. 2010, Delle Monache et al. 2011). The variance between model results also provides some estimate of uncertainty (Gurney et al. 2002, 2003; Berner et al. 2010). There is the danger that the same error exists in each model, but the estimate may be improved by postprocessing (Delle Monache et al. 2011).

Improvements on a basic ensemble methodology will also be possible within Phase 1. An improved ensemble framework could include weighting the impact of each model-retrieval result on final estimates according to how well each model matches observations. Implementation of the ensemble within a UQ framework (Sec. 7.2.4) would also allow greater exploration of model parameter space, with the capability to weed out model configurations with a poor match to observations as well as better quantify the real uncertainty, as also discussed in Chapter 6 in the context of data UQ.<sup>3</sup> These enhanced ensemble-UQ capabilities will be computationally more expensive but should be viable within existing supercomputing resources.

<sup>&</sup>lt;sup>3</sup> Model *calibration* may lead to improved accounting/description of the (type of) data used to support the calibration, but unless the UQ system can handle epistemic errors common to all models in the ensemble, there will be unquantified errors in retrieved emissions. This indicates the value of a larger, more varied, ensemble of models, as well as the importance of handling epistemic errors in the UQ system, as well as of an effort to improve models, as discussed above.

During the Phase 1 period and within the ensemble system, it should be possible to include several complementary global model-retrieval systems, e.g., CarbonTracker/TM5 that operationally retrieves biospheric  $CO_2$  fluxes (Peters et al. 2007), IMPACTER that has focused on fossil  $CO_2$  emissions, including stratospheric <sup>14</sup>C inputs (Cameron-Smith et al. 2009), and GEOS-Chem that has been used to retrieve biospheric  $CO_2$  using satellite observations (Nassar et al. 2011). These models rely on meteorological data input from weather models, of which there are several available to ensure diversity of the ensemble, including NCEP, GMAO, ECMWF, and the US Navy. These models would each need to be upgraded to retrieve both fossil and total  $CO_2$ , and perform retrievals with both in situ and remote observations, to the extent they do not do so already. Current grid resolution in these models is typically in the range of 100-400 km. An improved grid resolution of 50 km should be possible by the end of the Phase 1 period.

Higher resolution in regions of importance (a few km grid spacing) to better resolve atmospheric transport around regions of complex topography and large point sources can be achieved by including regional models, which are provided boundary conditions by global models (nesting) in the ensemble. Although running a model at higher resolution does not automatically imply a better simulation, it is generally found that the match to observations improves, especially in regions with complex topography (Wehner et al. 2010, 2009; Gent et al. 2009; Iorio et al. 2004; Duffy et al. 2003). The WRF regional model is one good candidate. It is used by the National Weather Service and widely used in many scientific communities. The large user and developer base means it is better tested than most models. It also means that there are several choices of parameterization for each of the important physical process, so that WRF can be configured with properties important to GHGIS, e.g., by selecting advection schemes that conserve tracer mass. It also means that an ensemble of different models can be created by mixing and matching different parameterizations (Cameron-Smith et al. 2009). WRF has been used to simultaneously assimilate both meteorological and chemical observations using the 4DVar data assimilation method (Carmichael et al. 2008, Chai et al. 2009).

Back-trajectory models would provide another addition to the ensemble for regional and local inversions that could be implemented within the Phase 1 period. Back-trajectory models are complementary to forward model-retrieval systems in many ways. In particular, when back-trajectories are available at many different times for a given observation site, they can provide the information footprint for that site. However, some effort will be required to combine forward-and back-trajectory models within a single ensemble system.

Biospheric emissions could be handled through either predetermined emissions from an observational climatology (e.g., Takahashi et al. 1997, Gloor et al 2003) or biospheric models (see Sec. 7.2.3) when they are readily available, e.g., the CASA model (Randerson 2001) in Carbon tracker (Peters et al. 2007) and biological parameterizations developed for WRF (e.g., Ahmadov et al. 2007, 2009; Nehrkorn et al. 2010).

The capabilities proposed for the Phase 1 capability already exist, even though some research and development is needed to determine the best way to integrate the results from the different types of models within the ensemble framework, in parallel with the development of the nextgeneration atmospheric (transport) models. In summary, in the course of the Phase 1 effort, a next-generation ensemble model-retrieval system could be constructed for GHGIS with multiple global, regional, and back-trajectory models combined with a UQ capability.

## 7.3.3 Accuracy of the Phase 1 GHGIS Model-Retrieval System

An important question is, "How accurate would the Phase 1 GHGIS model-retrieval system be?"

This is a challenging question because there are currently no models that come close to the GHGIS model-retrieval system proposed. However, there are some pointers that can be used to assess the possible accuracy of the GHGIS model-retrieval system that will be developed:

- 1. The Phase 1 <sup>14</sup>C observation network proposed in Chapter 5 will be broadly similar in distribution, frequency, and measurement accuracy to the CO<sub>2</sub> observation network used for the TransCom 3 study. Hence, the accuracy of the TransCom 3 model-retrieval intercomparison of  $\pm 200\%$  at the  $2\sigma$  level, discussed in Sec. 7.1.4, is a starting point for estimating the possible accuracy of our proposed GHGIS Phase 1 model-retrieval system. Needless to say, a significant improvement over that uncertainty level is required.
- 2. Existing model-retrieval systems are generally focused on biospheric emissions, which are larger but much more variable (diurnal, seasonal) than fossil-fuel emissions, so given the sensitivity of model retrievals to bias (see Sec. 7.2.1), inversions for fossil  $CO_2$  ( $CO_{2,ff}$ ) should be more accurate for the same observation network.
- 3. TransCom 3 was conducted almost 10 years ago, and improvements in atmospheric models and retrieval algorithms since then should have reduced biases, as discussed in Sec. 7.2.
- 4. Estimation improvements should result from an ensemble of models, inclusion of regional models and back-trajectory models, as well as UQ.
- 5. Presently available distributions of fossil-fuel emissions are better than for the biosphere (which have also improved since TransCom 3), reducing emission representation errors.
- 6. The incorporation of satellite  $CO_2$  observations from OCO, GOSAT, and, potentially, from improved near-surface retrievals of AIRS data (Chapter 3) will provide additional constraints in regions far from ground observation locations.
- 7. A negative is that emission regions of interest for GHGIS are, primarily, at the country level, whereas TransCom 3 partitioned continents into only a few regions. However, the large entities with the greatest emissions (China, United States, European Union, and Russia) are only a little smaller than the TransCom 3 regions. Using smaller regions can also be a positive: smaller regions require more observational information to constrain them (negative), but smaller regions reduce the emission representation bias (positive).

Overall, general improvements since TransCom 3, plus the GHGIS model-retrieval improvements proposed above, should significantly improve the accuracy of the Phase 1 model-retrieval capability. Unfortunately, the lack of a comprehensive error budget for any of the existing models, plus uncertainty in the value of each of the improvements, means that reliable estimates of the Phase 1 GHGIS cannot be given by extrapolating from what is currently known. However, an overall improvement in accuracy by a factor of 2 to 10 seems likely. At the top end

of this range, improvement by a factor of 10, while no small feat, would provide an accuracy of  $\pm 20\%$ , in accord with the GHGIS accuracy levels discussed in Chapter 2. This accuracy is also still far from the theoretical maximum accuracy that would be achieved for the TransCom 3 surface network without any bias, i.e.,  $\pm 4\%$ , as described in Sec. 7.5.1.

# 7.4 Phase 2

Again, as assumed elsewhere in this report, the Phase 2 GHGIS period would run for 10 years after the start of the GHGIS development project and, during its first 3 years, would run in parallel with the 3-year Phase 1 period.

## 7.4.1 Phase 2 GHGIS Model-Retrieval System

The Phase 1 GHGIS model-retrieval system outlined above can be expected to yield significantly better results than those from currently available capabilities. However, it will almost certainly be insufficient to meet the GHGIS requirements outlined in Chapter 2 for the quantification of national/regional anthropogenic emissions.

A number of further improvements to the model-retrieval system are possible that are aimed at a goal of  $\pm 5\%$  accuracy for the quantification of emissions from each large country during the Phase 2 development period.

Observational test beds will be important in meeting these goals and offer a number of opportunities. First, by densely instrumenting a small region, the high density of observations can provide a lot of data to assess the performance of the models used in the GHGIS ensemble, and identifying root causes of problems. This would be following in the footsteps of the DOE/CAPT project (Phillips et al. 2004) that uses observations from the DOE ARM sites (Ackerman and Stokes, 2003) to diagnose problems with subgrid-scale parameterizations in climate models, but with the automation advantages that the GHGIS UQ framework would offer. Second, overinstrumenting a region will allow OSSE experiments to determine the minimum density of observations needed for a given accuracy of emission retrievals for the test bed region, with observations not used in retrievals, used to assess the effectiveness of the UQ system to assign weights to different ensemble members. Third, a densely instrumented region would allow the impact of covariance between measurement locations to be determined, and the impact of that covariance to be quantified (see Chapter 6).

Several improvements to the Phase 1 GHGIS model-retrieval system could be achieved during the Phase 2 time frame.

1. Meteorological reanalysis data, and models themselves, generally improve over time through ongoing model development in many venues. Model resolution also usually improves over time. These improvements include the fidelity, detail, and computational performance of the models. Additional models could also be added to expand the ensemble. Not least, next-generation models that would result from a focused development program can be expected to become available during the Phase 2 period.

- 2. Implementing multiple/alternative parameterizations for each physical process in each of the individual GHGIS models will increase the depth and breadth of the GHGIS ensemble. This will provide the ensemble UQ framework a more comprehensive set of simulations with which to select the best simulations and to estimate uncertainties.
- 3. Additional retrieval methods, including variations on those described in Sec. 7.1.2, and any new methods that are developed will be implemented and tested. In particular, increasing use will be made of models and techniques that can jointly assimilate different chemical observation modalities and additional meteorological data.
- 4. A more comprehensive UQ system will be able to sample a larger set of model parameters. It should also be possible to implement a UQ capability to detect and compensate for various system biases (see Sec. 7.2.4). The characterization and propagation of uncertainties through interfaces between land, atmosphere, and ocean will also be needed to fully characterize the errors and uncertainties.
- 5. Atmospheric chemistry can be added to those individual models that currently lack it. This will allow the measurement of reactive species to expand the number of GHGs whose emissions can be retrieved, as well as provide sector information, and constrain and validate emission retrievals for  $CO_2$  (see Sec. 7.5.2).
- 6. Assimilation of observations of important physical processes such as boundary layer height (see Chapter 5) and oceanic surface pressure from satellites (see Chapter 3) will help constrain the transport and mixing within each model (e.g., Liu et al. 2009, Kang 2009).
- 7. Computational resources are expected to increase over the next decade, which will support the larger ensembles, more complex models, and higher-resolution simulations.

These improvements will enhance the GHGIS model-retrieval capability when ready, so the model-retrieval system can be expected to be continually improving throughout the Phase 2 period. All these tasks will involve some level of research and development, but the biggest challenges (and opportunities) lie in developing methods to (1) jointly assimilate observations of multiple tracers and additional meteorological data with multiple observational modalities, and (2) detect and correct GHGIS biases.

In the resource-limited development environment in which GHGIS is likely to be developed, a determination of which of these and other components/elements to emphasize over others will likely require additional work and study that fall outside the scope of the present study.

In summary, the Phase 2 capability would represent a significant leap beyond that envisaged for the Phase 1 GHGIS model-retrieval system.

## 7.4.2 Accuracy of Phase 2 GHGIS Model-Retrieval System

The benefits of the improvements proposed in Sec. 7.4.1 will all be positive and cumulative. These modeling improvements will also be coupled to improvements in the in situ and remote sensing observational networks (Chapters 3, 4, and 5), and improvements in emission distribution maps from primary inventory sources (see Appendix A) and the Phase 1 GHGIS.

The implementation of a well-distributed global surface observation network, such as  $^{14}$ C measurements at the sites of the Comprehensive Test Ban Treaty (CTBT) Radionuclide monitoring surface network, should reduce emission uncertainties by a factor of 2 over the TransCom 3 network, as described in Sec. 7.5.1. Significant extra value can be expected from satellite and aircraft observation systems specifically designed and implemented for GHGIS purposes that could be completed during the Phase 2 period, as described in Chapters 3 and 5.

Predicting the capabilities of the Phase 1 model-retrieval system requires an even greater extrapolation from present-day capabilities than for the Phase 2 system. However, given all the anticipated modeling and observational improvements beyond the Phase 1 system, an additional improvement factor of 4 to 10 seems plausible. This implies a combined improvement factor of 8 to 100. The most optimistic improvement factor of 100 would imply an accuracy of  $\pm 2\%$  in estimates of annual emissions of large countries, which would fall within the accuracy needed to meet GHGIS requirements. This is still above the  $\pm 1\%$  maximum accuracy possible with only surface <sup>14</sup>C observations at the 79 CTBT radionuclide sites (see Sec. 7.5.1), so it does not exceed that fundamental limit. Even the most pessimistic improvement factor of 8 would still be close to the accuracy needed for the first GHGIS requirement goal (Chapter 2).

Much better estimates of the Phase 2 capability will be possible once the Phase 1 GHGIS capability has been developed (both observational and model-retrieval system components), since the ensemble nature of the model-retrieval system will provide an estimate of its own accuracy that is comparable in design to the TransCom 3 study. Furthermore, the Phase 1 UQ capabilities will allow a more detailed analysis of the source of the errors in the system than is presently available. Hence, a much better prediction of the benefit of future model-retrieval improvements will be possible for the Phase 2 capability before the full roll-out of the Phase 2 observation capabilities, which will provide the opportunity to redesign, or reconsider the structure and framework of, the operational system.

# 7.4.3 OSSEs

To provide the most cost-effective system for GHGIS, a simulation of the effectiveness of prospective observation networks will be required, before assigning priorities and investing time and money in them. It also makes sense to reevaluate the observational network when new observation systems come available. For example, laser-based <sup>14</sup>C samplers may prove successful and become more cost-effective in the field than accelerator mass spectrometers, or next-generation satellites may render aircraft observations unnecessary (see Chapter 9 for more discussion). Alternatively, the space and time density of the observational system components could be increased in order to decrease reliance on the model-retrieval GHGIS components, as discussed in Chapters 3 and 6, should the modeling components continue to dominate uncertainties.

The model-retrieval systems proposed for GHGIS will be ideally suited to perform OSSEs, in which synthetic data with the characteristics of the proposed observation system are input into the model-retrieval system to predict the improvement in accuracy that can be expected from the new system. One advantage of an OSSE is that the "true" emissions are known, because they are used to generate the synthetic data for the new observation system, which makes it easy to determine the additional value of the proposed observations.

The model-retrieval system needed for a GHGIS OSSE capability is the same as that used to analyze the real observations, and only a moderate amount of additional code wrapping will be required to make an OSSE system that can quickly test a large number of potential observation candidates to identify and rank the most cost-effective observation components in a systems sense.

A related capability is network design, in which the OSSE capability could be extended to automatically find observation network configurations that satisfy multiple constraints, such as cost, effectiveness, and ease of location access. A preliminary analysis for an in situ <sup>14</sup>C flask network is discussed in Sec. 7.5.1.

# 7.5 Network Design and Multiple Tracers

# 7.5.1 Network Design

With sufficient <sup>14</sup>CO<sub>2</sub> measurements in both time and space, national-level fossil-fuel emissions can potentially be constrained using inverse-modeling techniques (NRC 2010a, Rayner et al. 2010). Very little work has been done on <sup>14</sup>CO<sub>2</sub> observation networks, but network design methods that have been used to assess biospheric CO<sub>2</sub> observing systems (e.g., Gloor et al. 2000, Patra and Maksyutov 2002, Hungershoefer et al. 2010, Lucas et al. 2010) can also be applied to <sup>14</sup>CO<sub>2</sub> measurement networks. These techniques enable quantitative assessments of different network layouts, sampling strategies, measurement modalities, and the impacts of measurement errors and biases on the retrieved surface fluxes. Furthermore, by applying objective analysis to the assessment process, various factors of network design can be optimized, including site selection, sampling frequencies, and network costs.



Figure 7-7. (a) Locations of the sites used for CTBT radionuclide monitoring (red circles) and Global-View  $CO_2$  measurement sites used in the TransCom 3 experiment (yellow circles). (b) Fossil-fuel emission basis function regions used in the <sup>14</sup>CO<sub>2</sub> inverse modeling and network assessment presented here.

Figure 7-7(a) shows two potential networks for measuring  ${}^{14}\text{CO}_2$ . The first network corresponds to the CTBT system used to monitor radionuclide levels in the atmosphere (79 sites, Medici 2001). The second network shows the sites from the Global View CO<sub>2</sub> network (GVTC3) used in the TransCom 3 study (56 unique sites, Gurney et al. 2003). Assessments of the effectiveness of monitoring fossil-fuel emissions with each of these networks was conducted by simulating fossil-fuel tracers using the EDGAR emissions inventory (Olivier et al. 2005) partitioned into the area regions shown in Fig. 7-7(b). The simulated tracers were sampled at the CTBT and GVTC3 sites and noise was added to create synthetic observations. An inversion method (MacKay 1999,

Bishop 2006) was applied to the forward simulations and synthetic observations, providing posterior distributions of fossil-fuel fluxes for the specified regions.

Figure 7-8(a) depicts errors in retrieved fossil-fuel emissions using the CTBT and GVTC3 networks, for different levels of observational noise (1, 5, and 10 ppm) and different sampling frequencies. As expected, retrieval errors for both networks are greater with less-frequent sampling, with the largest increase occurring from sampling once per day to once every other week. The retrieval error also increases with observational noise. For reference, Rayner et al. (2010) applied 1 ppm measurement noise (following Turnbull et al. 2009) in their <sup>14</sup>CO<sub>2</sub> network study. The assessment in this study indicates that CTBT reduces the error in the retrieved fossil fuel emissions by about a factor of 2 compared to GVTC3. Indeed, CTBT with monthly <sup>14</sup>CO<sub>2</sub> samples performs similarly to GVTC3 with daily samples. The CTBT network has slightly more sites, but site location is the major factor for the performance difference. Unlike GVTC3, the CTBT network has multiple sites adjacent to large emitting regions. This feature is expected to persist if transport model errors are included in the network assessment. These results are consistent with Rayner et al. (2010) and the OSSE in NRC (2010a) that assumed 84 sites around the USA, each collecting ten samples per month, and calculated that fossil CO<sub>2</sub> emissions could be retrieved for state-sized regions to within 10%. However, it is critical to note that these results were obtained with unbiased models (perfect models), which is significant since biases are the main cause for errors in model-retrieval emission estimates, as discussed in Sec. 7.2.1.

CTBT clearly outperforms GVTC3 in the presence of random measurement errors. However, Fig. 7-8(b) shows that the situation is altered by introducing a measurement sampling bias, whereby local noon observations are compared to daily average model values. This sampling bias greatly impacts the CTBT inversions because it has many continental sites affected by large daily fluctuations in the depth of the PBL. The results of this bias experiment underscore the need to properly account for the spatial and temporal representations of prior fluxes and observations in fossil-fuel inversion studies.



Figure 7-8. (a) CTBT and GVTC3 fossil-fuel emissions retrieval error as a function of sampling frequency and observational noise. Retrieval error is the sum of the standard deviations of the posterior fluxes weighted by the magnitudes of the prior fluxes. (b) The impact of a temporal measurement sampling bias on the CTBT and GVTC3 retrieval errors. The error bars show 1-sigma deviations using different random seeds for the observational noise.

Optimization methods can also be applied to network design. Figure 7-9 depicts the fossil-fuel retrieval error for different location configurations of a 40-site  ${}^{14}CO_2$  observing network. A global, stochastic optimization method is used to search for location configurations, and the algorithm begins to converge after about 1000 iterations. This demonstration shows that a 40-site observing network can achieve retrieval errors comparable to the 79-site CTBT network by optimal positioning of the measuring sites. Such optimization methods can be extended to simultaneously minimize other network objectives, such as sampling frequency and sensor density, which will be critical in the design of future GHG observing systems.

# 7.5.2 Use of <sup>14</sup>CO<sub>2</sub> and Other Chemicals to Discriminate Fossil Emissions from Biospheric Emissions

Measurements of the carbon-14 isotope of  $CO_2$  can help discriminate between  $CO_2$  from fossil emissions (fossil-fuel combustion plus cement manufacture) and other  $CO_2$  sources; fossil emissions are depleted of <sup>14</sup>C because of radioactive decay (e.g., Turnbull et al. 2009, Graven et al. 2009). See Chapter 5. A model-retrieval system that incorporates measurements and transport modeling of <sup>14</sup>CO<sub>2</sub> can be used to help quantify and attribute fossil-fuel emissions consistent with the difference between pairs of <sup>12</sup>CO<sub>2</sub> and <sup>14</sup>CO<sub>2</sub> measurements, while simultaneously retrieving total CO<sub>2</sub> emissions.<sup>4</sup> Such a model-retrieval system would use fossil emission inventories as priors. A variety of fossil-fuel inventories, both sector-based and high-resolution gridded products, are available as input sources, e.g., EDGAR emissions (Olivier et al. 2005), VULCAN emissions (Gurney et al. 2009), and other products (Rayner et al. 2010). See also Appendix A: Inventories.



Figure 7-9. Demonstration of optimization methods applied to the problem of selecting measurement locations for a 40-site <sup>14</sup>CO<sub>2</sub> observing network. The algorithm converges after about 1000 iterations. The retrieval errors of the larger CTBT and GVTC3 networks are also shown.

In addition to  ${}^{14}CO_2$ , other species are emitted in association with fossil-fuel combustion, e.g., CO, NO<sub>x</sub>, black carbon; with biospheric activities (biogenic hydrocarbons), and certain economic

<sup>&</sup>lt;sup>4</sup> Recalling the caveats regarding <sup>14</sup>C discussed in Chapter 5, <sup>14</sup>C-depleted carbon is also emitted by volcanoes and/or other nonanthropogenic deep/old carbon-emission sources. Carbon isotopes are also generated in nuclear reactors, whose emissions can complicate interpretation of the <sup>12</sup>C:<sup>14</sup>C signal and fossil-fuel combustion attribution.

sector activities, e.g., hydrofluorocarbons (HFCs) and chlorofluorocarbons (CFCs) for refrigerants; methane (CH<sub>4</sub>) from natural-gas distribution leakage; sulfur and heavy metals from coal burning, and SF<sub>6</sub> from electricity distribution. Measurements of these species could be used in a model-retrieval system to corroborate and constrain  $CO_2$  emissions from different sources.

These other species offer several advantages and disadvantages for GHGIS that are complementary to  ${}^{14}\text{CO}_2$ : they are generally easier to measure (see Chapters 3, 4, and 5); are often already measured for air-quality purposes; can discriminate between different sources; and many of the chemicals are reactive and therefore relatively short-lived (which will allow GHGIS to distinguish between close and distant sources). Disadvantages include the need to know emission factors (ratio of chemical to CO<sub>2</sub> produced by combustion processes) to constrain CO<sub>2</sub> emissions.

Measuring these gas species offers other major advantages: (1) the transport of these gases in the atmosphere is correlated (because they are all convected by the wind field) and, as a consequence, can help constrain certain model-transport errors, (2) some of these species are GHGs in their own right (e.g., CH<sub>4</sub>, nitrous oxide (N<sub>2</sub>O), ozone (O<sub>3</sub>), CFCs, HFCs, SF<sub>6</sub>), and (3) some of these gases are of interest to other science fields, such as air-quality and as markers of interactions with and within the biosphere.

Measurements of CO along with  $CO_2$  have already been used to revise anthropogenic  $CO_2$  emissions derived from bottom-up estimations, including attributing emissions to different countries (China, South Korea, Japan, and Malayan forest fires) based on their different CO:  $CO_2$  emission factors, and airborne flask measurements from the NASA/TRACE-P campaign (Suntharalingam et al. 2004, Palmer et al. 2006). CO inversions using measurements from the NOAA/ESRL *in situ* sensor network have also been performed (Kasibhatla et al. 2002, Petron et al. 2002). Such inversions have also been conducted using satellite data (Kopacz et al. 2010).

A particularly useful tracer for identifying model errors is  $SF_6$ , which is very long-lived (basically, chemically inert in the atmosphere) and a purely anthropogenic gas (used as an insulator in high-voltage electrical equipment).  $SF_6$  can be measured with great precision at high frequency and, as a result, has been used as a surrogate for anthropogenic  $CO_2$  (e.g., Levin et al. 2005, Rivier et al. 2006, Turnbull et al. 2006). However, these studies have had mixed results because  $SF_6$  and anthropogenic  $CO_2$  have different emissions patterns. Nonetheless,  $SF_6$  will still be valuable for constraining atmospheric transport (e.g., Lac et al. 2006).

Multiple tracers may be assimilated into the model-retrieval system by folding them into a single cost function (e.g., Pison et al. 2009), or by formulating a vector of separate cost functions for each objective of interest (e.g.,  $CO_2$ ,  ${}^{14}CO_2$ , and  $SF_6$ ) and minimizing different combinations of the vector components. The latter can explore trade-offs by differential weighting of the vector components (i.e., individual tracers). To infer fossil-fuel emissions, for example, it may be better to emphasize model-data mismatches for a non-fossil-fuel-based tracer with fairly well known emissions over  $CO_2$  or  ${}^{14}CO_2$  mismatches.

# 7.6 Benefits to Other Science Fields

The observations, capabilities, and results generated by GHGIS will also be of great value to scientists and policy makers in other fields. It is beyond the scope of this report to try and list all the ways that GHGIS will benefit other fields. However, obvious examples include:

- air pollution, especially long-range transport and source identification;
- carbon-cycle modeling; and
- atmospheric model improvements and validation, which can lead to improved climate predictions and weather forecasts.

# Chapter 8. GHGIS Mission Operations Center (GMOC)

# **Chapter Summary**

The goal of the proposed Greenhouse Gas Information System (GHGIS) Mission Operations Center (GMOC) is to support an operational capability to integrate the myriad data, information, and technical analyses necessary to systematically, reliably, and continuously assess actions taken by countries related to greenhouse gas (GHG) treaty commitments. The spectrum of GHGIS operational responsibilities may include assessing treaty commitment fulfillment; assessing the effects of these actions on anthropogenic GHG emissions; identifying GHG climatic effect mitigation strategies of actions that might exceed treaty obligations; and monitoring economic-sector activities, especially as they relate to energy production. This capability will support a variety of stakeholders, including policy makers and analysts, technical and economic analysts, scientists, and other users.

# Findings

- 1. Today's data centers related to carbon, carbon cycle, GHG emissions, and related monitoring were designed to support scientific research goals rather than the operational GHGIS mission responsibility to perform data access and analysis, with continuous operational acquisition, processing, analysis, reporting, and dissemination of GHG monitoring information.
- 2. Potential customers of the GMOC products will be US policy analysts, policy makers, and administrators for GHG treaty negotiation and monitoring, program managers responsible for future investments in research/development/technology, many government officials, and, not least, scientists and researchers. These customers will require reliable, objective, and traceable reporting of data products and analyses.
- 3. The proposed GMOC will integrate and analyze a variety of data streams and information to provide system analysis summaries and reporting of emissions and the effects of mitigation actions taken, along with country- and perhaps subcountry-level trends of anthropogenic GHG emissions.
- 4. Sensing assets in place today, as well as established data centers already collecting and integrating data, will allow deployment of an initial GMOC prototype capability within the Phase 1 period of a GHGIS development project, i.e., within 3 years following Authority to Proceed (ATP). The GMOC will evolve during the Phase 2 period and over subsequent years, as additional GHG measurement, modeling, and analysis capabilities are developed and mature to operational status, following a phased and modular development methodology. This modular approach will allow GMOC and GHGIS enhancements to meet customer needs and evolving technologies, while maintaining necessary uptime and capabilities.
- 5. An initial GMOC system architecture, based on available technology, has been proposed to serve critical roles within GHGIS: (1) data acquisition and storage, (2) processing and analysis, and (3) reporting and dissemination of knowledge to support decisions. Key system qualities include scalability to accommodate increasing data volumes, reliability

to support operational requirements, flexibility to incorporate new and different future data streams, and traceability to support audits of reported results.

## **Recommendations (Phase 1 GHGIS Development)**

- 1. The proposed prototype GMOC will leverage established capabilities and methodologies already in place at existing data centers and other information sources. Several analogous operational monitoring systems such as the Comprehensive Nuclear-Test-Ban Treaty Organization (CTBTO) International Data Centre (IDC), the United States National Data Center (USNDC), the National Earthquake Information Center (NEIC), provide templates, development strategies, technologies, architectures, and lessons learned that could be used by the GMOC.
- 2. Although existing climate and GHG-related data centers, such as the Atmospheric Radiation Measurement (ARM) program and the Department of Energy (DOE) Carbon Dioxide Information and Analysis Center (CDIAC), do not have an operational monitoring mission focused on policy analyst users, the data and analytical capabilities at these and other centers provide a foundation for GHG monitoring efforts. The GMOC will utilize such existing technologies when feasible.
- 3. Because of the time necessary to develop and establish an operational, trustworthy, and reliable data-collection and -processing system, design and development should begin immediately, as soon as ATP is granted, to establish baseline levels of anthropogenic emissions as soon as possible.

# **Recommendations (Phase 2 GHGIS Development)**

- 1. The GMOC will be designed, developed, and deployed following a phased and iterative approach, as recommended by the recent Federal CIO Implementation Plan (Chandra 2010). Also referred to as "spiral development," this approach will create initial operational capabilities as quickly as possible and expedite incremental updates to system capabilities.
- 2. As the GHGIS evolves, the GMOC will identify gaps in existing data collections, which can be addressed with new sensor development, placement, and interfaces to the GMOC. Over time, the GMOC will perform sensor and model down-selection as priorities evolve to create a system tailored to the functions and specifications required to operate GHGIS.

If existing monitoring systems are to serve as a guide (e.g., the CTBTO IDC), enhancements beyond the end of the Phase 2 period (10-year time frame following ATP) would likely be indicated to address evolving needs and advances in science, technology, and sensing capabilities, and not least, the need to monitor and quantify anthropogenic emissions that, if emissions treaties are successful, will represent a decreasing fraction of natural/biogenic carbon fluxes.

# 8.1 Introduction

## 8.1.1 GHGIS Mission Operations Center (GMOC)

The GMOC is the GHGIS component responsible for integrating data streams and utilizing advanced processing and analysis capabilities to provide required information to end users. The GMOC will provide an integrated and operational capability for stakeholders including policy analysts, technical analysts, and other users to systematically, reliably, and continuously assess the state of GHG emissions at country and subcountry levels and (economic) sector levels. The GMOC will support:

- Continuous acquisition and integration of observables and other relevant data;
- Processing and analysis of incoming data using operationally validated algorithms and models;
- Situational analysis and characterization of trends in GHG emissions, including modeling, uncertainty analysis, and uncertainty quantification; and
- Reporting of these results periodically and regularly to key stakeholders.

Reporting from the GMOC will provide stakeholders with awareness and understanding of the degree to which different countries adhere to their commitments to reduce GHG emissions and undertake emissions mitigation actions. Establishing reliable baselines as part of an operational GMOC is necessary to assess trends in GHG emissions and the effectiveness of mitigation strategies. This baseline will also aid policy analysts with negotiations involving potential future climate treaties.

# 8.1.2 Overview of Current State of GHG Data Collection, Integration, and Analysis

Systems exist today that support the collection and integration of a variety of different GHG, climate, meteorological, and other observable data and metadata, as well as in support of model inputs and results. Many of these systems produce high-quality and high-fidelity data, and have some form of data integration and archive capability. However, many of the sensors and systems focus on science explorations and research applications and were not designed to support GHG operations in a manner useful for enabling regular, long-term GHG policy-level decisions. Additionally, most of the existing sensor and analysis systems were not designed for operational use, such as for treaty monitoring or similar purposes.

These systems are funded, operated, and used for a variety of purposes and by a variety of organizations. As a consequence, there is insufficient uniformity in the level of rigor applied to the calibration and validation of the measurements, and results can vary greatly from sensor system to sensor system or even through time at any given site, as research questions evolve. Measurement disparities and differing localized or intermittent sampling methods create issues for operational systems that require data quality (quality assurance: QA) and data control (quality control: QC) standards to maintain operational capability and provide many years of continuous and sustained monitoring. On the other hand, some of these issues have been addressed and

resolved within existing data center designs. These solutions, when applicable, will be utilized during the development and deployment of the GMOC.

The large-scale and evolving nature of GHGIS will require a GMOC that is designed, developed, and deployed through an iterative and phased process. An initial prototype capability will be developed early in the process while working toward a flexible and adaptable, fully operational system. Such an approach will allow the early establishment of a trusted baseline of key observables, archiving and retrieval of key data and parameters for later reanalysis, continuing enhancements to analytical functionality over time as such capabilities are developed and become available, and a flexible and extensible architecture allowing the system to meet key and evolving requirements over time. Existing national data center capabilities that provide GHG and other relevant information will be considered and incorporated into the GMOC architecture, design, and deployment. Lessons learned, architectural constructs, and system development processes associated with similar operational monitoring systems will also be used.

The remaining sections of this chapter describe the GMOC in further detail. An analysis of user needs and requirements for the GMOC is presented in Sec. 8.2, followed by a summary of relevant existing data centers that could be potentially leveraged for a GMOC in Sec. 8.3. Sec. 8.4 presents the envisioned concept of operations (CONOPS) for the GMOC, while Sec. 8.5 describes a conceptual architecture to fulfill the expected user needs. Finally, Sec. 8.6 describes a general program plan for designing and building the GMOC using a phased, iterative approach.

# 8.2 GMOC User Needs and Requirements Analysis

## 8.2.1 User Needs

The GMOC will serve and interface to a variety of stakeholders. Potential customers of the GMOC include US policy analysts and administrators for GHG treaty negotiation and monitoring; program managers responsible for future investments in research, development, and technology; and other government officials. These customers will require periodic, objective, and comprehensive reporting of key parameters and analyses. Specifically, the GMOC should provide system analysis summaries, continuing updates to system capabilities and data collection, and, most importantly, country- and subcountry-level reporting, as well as sector-level summaries and trends in anthropogenic GHG emissions and mitigation actions.

The proposed GMOC capabilities in support of the controlled acquisition, integration, and organization of relevant GHG observables over time will naturally allow it to provide important data sets and analyses to research and science communities, and potentially to the general population at large. While the research and science community is a secondary, but very important, potential customer of the GMOC, the GMOC will augment and support, but not replace activities and capabilities presently in place in the research and science communities, integrating, reconciling, and archiving results of these activities beyond today's capabilities.

## 8.2.2 GMOC System Requirements

To provide continuous, long-term support to its stakeholders, the GMOC will need to develop key system qualities and capabilities. These are itemized below and depicted in Fig. 8-1.

**Reliability:** The system must provide trusted information when needed by policy analysts and other stakeholders. For information to be trusted, the integrity of that information must be preserved via data security mechanisms that prevent tampering with or accidental corruption of that information.

**Flexibility:** Policy and science needs will change over time, as technology evolves and new agreements are brought into consideration; therefore, the GMOC must be able to incorporate new inputs, models, and algorithms to meet these new needs and provide updated reports as needed.

**Traceability:** The ability to reanalyze and reprocess historical data and conclusions will be critical. Additionally, the results and products generated by the system must be able to withstand audits at the highest levels of scientific scrutiny.

**Scalability:** The number and variety of sensors will increase to support the need for characterizing emissions by country, sector, and possibly by region. Therefore, the GMOC will have to be able to scale its interfaces, acquisition and storage of increasing volumes of data, and analytical capabilities.



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Figure 8-1. Key GMOC system qualities and capabilities.

## 8.2.3 GMOC Subsystem Requirements

To provide an operational analysis of the GMOC user needs and requirements, the proposed system has been divided into the following functional subsystems: (1) data acquisition and storage, (2) processing and analysis, and (3) reporting and dissemination. For each of these, key roles and responsibilities are highlighted below.

#### Data Acquisition and Storage

**Role:** The GMOC will be the primary collection and integration point of GHG observables within GHGIS for support of GHG monitoring at the required spatial, temporal, and sectoral scales. This role includes aggregating and archiving key data and metadata; enabling access to data and metadata at other trusted repositories; and managing the provenance for all acquired data and metadata, as described in Chapters 3 through 5, and processing tools within the GMOC, in coordination with the data fusion and reconciliation and UQ activities described in Chapter 6 and the modeling and modeling UQ activities described in Chapter 7.

**Responsibilities:** The GMOC will provide continuous and ongoing acquisition and storage of GHG and related data for US monitoring purposes, including the long-term archiving of all relevant data. The GMOC will ensure and support data QA, including authentication, validation, and metadata support of those data that are already archived, or will be archived elsewhere; examples of the latter are discussed below.

Benefiting from experience of large data centers and data-distribution centers, the decision will need to be made whether to mirror all data on which the GMOC will rely for its reports, or access them remotely. Three considerations will be taken into account in making this decision.

- 1. Experience in high-performance computing operations, especially data-intensive operations and applications, indicates that resources required to move large volumes of data through networks can easily exceed those required for the computational analysis performed based on that data. The computation is typically best performed at the site where the data reside, moving the data needed from its large, archival-storage media, to faster-access (cached) storage in support of the high-end computations needed. While it is yet to be determined what hardware resources are needed to support GMOC's operational mission, the data needed by computationally intensive algorithms should be collocated with the machine(s) executing those algorithms.
- 2. Support of the GHGIS and GMOC operational requirements may dictate a decreased reliance on data centers that were designed and established to meet scientific research needs.
- 3. While, at least initially, the volume of GHGIS-relevant data that will reside at other sites will easily exceed what will be required to be stored in the GMOC to support GHGIS needs, that balance will almost certainly shift with time, so the GMOC will need to be scalable, as discussed elsewhere, to accommodate a high-volume and diverse data set.

#### Processing and Analysis

**Role:** The GMOC will provide data-processing and -analysis capabilities to US policy makers and analysts on GHG observables, including traceable workflow provenance history of all output

products. The GMOC will provide a trusted and objective situational analysis capability to calculate anthropogenic emissions in support of US policy development and implementation. This analysis will assess changes in emissions over time to evaluate the degree to which a country is adhering to its commitments.

**Responsibilities:** The GMOC will operate a systematic process for the implementation and execution of operational analytical algorithms for increasingly refined analysis of key data sets. The GMOC will be capable of analyzing observable data to provide ongoing status of spatial, temporal, and sectoral representations of GHG emissions and the results of mitigation actions. Specifically, the GMOC will provide:

- Analytical capabilities to conduct inverse modeling to support country-level attribution of GHG emissions, as described in Chapter 7.
- Analytical and modeling capabilities to discriminate anthropogenic emissions from those from natural sources.
- Systematic and traceable offline analysis of country-level, high-fidelity, high-resolution assessment of GHG emissions and emission changes.
- Uncertainty quantification and sensitivity analysis capabilities to identify key input data uncertainties and provide guidance to support systematic reduction of uncertainty for both data and modeling results.

#### Reporting and Dissemination

**Role:** The GMOC will provide periodic reporting of emissions to its key customers and stakeholders at regular intervals, as defined by customers and their needs. In addition, the GMOC will have the capability to support and respond to ad hoc, out-of-sequence, requests for data and analyses to support evolving policy and application needs.

**Responsibilities:** The GMOC will synthesize and document information necessary to support policy analysts' situational assessments of GHG emissions and emissions mitigation actions. These assessments will incorporate relevant data into a product that characterizes the state of country-level emissions and mitigation-action commitments at a specified temporal resolution. The GMOC will provide an interface to facilitate efficient reporting and dissemination of this information. Additionally, the GMOC may provide an interface to the science and research community to disseminate data sets at various levels of processing and analyses (both automated and on-request) to authorized users.

# 8.2.4 Summary of Existing Gaps in Operational GHG Monitoring

From an information systems perspective, there are a number of gaps that exist in current GHG monitoring efforts. The GMOC will be designed to fill such gaps. Specifically:

• Existing systems were not designed to collate, reconcile, and synthesize information necessary to support policy analysts; existing GHG data systems were designed for science and research.

- Existing data centers were not designed to support an operational mission responsibility for performing data integration and evaluation, with continuous operational acquisition, processing, analysis, reporting, and dissemination of GHG monitoring information. In addition, existing data centers may not have incorporated rigorous data security procedures needed by an operational monitoring center.
- Today's processing systems cannot meet the requirements for implementation, execution, and integration of automated and operational (validated and verified) analytical algorithms to provide continuous GHG monitoring and assessments.
- Today's enterprise architecture cannot facilitate systematic and traceable analysis of country-/subcountry-/sector-level, high-fidelity, high-resolution assessments of GHG emissions and emission changes.
- Operational-level baselines are not available today to establish country-/sector-level monitoring goals and inform policy analysts.

# 8.3 Summary of Existing Data Centers

# 8.3.1 Existing Collection and Integration Centers for GHG Data

The GMOC will be developed to provide comprehensive and reliable services to stakeholders at no later than the time specified by GHGIS users. For this to happen, well-characterized capabilities and methodologies in place at existing data centers will be leveraged for immediate use. Although these existing data centers do not have an operational monitoring mission, as noted above, the data and analytical capabilities at these centers provide a solid foundation that could be leveraged for GHG monitoring efforts. The GMOC will use existing technologies, protocols, and formats, when feasible and appropriate. This does not preclude proprietary GHGIS sensor networks from interfacing with and providing data to the GMOC in the future. On the contrary, as GHGIS evolves, gaps noted in sensing and data collections can be addressed with new sensor development, placement, and interfaces to the GMOC.

The following is a partial listing of relevant data centers funded by US government agencies that can possibly be leveraged by the GMOC. Many of these provide access to global data and, in some cases, to international data providers.

• Department of Energy (DOE) Carbon Dioxide Information Analysis Center (CDIAC) – CDIAC is the primary DOE data center for GHG-related information. It produces nation-level and gridded fossil-fuel emissions estimates by integrating inventory and economic data from a wide range of sources, particularly in collaboration with the United Nations. CDIAC also assembles data from Ameriflux network flux towers and uses that to create standardized format and gap-filled flux data products, working in collaboration with flux tower networks in other countries. CDIAC has also assembled the world's most comprehensive data system for ocean carbonate chemistry, assimilated from a broad range of US and other nation sources, that are used for physical fate and transport modeling of carbon dioxide (CO<sub>2</sub>) absorption in the ocean.
- **DOE** Atmospheric Radiation Measurement (ARM) Program The DOE ARM program, including the ARM Archive, is part of the ARM Climate Research Facility (ACRF), and makes measurements on cloud formation, cloud dynamics, and interactions between solar radiation and the atmosphere. The ARM program includes an operational data processing and data management facility with three fixed measurement locations around the world, two mobile measurement facilities, current data holdings over 200 terabytes (TB), and a current data ingest rate of multiple TB/month (due to new equipment funded by the American Reinvestment and Recovery Act). The ARM program produces standardized data products and supports a variety of *ad hoc* data queries and data manipulations, although on a narrower range of science and data sources than GMOC will support.
- DOE Earth System Grid (ESG) ESG is a software toolset in use by an internationally distributed network of data centers. It provides climate researchers with access to data, information, models, and analysis tools required to digest and help interpret huge climate simulation datasets. It is particularly targeted at managing and distributing the petabytes of climate simulation results used by the Intergovernmental Panel on Climate Change (IPCC) assessment reports. ESG development is led by the Earth System Grid Center for Enabling Technologies (ESG-CET) and is an example of the kind of data and system interoperability that can be achieved by consistent application of metadata, data, and protocol standards. The Climate Data Analysis Tools (CDATs) and Ultrascale Visualization Climate Data Analysis Tools (UV-CDATs) under development by ESG collaborators are examples of the type of provenance-aware, scalable visualization and analysis tools that will be used by the GMOC. Internally funded research and development efforts at the Jet Propulsion Laboratory, at present, are collaborating with this data network framework to provide access to and make spaceborne sensor data available through it.
- National Aeronautics and Space Administration (NASA) Earth Observing System Data and Information System (EOSDIS) – EOSDIS processes and distributes data from NASA Earth-observing satellites, airborne platforms, ground- and sea-based sensors, and field campaigns. EOSDIS also integrates data from other space agencies, such as the European Space Agency (ESA) and the Japan Aerospace Exploration Agency (JAXA), and data from other disciplines and activities, such as socioeconomic data, where those data are needed for the NASA Earth science research mission. The extremely broad range of EOSDIS data products are primarily distributed through a set of 12 discipline-focused data centers, sometimes referred to as the Distributed Active Archive Centers (DAACs), at various NASA and other centers. One of those is hosted at Oak Ridge National Laboratory.
- National Oceanic and Atmospheric Administration (NOAA) Earth System Research Laboratory (ESRL) – ESRL hosts a range of climate and GHG data as well as several analytical and reporting capabilities such as CarbonTracker, which combines available CO<sub>2</sub> measurements with atmospheric-transport modeling to estimate and assess carbon (CO<sub>2</sub>) sources and sinks. ESRL also includes the Global Monitoring Division, which hosts data from the existing tall towers and flask measurement projects.

- NOAA National Environmental Satellite, Data, and Information Service (NESDIS) The NESDIS provides timely access to global environmental data from satellites and other sources as well as information services including Earth-system monitoring, official assessments of the environment, and related research results. The National Climatic Data Center (NCDC) and National Oceanographic Data Center (NODC) are parts of NESDIS. NCDC produces numerous climate publications, responds to data requests from all over the world, operates the World Data Center for Meteorology, and supports a three-tier national climate services support program including the following partners: NCDC, regional and sectoral climate centers, and state climatologists. NODC provides scientific and public stewardship for national and international marine environmental and ecosystem data and information, including ocean-wind measurements.
- *Mercury metadata toolset* Existing data centers often use different standards for metadata, depending on their history and the practices of their particular communities. Mercury is a toolset for creating a virtual internet repository of metadata, creating a consistent and easy-to-use search infrastructure across multiple metadata standards. Where the metadata specifies data access methods using common standards (such as OPeNDAP and OGC web services), Mercury can provide both user interface and programmatic direct access to that data.
- **The AirNow website** AirNow is a collaboration involving the Environmental Protection Agency, NOAA, National Park Service, tribal, state, and local agencies, and an example of rapid assimilation of measurements made by a variety of different organizations to provide hourly input to a variety of stakeholders, including data needed for decision support. While GHGIS does not need to provide feedback on the same time intensity as AirNow, this system, as well as the data assimilation and modeling associated with weather prediction, are examples of existing tools and patterns that will be considered in more detailed GMOC design work.
- *National Ecological Observing Network (NEON)* NEON is at the early stages of implementation. However, considerable design work has gone into the selection of sites and relevant protocols, standards, formats, and interfaces necessary for NEON's information system. Data from NEON are and will be relevant to GHGIS, and lessons learned from the information systems design will be considered in GMOC development.

### 8.3.2 Analogous Operational Monitoring Systems

While existing GHG data centers can provide the GMOC with the data, processing, and analysis tools necessary to support GHGIS, concepts from existing non-GHG operational monitoring systems with similar missions and globally distributed sensor networks can also be leveraged when designing and developing the GMOC. Operational monitoring centers have missions that include continuous monitoring of the sensor network and the system, continuous data acquisition and processing, data analysis using operationally validated algorithms, and dissemination of information that can inform and support decisions by the US government executive branch and policy community, as well as provide support for further technical analysis. The following is a listing of relevant existing monitoring systems with operational missions that provide system concepts that could be leveraged when designing the GMOC.

- Comprehensive Nuclear-Test-Ban Treaty Organization (CTBTO) International Data • Centre (IDC) and International Monitoring System (IMS) – The CTBTO has developed a sensor network and processing and analysis framework for international ground-based nuclear-explosion treaty-monitoring (Sullivan 1998). The IMS is a globally distributed, heterogeneous sensor network of seismic, hydroacoustic, infrasound, and radionuclide sensors. The IDC's goal is to provide member states' information needed to establish whether an event has taken place that could have been a nuclear explosion. The operational mission of the combined IDC and IMS is similar in nature to GHGIS, although the reporting timelines are quite different. The IMS sensor network comprises a suite of 321 monitoring stations and 16 radionuclide laboratories. Data are continuously acquired from these sensors and the state of the sensor network as a whole is continuously monitored to assure the system is operating as required. The IDC must process and exploit data, both as it arrives and during offline analysis; disseminated reports provide derived data product information to the appropriate communities to inform further decision making.
- United States National Data Center (USNDC) The USNDC is the US-only counterpart to the IDC. The function of the USNDC is similar to the IDC. However, the customer for USNDC-derived products is the US executive and policy communities as opposed to international member states. This perhaps provides a useful analogy for the GMOC to consider because of its requirement to report to the US executive and policy communities, in addition to the reasons listed for the IDC.
- US Geological Survey National Earthquake Information Center (NEIC) The NEIC is a US system for processing real-time data from over 1,300 globally distributed seismic stations (NEIC 2010). This system has a 24/7 operational mission and must quickly disseminate the location and magnitude of all potentially destructive earthquakes detected worldwide.
- United States Nuclear Detonation Detection System (USNDS) USNDS is a satellitebased (optical) nuclear-explosion treaty monitoring system, augmented with data from ground stations. It requires continuous data acquisition and analysis and the generation of reports from that data. The system, both space and ground segments, was developed iteratively with increasingly expanding capabilities, over a period of several decades.

An examination and assessment of these operational systems reveals concepts that these operational systems have in common that are applicable to the design of the GMOC. In the context of the GMOC, an operational system possesses the following qualities: high reliability, traceability, thoroughly validated and verified algorithms/models/tools, increasingly refined levels of processing and analysis including capabilities for higher-complexity situations, secure system guaranteeing data and product integrity, historical tracking to support reprocessing and reanalysis, and reliable and robust operation. These qualities apply to all analogous systems.

Each of these systems also monitors their state of health (SOH) and the SOH of related systems and sensor networks to enable quick resolution of issues with data sources and to be aware of concerns that may affect data quality. Data are continuously added to these systems. These systems have dedicated staff that work to ensure the system is available and continues to produce their required products over time. A quality of these systems that enables them to meet their operational requirements goals is a strict focus on the needs of their stated customer. This requires working with the operational customer to develop several key system documents such as an operational requirements document, a system specification, and high-level use cases. Requirements can then be derived from these documents. An iterative development process can be used that involves regular deliveries to solicit customer feedback followed by continued development and incorporation of that feedback. By tailoring the system to customer needs regarding data and products, these systems produce predictable, dependable, high-quality, customer-driven outputs. These systems also have program plans devoted to ensuring that their customers' needs are met by providing support and incorporating feedback regarding needed enhancements and improvements to the system over time (as sensors and situations evolve). To the extent possible, the GMOC design and development efforts will incorporate lessons learned as well as successful concepts from these analogous operational systems. Sec. 8.6 will describe a general program plan for the development of the GMOC.

## 8.4 GMOC Concept of Operations

As introduced in Sec. 8.2, the GMOC serves several critical roles in GHGIS. The roles can be broken into three subsystems: data acquisition and storage; processing and analysis; and reporting and dissemination of knowledge to support decisions. Each subsystem's key responsibilities are listed below.

### 8.4.1 Operational Functions

#### Data Acquisition and Storage Operations

- Collect observables from sensors and other data sources. Where those data exist at trusted US repositories, GMOC will need to decide whether to enable remote access to those data, or maintain a duplicate copy.
- Authenticate and validate the data to assess and ensure the quality of the data.
- Store and archive the data, including metadata and origination provenance information.

### **Processing and Analysis Operations**

- Automatically analyze the data; this includes fusion, reconciliation, exploitation, and uncertainty analysis, as discussed in other parts of this report.
- Conduct offline analyses to provide situational characterization at needed levels of temporal and spatial resolution, and model fidelity.
- Provide interpretations of analyses to summarize the current GHGIS system state and compare to previous system states.

GMOC

### Reporting and Dissemination of Knowledge to Support Decisions

- At a specified frequency (i.e., monthly, quarterly, annually), provide formal reporting of information to the US executive and policy stakeholders, including GHGIS-system status, data-collection status, and emissions analyses.
- Provide an automated interface to serve data to external users as needed.
- Field and support requests for analysis and reports.
- Report anomalies of interest to key stakeholders.
- On a case-by-case basis, support data requests from external users.

The envisioned GMOC data flow and interactions between subsystems are depicted in Fig. 8-2.



Figure 8-2. Operational functions of a GMOC resulting in reports that transform data into useful information and knowledge.

## 8.4.2 Data Acquisition and Storage

The GMOC data acquisition and storage subsystem is responsible for acquiring and archiving various types of data. These data encompass a wide variety of information such as observational data (e.g., concentrations, meteorological observations), self-reported country-level emissions data, reported inventories, socio-economic data, and other data relevant for monitoring state actions towards reducing GHG emissions. Such information is needed to provide executives as well as policy and other analysts with GHG information for specified temporal (i.e., quarterly, annually) and spatial/sectoral (i.e., regional, country-/subcountry-level, economic) domains. Information of interest includes, but is not limited to, global trends for a specific GHG, total emissions, emissions by economic sector, GHG concentrations, emissions mitigation actions, and country-level reports on a country's emission of anthropogenic GHGs, compared to their commitments and reported inventories.

The magnitude of the volume of data accessible to GHGIS is expected to grow rapidly during early phases. The system will therefore be designed for scalability (to accommodate increases in magnitude and frequency of data) and flexibility (to accommodate GHG and complementary data). For the initial phase, the network of currently available sensors will be leveraged by GMOC to provide the earliest support to help meet the GHGIS requirements. The sensors will send GHG and other data to their respective data centers. At these centers, the data will be processed, reduced, and archived in response to each center's original mission. Data necessary for GHGIS to fulfill its mission will then be transferred to the GMOC data-acquisition system. Origination or pedigree (QA/QC) metadata and any processing provenance information imparted and attached to the stored data will be associated and saved in the provenance database for later access during the processing and analysis, as well as the reporting and dissemination phases.

The stored provenance information enables analysts to look back and find information about the data sets, operations, and algorithms that were used to produce an end product. Archiving of such data along with their metadata will also allow a particular analysis and ensuing report to be traced to original data, calibrations, auxiliary analyses, models, etc., required to produce it. An improved calibration or model, for example, would allow for a reanalysis and an improved product that would, in turn, be traceable to the particular inputs and tools used to produce it.

Data will be continuously flowing into the GMOC from several data sources. Any event that might interfere with this data flow, such as an interruption of service, communications failure, or a compromise of data integrity, must be detected and resolved quickly to ensure the GMOC's continued access to high-quality certified data. In addition, the GMOC will have an automated processing capability responsible for activities such as acquisition, processing, archival, and analysis. This level of processing will be monitored to ensure that data are acquired and processed in a reliable and consistent fashion. The system can have a 24/7 operational availability in its data-acquisition and -storage capability, should data needs mandate this capability.

A yearly baseline dataset will be an important product of these data holdings. To monitor changes in emissions, analysts must establish reliable, traceable baselines that, if need be, can be revised as additional data on archived measurements or improved modeling and analyses become available. No such baselines exist today.

### 8.4.3 Processing and Analysis

Different levels of processing and analysis generate different levels of product output. Depending on the level of the output, processing and analysis can either be automated or require analyst intervention. The GMOC anticipates different analysts to support the US executive branch, policy analysts, and GMOC analysts. Executive and policy analysts will have access to much of the functionality of the GMOC and can pose questions to be answered by the GMOC. GMOC analysts monitor the state of GHGIS and the GMOC, generate periodic reports, and utilize the GMOC to answer questions posed by policy analysts. Policy analysts may also use a distributed software interface (e.g., a web portal or other web-based service) to directly access GMOC analysis capabilities and perform their own analysis, if desired. Furthermore, if GHGIS sponsors desire, authorized scientists and researchers may also have access to unlimited-release data sets and may query the system via a distributed software interface. After data have been ingested into the GMOC, the lowest level of the automated processing and analysis subsystem is responsible for GHG data processing, reduction, and storage. Automated analysis will include monitoring the SOH of the data and sensor system, and low-complexity processing. Sensor or data feed problems will trigger automated alerts to allow GMOC operators to initiate troubleshooting activities and notify the appropriate stakeholders.



Figure 8-3. GMOC analysis scenario.

For higher-level outputs, the majority of the analytical responsibility will reside with the GMOC analysts. GMOC analysts will be able to process multiple types and sources of data to generate products that can be used in the GHG emissions and related-activity monitoring effort. These products will be accompanied by metrics such as uncertainty, reliability, and QA/QC metadata. GMOC analysts will have the ability to analyze data utilizing available GMOC resources and workflows, or, when necessary, have access to high-performance computing capability as part of the offline analysis workflow. Processed data will be analyzed by GMOC analysts at an appropriate level of granularity and at a pace that supports reporting and dissemination requirements for GHGIS customers. All analytic processes will use scientific workflow management systems to record hierarchical provenance of interacting processing tasks that ultimately provide products for dissemination and reporting. That provenance information may include a history of specific versions of processed data and processing algorithms used, along with the order in which algorithms were applied, in order to produce a version-controlled end product. Saving such provenance information is critical for reanalysis and reprocessing at later times, as additional, or improved, information becomes available, as well as to be able to provide traceability of analysis and results. A sample GMOC analysis scenario is portrayed in Fig. 8-3.

In addition to the routine analysis performed by both system and GMOC analysts, there will be a need for higher levels of interactive offline analysis, as discussed above. Offline analysis will include processing that requires high-performance computing resources and any processing that is too complex to automate, such as large-scale atmospheric transport modeling. The scope of this analysis and high-performance computing requirements are yet to be determined. Regardless of the scope or location of the processing, workflow and provenance will be as important at an offsite facility as they were at the GMOC.

The processing and analysis subsystem will also provide a variety of GMOC tools to support analysis of the large volume of data associated with monitoring GHG emissions and related activities such as running climate models. Analysis tools will be needed to carry out tasks such as generating simple plots and trends, performing comparisons, and visualizing, analyzing, and interacting with data of interest. Because data from different sources will be available at different times, these tools must be able to reprocess previously used data in conjunction with newly available data. In addition, as the tools and algorithms evolve, analysts may reprocess data to produce improved results with updated version-control metadata.

The dynamic nature of GMOC responsibilities dictates that analysts must also be responsible for providing feedback to guide system improvements. Such feedback could include defining new functionality needed to support changes in verification requirements, modifications or updates to algorithms in the pipeline, introduction of validated new software into the system, enhancements to improve system performance, or suggestions for new sensor placement based on observed monitoring gaps.

### 8.4.4 Reporting and Product Dissemination

The reporting and dissemination GMOC subsystem will be releasing all levels of data and information products. Interfaces will be provided to facilitate the generation of spatially and temporally bounded reports, both at regular intervals and as needed at the request of GHGIS customers. These reports must be objective and unbiased, traceable, technically credible, reliable, and accompanied by relevant supporting information. Elements of traceability are rigorously enforced using metadata, pedigree, provenance principles, detailed version control, and processing workflows. Building on the discussion above, these elements include documentation of each step of report generation including, but not limited to, the process used to generate each report, data version and data UQ, the specific algorithms applied to process the data, and a justification for and documentation of any omitted data.

Outside of the analysis and processing of new data, it will be necessary to provide the ability to query the system. Three primary motivations for system queries are envisioned:

• Automatic queries resulting in periodic reports. The requirement for frequency of reporting will be determined by the GHGIS customers. When a customer requests a GMOC data product, an internal GMOC analyst is responsible for fulfilling this request. Select GHGIS customers will also have the option to generate automated reports directly through remote interfaces.

- Queries stemming from special requests for in-depth analysis of an activity or anomaly of interest, or equivalent, resulting in a special report. This will be initiated by a GHGIS customer, or policy analyst, and executed by a policy or GMOC analyst.
- Research and development community queries or other requests for data/analysis resulting in the dissemination of a data or analysis product, including provenance. This could be initiated by a climate scientist/researcher (or equivalent) and facilitated by a GMOC analyst, as necessary.

# 8.5 Conceptual GMOC System Architecture

The GMOC system architecture represents the infrastructure necessary to satisfy operational requirements and system qualities ensuring that all facets and goals of the GMOC are met. While the GMOC is composed of multiple subsystems, not all subsystems must necessarily reside in a single, centralized facility; technologies such as virtualization or cloud computing (Chandra 2010) could be used to allow consistent GMOC access from multiple locations, as well as allowing GMOC to access reserve capacity for peak processing demands. The decision for local storage and processing must be made with an eye to the three considerations outlined above.

The following subsections present a high-level system overview, followed by a more detailed look at the various subsystems within the GMOC, illustrating how the GMOC will fulfill its expected roles and responsibilities. The section concludes with an overview of some of the technologies that will be utilized throughout the GMOC.

### 8.5.1 GMOC System Overview

An overview of the GMOC system and its key interactions in Phase 1 and Phase 2 is presented in Figure 8-4. The GMOC must interface with many components of the GHGIS system including existing data centers, sensors, analysts, the research community, and the global Earth-science community. The Phase 1 prototype focuses on data derived from existing and planned near-term assets, while the Phase 2 operational system includes data from additional sensors designed and built for GHGIS purposes and other GHGIS-specific capabilities. During Phase 2, the GMOC will perform sensor and model down-selection with time and evolving priorities to create a system tailored to the functions required by GHGIS. The GMOC will be continually enhanced using an iterative approach, described in Sec. 8.6. Sensors and algorithms will be incorporated into GHGIS and the GMOC, as they become available, without a need to wait for the end of a phase before taking advantage of new capabilities.



Figure 8-4. GHGIS system concept overview and interactions.

### 8.5.2 GMOC Subsystems Descriptions and Interfaces

As discussed in Sec. 8.4, the GMOC key subsystems include data acquisition and storage; processing and analysis (including synthesis and assimilation); and reporting and dissemination. Some of these subsystems are broken down into finer-grained components, which are described briefly below. Fig. 8-5 depicts the primary roles and responsibilities of these subsystems.

### 8.5.3 Data Acquisition and Storage

The data acquisition subsystem is primarily responsible for ingesting, tagging, and archiving data from a large set of heterogeneous sensors and data centers. Primary functions of the acquisition subsystem include managing various modes of transmission and receipt, authentication, sensor testing, sensor calibration, and SOH monitoring. The acquisition system will be configured to accept data and information sources of arbitrary format or delivery mechanism.

The data storage subsystem is primarily responsible for storing acquired GHG, sensor, and related data. Primary functions of the data-storage subsystem include handling interactions with the on-line and off-line databases, archiving data to a long-term storage repository when the data are no longer needed, and SOH monitoring of the storage system.



Figure 8-5. GMOC conceptual design (subsystems).

To facilitate use of these data, this subsystem will provide an interface that allows users to access direct GHG observations, model outputs, inventory data, industrial/economic data, and other information. The interface will provide both storage input and output functionality, metadata and provenance definition and access, multi-format sensor data output, and input and output of all analysis and reporting results. The data-access subsystem will also include interfaces as required to support data requests by various national-asset organizations as well as the scientific community and other authorized users.

### 8.5.4 Data Processing and Analysis

The data processing and analysis subsystem performs the primary work of turning acquired multivariate data into output products and reports. A routine analysis schedule is envisioned that will likely require significant processing. Various types and amounts of trend or anomaly processing may occur based on results discovered in routine processing, as enhanced by automatic tagging to identify anomalies and unexpected behavior of any kind. This would prompt a re-examination of the data and its quality that may have been responsible for the

variance from expected behavior, and a re-examination of the modeling that was relied upon to produce these results, or other causes. This would support the primary goal of the analysis subsystem that is the attribution of emitted GHGs of interest to anthropogenic causes, e.g., as opposed to a volcanic eruption, that are at least at a country-level resolution. The required analysis to perform this task properly, while staying below a specified level of uncertainty, will be significant and will require interaction with the modeling and simulation and data UQ quantification GHGIS components.

### 8.5.5 Reporting and Dissemination

Finally, the reporting and dissemination GMOC subsystem will primarily be designed to synthesize the analysis output from the acquisition and processing steps into a set of results and reports for defined customers and policy analysts. These reports can be either generic in nature, e.g., for potential public/international release, or specifically tailored to a defined customer's exact needs and requirements. Additionally, internal reports, used to understand overall GMOC performance, SOH, resource usage, and other parameters of interest, will be produced, enhancing the overall robustness and reliability of the GMOC system.

Comprehensive data provenance to ensure traceability and repeatability will be built into all acquisition, storage, processing, analysis, and reporting functions performed by the GMOC. Sophisticated provenance aids in tracking and tagging the history of all results and reports and will be necessary to build trust in the policy and research communities on the validity of the GMOC-produced results and reports. Such information will also facilitate reprocessing.

### 8.5.6 Technologies

The GMOC subsystems will utilize existing technologies when applicable. Many of the existing data centers use various forms of the noncomprehensive list of technologies listed below.

### Metadata

Metadata provides information about data, including where the data originated, when the data were generated, relevant units of measurement, traceability to raw and calibration data, annotations from other analysts, and minimum and maximum elements. This information will be stored in an easily searchable format to allow analysts to quickly identify, locate, and retrieve data of interest. Delivered data products will be self-documenting through inclusion of the appropriate metadata.

#### Data Provenance

Data provenance will be used to track data QA/QC, data UQ, the derivation history of a data product (which includes the original input data sources as well as the history of operations), and modeling performed with that data that ultimately produces an output product. As mentioned earlier, a complete record of data and analysis provenance is crucial to provide process credibility, maintain traceability, and enable reanalysis.

#### Workflow Engines

Workflow engines can be used to construct and then automate much of the routine processing that must take place at the GMOC. Workflows provide mechanisms to chain tasks together, where each task takes input data from previous tasks, pertinent parameter and property settings, and other data from external sources, ultimately forming a traceable task output. Each such output records critical provenance information for the task process, authoritatively documenting the lineage of the result.

#### Visualization

Many different types of data must be considered when comparing a country's emissions and mitigation actions to their stated commitments. These data must be presented in a way that is useful to users and can inform assessments and decisions. To this end, a range of visualization tools must be made available to the users of the GMOC.

### Gateways/Portals

It is not reasonable to attempt to store every existing bit of climate data. Instead, an infrastructure is needed where complete metadata representing accessible data are available. When data are needed as part of the report-generation process, either the data or the process to retrieve that data through a gateway or portal can be stored at the GMOC.

The ESG-CET aims to build a virtual federated environment that combines model output, observational data, and analysis and visualization tools in order to facilitate and empower access by all user communities. To this end, the ESG-CET team operates and supports a global infrastructure for the management, access, and analysis of climate data. This infrastructure will be essential to providing the GMOC with access to a variety of data sources and tools.

# 8.6 General Program Plan for GMOC Development

The GMOC will be designed, developed, and deployed following a phased and iterative approach. Also referred to as spiral development, this approach will facilitate creation of the initial Phase 1 prototype capabilities, enable incremental updates to system capabilities in shorter time frames, and allow the development of the Phase 2 operational capability while minimizing disruption of services and products delivered before the end of that period. Added benefits include encouraging user engagement and feedback throughout the development process, allowing system development to be more agile and adaptable to changing user needs, and creating a system that is responsive to and can accommodate new/additional data sources. As described in Sec. 8.5, the conceptual architecture was designed to address the anticipated long-term needs of GHGIS. If the CTBTO monitoring systems are to serve as a guide, the GMOC can be expected to be continually enhanced over time to meet evolving operational needs.

Section 8.6.1 defines a program plan for system development in Phase 1, addressing what can be accomplished within a 3-year time frame, from project start. Sec. 8.6.2 then describes a high-level plan for enhancing the GMOC to meet the Phase 2 goals. Lastly, Sec. 8.6.3 proposes a general plan for the integration of emerging technologies from the research communities into an operational GHGIS and the GMOC in particular.

### 8.6.1 Phase 1 System Development

Early in the development cycle, the GMOC team will design an enterprise architecture to establish operational-level baselines of GHG emissions, forested areas, emissions-mitigation actions, and emissions changes. These baselines will be used to establish country-level monitoring goals. Since this system will support an operational mission, the GMOC will also establish metrics for operational performance and effectiveness to guide future enhancements. The enterprise architecture will facilitate the implementation, execution, and integration of automated and operational (validated and verified) analytical algorithms for continuous GHG monitoring and assessments.

Phase 1 of the GMOC will borrow lessons learned and successful concepts from the agile development of other operational systems. Importantly, this new capability will integrate existing capabilities and products from existing data centers. By the end of Phase 1, the GMOC will perform continuous evaluation and data acquisition from existing data centers. GHG monitoring information will then be processed, analyzed, reported, and disseminated to key stakeholders at regular intervals, along with associated data and modeling UQ. While, as discussed in Chapter 2, Phase 1 products are unlikely to meet the GHGIS requirements, the experience gained and the interaction with GHGIS users will provide invaluable feedback and guidance for Phase 2 GHGIS developments.

Before deployment of the Phase 1 GMOC prototype, functionality will be developed to demonstrate the Phase 1 capabilities and scalability to Phase 2. By following this notional roadmap, the GMOC will reach an initial prototype capability within the Phase 1 time frame (0–3 years from project start).

### 8.6.2 Development Beyond Phase 1

During Phase 2 (0–10 years from project start), the GMOC will build on the system developed in Phase 1 to move to full operational capability. This phase will continue iterative development, testing, validation, and integration of enhancements toward an operational GMOC. An operational GMOC will monitor country-level emissions and/or emissions changes against the baseline agreed upon and established during Phase 1. To maximize efficiency and minimize redundant development efforts, the Phase 1 GMOC will evolve into the Phase 2 GMOC.

The Phase 2 GMOC will acquire, validate, and store data from existing and newly deployed data centers/sources. Processing and analysis operations will scale appropriately to the magnitude and complexity of the data and/or physical processes governing GHG trends. As needed, higher-level offline analysis routines will be promoted to other GMOC resources, as necessary. The modeling and simulation required to perform GHG attribution analysis will also be integrated into the GMOC. Reporting frequency will be established and formal reports will be generated and disseminated to key policy stakeholders.

# 8.6.3 Technology-Insertion Program: Collaboration between Science/Research and the GMOC

Insertion of new technology or features into the GMOC will follow the program presented in Fig. 8-6.



Figure 8-6. GMOC technology insertion.

In requesting new technology, principal stakeholders will consider user needs. additional/purpose-built sensing assets, emerging technical and political issues and priorities, and operations needs. These needs will drive the direction of applied research, which may be funded by many stakeholder agencies/entities. Results from the research and industrial communities (e.g., algorithms, hardware design and implementation) are then considered for the GMOC. At this point in the iterative design process, reworking and refocusing these results toward the GMOC mission may occur. The technical operations stakeholders will evaluate algorithms or hardware upgrades and initiate integration into the GMOC as necessary. Once the new capability is demonstrated, validated, and verified, it will be delivered to the operational agency to enhance the operational system. The operational agency, where the GMOC resides, will then have a new baseline capability with improved performance and new mission capabilities. The process continues, enabling the GMOC to evolve over time, benefiting from the latest developments. In the context of GHGIS efforts, this technology insertion model may be used to incorporate the latest advances of the uncertainty quantification and inverse modeling efforts. For example, new algorithms may be transformed from research into operational-level software for use in the GMOC processing and analysis system.

By this method of technology insertion and infusion, it is easier to identify and plan for areas of focused research and development. The technology-insertion process has implications for GMOC budget and schedule. Experience shows that the following principles apply:

Given the long-term project-development period, a stable/predictable budget will be critical for development, operations and maintenance, integration, and testing. When stable budgets are augmented by additional development funds from other government agencies and programs, enhancements can be accelerated, augmentations can be incorporated, and mission-capability scope can increase.

A 12- to 18-month delivery cycle provides rapid evolution of mission-enabling capabilities.

In summary, it is anticipated that GHGIS, in general, and the GMOC, in particular, will evolve over time, with Phase 1 providing initial baseline and prototype capabilities, followed by iterative enhancements during Phase 2 that will deliver the first fully operational system, with new purpose-built sensors and advanced modeling.

# Chapter 9. Systems Engineering and Integration

# **Chapter Summary**

The role of system engineering and integration is to ensure that the combined system meets the requirements set by the Greenhouse Gas Information System (GHGIS) customers and users, and therefore their needs. Driving considerations in setting these requirements are system performance, cost, and schedule. The GHGIS is a highly complex system, and a system-level perspective will be important in ensuring that the combination of a large variety of data sources is well integrated, processed, analyzed, and disseminated to provide the products the end-users require, in time, at as low a cost as possible.

# Findings

- 1. The proposed GHGIS system architecture includes a centralized, operational GHGIS Mission Operations Center (GMOC) described and discussed in Chapter 8. It integrates relevant top-down and bottom-up data, processes, archives, analyzes, and disseminates information products to users.
- 2. The GHGIS implementation plan focuses on a near-term capability-based Phase 1 deliverable for a prototype GHGIS (3 years after development project start) and a requirements-driven operational Phase 2 GHGIS (10 years after project start).
- 3. The Phase 1 capability will integrate data from existing sensors and information sources as well as those that can be deployed within the Phase 1 period, in the (yet-to-be) designed and implemented GMOC.
- 4. The Phase 2 operational capability will consist of an expanded sensor network with purpose-built sensor types and locations driven by requirements dictated by user needs, system performance as determined by a system design tool, constraints stemming from access considerations, and a need to keep costs down.
- 5. As also discussed in the preceding chapters, an evolutionary development approach will be followed given that user needs may well adapt to GHGIS capabilities, as those evolve, and further research and development (R&D) is likely to provide enhanced performance at reduced costs, and the funding profile is likely to be spread over time.
- 6. Given the complexity of the GHGIS system and uncertainties inherent in the discrimination and attribution of anthropogenic emissions, collaboration with relevant science and technology R&D communities will be essential to maximize the efficiency of the GHGIS operation and the quality of delivered information products.

# **Recommendations (Phase 1 GHGIS Development)**

- 1. Establish a first set of GHGIS requirements and specifications.
- 2. Design, develop, and deploy the GMOC.

- 3. Negotiate access to existing greenhouse-gas (GHG) data, proxy and bottom-up data (energy, infrastructure, activities by economic sector, etc.), and other relevant information.
- 4. Establish a first set of anthropogenic-emissions and carbon-stock baselines, as best as feasible, against which future emissions reductions and mitigation actions can be referenced.
- 5. Develop network-design guidelines for new purpose-built sensors and expand and augment existing sensor networks on an as-necessary basis.
- 6. Develop and implement a basic data analysis capability to combine a priori information, self-reported (bottom-up) inventory data, and GHG measurements to detect significant changes in anthropogenic emissions and reporting anomalies.
- 7. Begin the investment in next-generation atmospheric and other models for atmospheric transport and attribution of anthropogenic emissions that can be verified and validated.
- 8. Pausing on the last bullet, such an investment is within the purview of the DOE-SC, National Aeronautics and Space Administration (NASA) Earth Science, National Oceanic and Atmospheric Administration (NOAA), and other agencies. Its benefits will transcend the needs of GHGIS and have a great impact, not only scientifically, but also is many other contexts.

## **Recommendations (Phase 2 GHGIS Development)**

- 1. Identify users and needs, revise requirements and specifications as necessary, and maintain communication as users and needs evolve/change.
- 2. Continue the investment in the intensive model development for atmospheric transport, data inversions, and attribution of anthropogenic emissions.
- 3. Develop a sensor (land, sea, air, space) network design and performance analysis tool based on an Observation Systems Simulation Experiment (OSSE) approach.
- 4. Invest in sensor technology development and measurement capabilities to support an extensive purpose-built sensor network.
- 5. Collaborate with and manage R&D efforts to develop and test new measurement technology and techniques, and new analysis and modeling tools.

## 9.1 Introduction

The main value of the GHGIS will be determined by the degree to which the system fulfills the primary need to monitor actions and the effects of actions taken by countries to reduce anthropogenic GHG emissions. While many other benefits will derive from its development, the ability of GHGIS to meet this and other needs will ultimately depend on a large number of factors, including:

• An understanding of GHGIS-customer needs, the resulting system requirements, and system-component specifications.

- Access to needed information, whether GHG observational data, energy, infrastructure, or other types of relevant information.
- The ability to determine the type, number, and locations of new purpose-built sensors to address the needs for discrimination and attribution of anthropogenic emissions to specific countries, regions, economic sectors, and times.
- The ability to deploy and integrate measurement data from the new sensors deployed.
- The reliability and trustworthiness of the collected data.
- Robustness of the entire system, i.e., the extent to which the system and final products degrade as a result of the failure of a system component.
- The capability of the analysis and modeling tools to infer anthropogenic emissions from observational GHG data and related information.
- The ability of the overall system to reliably assimilate relevant data and deliver information products to the users in a timely fashion.

The task of systems engineering and integration throughout the scoping, design, development, implementation, and operation of GHGIS is to identify users' needs, translate these needs into system requirements, develop a system architecture that will best satisfy these requirements, flow requirements down to the system elements and component specifications, and ensure that the implemented system continues to meet the requirements and consequently meets the users' needs.

The task of the present GHGIS Scoping Study described in this report was to determine the major issues with the design, development, and implementation of GHGIS and propose a path forward. This chapter provides a systems-level overview of the major concerns and challenges that should be addressed to ensure that GHGIS will meet its system requirements.

This study focused primarily on direct GHG measurements, and earlier topic-specific chapters provided detail on the types of observations and analysis that could be performed in the near term and what kind of observations and analysis would be needed to meet the requirements on GHG flux uncertainty and spatial and temporal resolution assessed in Chapter 2. One can already state, however, that meeting users' needs will involve creating an all-source information system that integrates a wide variety of information, in addition to GHG measurement data, such as energy, economic, infrastructure, and inventory data.

This chapter will discuss:

- 1. GHGIS goals and requirements, and a system architecture that addresses them;
- 2. issues with the deployment and integration of a highly complex system like GHGIS;
- 3. the need to develop a system-performance analysis tool and the recommended process for designing GHGIS; and
- 4. a proposed development plan and path forward.

# 9.2 GHGIS Goals and System Architecture

### 9.2.1 GHGIS Goals

As stated above, the success of GHGIS will ultimately be determined by its ability to meet users' needs. Both users and their needs are currently only partially identified and only in a framework sense (cf. Chapter 2). With the expectation that the needs will depend on both national and international politics, as well as Earth and perhaps other science, the GHGIS system design, as well as the implementation plan, must be flexible and capable of adaptation. With uncertainty in users' needs, at present, this scoping study focused on a requirements framework for detecting deviations from commitments to reduce GHG emissions, as described in Chapter 2, with the final requirements to be chosen by customers, based on the desired performance, available resources, and time to complete an operational GHGIS during Phase 2 of the proposed development effort. As is the case with many complex systems, there will likely be a continued evolution of needs and requirements throughout system scoping, design, and development of GHGIS.

Absent clearly defined user-provided needs, the GHGIS scoping-study team developed goals that will drive the design and development of GHGIS. One of the primary perceived needs and long-term goals of GHGIS is to provide the capability to globally monitor GHG concentrations, discriminate anthropogenic emissions from those from natural sources, attribute emissions to country of origin, or, in the case of large emitters and countries with large areas, at subcountry level, attribute emissions to economic sectors, and integrate relevant international economic, infrastructure, and other monitoring information. Targeted users are primarily the executive, policy, and science research and advisory communities that are focused on monitoring actions and effects of actions taken in relation to GHG emissions and future treaties.

Monitoring actions taken will benefit from an all-source approach that includes a large variety of observational data, but monitoring the effects of these actions on the emissions of GHGs will require direct, to-purpose, GHG-related observations.

Given a need for integrated information on anthropogenic GHG emissions, the proposed plan is to stand up a GHGIS that provides as much value as possible to users, subject to cost constraints, in the shortest time possible, and then evolve in capability as specific needs are identified and additional purpose-built sensors are developed and deployed, and more information from additional sources becomes accessible and available, as discussed in Chapter 8. It is proposed that near-term capabilities be focused on monitoring actions given that information sources based on imagery or infrastructure data are more developed than for near-surface GHG emissions detection at this time. The speed with which GHGIS can address the need to directly monitor anthropogenic GHG emissions and provide discrimination and attribution to the country of origin will depend on resources provided to develop an adequate sensor network and integration, and an operations center, as described in previous chapters.

### 9.2.2 System Architecture

A high-level overview of the proposed GHGIS system architecture is shown in Fig. 9-1, and is discussed in Chapter 8. Direct GHG observations will be made by space observational assets

(Chapter 3), airborne sensors (Chapter 4), and ground-based sensors (Chapter 5). Data will be sent to the centralized GMOC discussed in Chapter 8, assessed for uncertainty quantification (Data UQ, as discussed in Chapter 6), providing input to modeling, modeling UQ, and attribution analysis (Chapter 7). Meteorological data will be acquired for use by transport and modeling tools to help attribute emissions. This all-source data integration will also include energy, infrastructure, inventory, and other data that will provide both self-reported data as well as proxy information that can independently corroborate the information gathered through direct observations.



Figure 9-1. System overview of the proposed GHGIS (with direct GHG observations and other useful data integrated and analyzed in the GMOC, with delivery of data and information products to the executive, and policy and scientific communities).

As discussed in Chapter 8, the proposed GMOC will support data archiving, processing, analysis, and exploitation. Intensive transport, inverse modeling, and related analyses could be performed off-line, depending on computational resources required and available, and where it is decided that GHGIS data will reside and be distributed, if not all at the GMOC. Informational products will be delivered regularly to GHGIS users. Queries of GHGIS will allow users to

address needs as they arise. A GHGIS information-flow diagram is shown in Fig. 9-2. More details of the data integration and dissemination were given in Chapter 8.

As discussed throughout the report, in the near term (Phase 1), GHG data will be acquired from existing and expanded sensor networks, as well as new planned sensor deployments. In addition, meteorological data will be acquired by establishing access to existing meteorological data, e.g., the MERRA reanalysis products from NASA, or from dedicated sensors deployed for GHGIS use as soon as feasible. The long-term (Phase 2 and beyond) plan for GHGIS implementation assumes the system architecture shown above, but an expansion and augmentation of existing sensor networks, improved data analysis tools, and a shift from shared R&D sensor assets to dedicated purpose-built operational assets. Data from the latter will also be made available to wide user communities, as appropriate.



Figure 9-2. Simplified GHGIS information flow.

### 9.2.3 Concept of Operations

The GHGIS concept of operations (CONOPS) involves the regular dissemination of information products and the ability to respond to customer queries. It is assumed that communication between direct GHG observation sensors and data centers will be one way, when available, and GHG data will be sent to the GMOC, along with relevant metadata such as sensor state of health (see Chapter 8 for more details). Relevant all-source data (energy, infrastructure, inventory, etc.) will also be obtained regularly by the GMOC, with interfaces negotiated to provide additional information and analyses when needed.

As described in Chapter 8, GMOC will perform regular analyses on anthropogenic GHG emissions for specified countries and time periods using relevant acquired data, as requested by GHGIS customers. The time between the GHG observations and acquisition of data by GMOC will necessarily vary for different observational assets. This variability in data latency will lead to a continuously improving assessment of GHG emissions as new data become available, are certified, and their uncertainties quantified (cf. Chapter 6). In addition, data quality and

trustworthiness will vary, and a data certification process will need to be implemented to assess the value of the data and how they will be used in analyses and reporting, as discussed above and elsewhere in this report. Ideally, dedicated GHGIS sensors will be deployed, designed to meet data-latency requirements and maximize data quality and trustworthiness, within cost constraints.

GHGIS must be able to respond to user queries, as unforeseen needs arise and specific information is requested. As discussed in Chapter 8, GMOC operational analysts will respond to queries and run off-line intensive simulations and analyses, as appropriate and required to respond to the query. A notional GMOC analysis is illustrated in Fig. 8-3. Simple queries for accessing observational data by the policy or science communities can be automated. Off-line intensive processing centers would require significant computational resources to perform detailed simulations. Models and codes used will be certified and agreements would be in place to certify on-site and off-line analysis centers as operational elements of GHGIS on a periodic basis.

To ensure reliable delivery of valuable information products and responses to queries, GMOC must meet appropriate availability requirements that will require careful consideration of operations and maintenance processes, redundancy of critical computational/processing resources, communications and network infrastructure, and, not least, cybersecurity measures and best-practices to mitigate against such threats and ensure data, model, and analysis integrity.

### 9.2.4 Implementation Timeline

The implementation plan for GHGIS is focused on a capability-driven Phase 1 (3 years from project start) and a requirements-driven Phase 2 (10 years from project start), referenced to the beginning of funding for GHGIS design and implementation. The goal is to provide significant value in 3 years with the integration of existing information into a prototype Phase 1 system and evolve GHGIS to meet the longer-term GHG detection, discrimination, and attribution performance requirements within the Phase 2 period, aimed at an operational system. Following an evolutionary development plan will allow user feedback and system design analysis to direct continuous improvements and development, in support of attaining the necessary system performance to most efficiently and cost-effectively reach the long-term GHGIS goals and meet its requirements.

The envisioned GHGIS implementation plan is illustrated in Fig. 9-3. The scoping study depicted at the beginning is the study that has been conducted and is documented in the current report. Phase 1 and Phase 2 developments begin concurrently, the former aimed at the GHGIS prototype delivery, while the latter is aimed at the operational GHGIS delivery. The three arrows represent the parallel efforts of

- 1. development, implementation, and operation of GHGIS;
- 2. GHGIS R&D directed towards improved tools and methods for producing higher confidence and quality information products; and
- 3. basic science and technology R&D outside the GHGIS effort on which the Phase 2 GHGIS will rely for its ultimate delivery.

Though the Phase 1 capability will depend largely on existing and near-term sensor networks and analytical tools, directed R&D should begin immediately focused on data fusion/integration and analytical tools needed to meet the long-term requirements that will drive the operational Phase 2 capability. The development of GHGIS analytical tools and sensor network design considerations can benefit directly from the national and international science communities through close cooperation with scientists focused on related basic and applied research.



Figure 9-3. GHGIS implementation plan and the role of R&D in further development.

### Phase 1

The capability-driven Phase 1 (3-year) plan is to integrate existing information sources and sensors and begin delivering preliminary information products. Given the maturity of non-GHG forms of sensing such as optical and infrared imaging and the wealth of existing energy, industrial, infrastructure, and other types of data, the capability of a prototype GHGIS at the end of the Phase 1 development period will benefit strongly from the all-source approach to data integration. However, it will be imperative to begin integrating existing GHG sensors and assets as soon as possible, and begin providing comparative analyses of GHG data with other kinds of related data. As discussed in Chapter 2, where the requirements framework is presented, and in the subsequent chapters on measurements, data UQ, and modeling, it will not be possible to provide high-confidence attribution using existing sensor networks, though it may be possible to detect anomalies or significant misreporting of GHG inventories.

The types of questions that can be answered by the Phase 1 GHGIS will primarily depend on

- the amount and quality of information that can be obtained on countries' actions from all relevant sources: self-reported inventories, energy, infrastructure, remote-sensing or other types of "proxy" data;
- the number, type, and locations of sensors that can be exploited, or deployed, within the Phase 1 period; and
- the sophistication of the analysis and modeling tools that can be deployed within the Phase 1 period.

Information in addition to direct GHG measurement data will be useful both to provide evidence for and perhaps verify a country's compliance with actions committed to in a treaty and to reduce

a priori representation error in inverse modeling, reducing the uncertainty with which measured GHG concentrations can lead to attribution of GHG emissions.

Capabilities for ground, air, and space sensing that would be deployed during Phase 1 are described in Chapters 3 through 5. Existing tall-tower networks could be expanded, if that is deemed advisable; upgrades could be made to air quality/pollution observation platforms; and data retrievals from space platforms could validate near-surface measurements, both in the infrared and reflected sunlight, e.g., with OCO-2. Given the long lead time, near-term space capabilities will be limited to existing on-orbit assets, with OCO-2 currently planned for launch in 2013. Airborne measurement programs could be expanded and commercial aircraft-hosted GHG monitoring programs could be pursued. Increased  $\Delta^{14}$ C analyses could be performed from established whole air-collection sites. Standardized protocols and quality-assurance and -control procedures for field and lab measurements would be developed and adopted.

Analysis, modeling, and uncertainty quantification capabilities planned for Phase 1 are described in Chapters 6 and 7. Combinations of measurement data from various sensor modalities would be combined to improve calibration, and to detect outliers as well as potential instrument errors. Analysis and modeling efforts in Phase 1 will focus on integrating existing information on emissions sources and fluxes coupled with meteorological data and atmospheric transport modeling to provide comparisons between predicted and measured GHG concentrations. This initial capability will focus not on inverse modeling to infer emission source locations and fluxes, but instead to detect and attempt to assess significant deviations between actual and selfreported emissions. Further, if limited to urban domes, techniques based on estimation of airborne pollutants can be adapted to infer anthropogenic carbon dioxide ( $CO_2$ ) emissions (see Chapters 6 and 7).

Even without additional sensor deployment, valuable information will likely result from the dedicated assimilation and integration of currently existing data sources for the purpose of GHG treaty monitoring. The GMOC will provide this capability and can be designed, developed, and implemented as a prototype operational center during Phase 1. Interfaces to existing data sources must be negotiated, and data processing and analysis tools will need to be developed and implemented. More details can be found in Chapter 8.

### Phase 2

The requirements-driven Phase 2 (10-year) plan is to extend the GHG-sensing network to meet high-performance GHG detection, discrimination, and attribution requirements, towards the development of an operational GHGIS. Analysis, modeling, and simulation tools will continually evolve during Phase 2, and the increasingly complex integration of sensor data will be accommodated by building in scalability and flexibility into the GMOC, as discussed in Chapter 8. GHGIS will be designed to provide independent attribution of anthropogenic emissions to the country or region of origin through direct GHG emissions. Direct GHG detection will provide independent and high-confidence knowledge of country emissions in addition to providing a means to assess the efficacy of a country's actions to reduce anthropogenic GHG emissions or increase sinks. Purpose-built capabilities for ground, air, and space sensing that could be deployed during Phase 2 are described in Chapters 3 through 5. The primary increase in observational capability during the Phase 2 period will result from a directed and coordinated effort to deploy dedicated operational ground-, air-, and space-based sensors, and perhaps also seaborne in special circumstances and locales, to efficiently provide discrimination of anthropogenic from natural/biogenic emissions and attribution of these emissions to the country of origin, economic sectors, etc., as discussed above.

Analysis, modeling, and UQ capabilities planned for Phase 2 are described in Chapters 6 and 7. Increased capabilities will arise from improved models and modeling techniques, such as multivariate assimilation through the combination of GHG and locally measured meteorological data. Additional analytical techniques will be used to constrain flux estimates based on combined GHG and related tracer gas measurements from various sensor modalities. Advances in algorithms and computational power could enable fully integrated model calibration and uncertainty estimation, improving estimates, and enabling improved system design strategies for optimizing the sensor network design.

As described in Chapter 8, Phase 2 plans for the GMOC consist primarily of adapting to a large increase in sensor data, interfaces, and processing needs. Scalability and flexibility are key attributes of the GMOC design to accommodate expected changes in the number and types of sensors and information sources, as well as changes in the type and format of the data. Changes in users' needs will require highly flexible computational capabilities, user interfaces, and an infrastructure to allow for agile response.

### 9.2.5 Evolution of Capability

The capability of GHGIS to monitor countries' actions and the effects of these actions on anthropogenic GHG emission fluxes will depend on the amount and type of information available. In the case of direct GHG measurements, a useful sensor type, location, and measurement frequency must be determined, the sensor system must be deployed; the sensor system must function as designed; the data must be assessed, their UQ established, and then communicated to the GMOC in a timely manner; and the data must be certified as free from tampering at any stage in the course of this path. Failure at any of these steps will prevent GHGIS from achieving the desired performance and delivering on its requirements.

Evolving the capability of GHGIS will be achieved primarily through a combination of analysisbased sensor network design (including ground, air, and space), negotiation of site access and trusted communication of data, and sensor deployment at desired/accessible sites. Continuous interaction between the GHGIS team and science researchers and developers of new sensing technology will help ensure that GHGIS continually provides maximum value for minimum cost. For instance, development of precise in situ <sup>14</sup>C measurements could significantly enhance system performance and attribution to anthropogenic sources, if resources and sites were available for worldwide deployment. This would provide a valuable GHGIS component, in concert with other components, even though, as discussed in Chapter 5 and elsewhere in this report, it would by no means provide the sole means of attribution. To adapt to continuously changing sensor networks, improved analysis tools, scientific understanding, changing user needs, etc., flexibility will be essential to the design of GHGIS and the GMOC. It is likely that with user feedback and recurring analysis of system capability there will be a desire for frequent upgrades to GMOC software as well as updated recommendations for sensor placement.

To achieve this evolution of capability, a sustained intensive effort must be made, with sufficient resources applied to the development of the data integration and analysis capabilities, and the design and deployment of a sensor network dedicated to the discrimination and attribution of anthropogenic GHG emissions. Access to sensor data from foreign-controlled sensors will require continued cooperation and clear benefit to the country providing the data, namely access to other countries' data in return.

### 9.2.6 Collaboration with Research and Development Efforts

Collaboration between the GHGIS effort and more basic scientific R&D efforts will be important to ensure that GHGIS benefits from the highest-quality knowledge, tools, and methods available for discriminating natural from anthropogenic emissions and providing attribution to sources for these emissions. Regional studies are particular useful for experimenting with multi-sensor measurements, data integration, and analysis to understand how well the system at a local level can discriminate and attribute the anthropogenic emissions.

There are numerous research groups and collaborations around the globe that focus on the carbon cycle and related GHG science. Some notable examples are the North American Carbon Program and CarboEurope. These research programs are pushing the boundaries of current scientific knowledge and measurement technology, and collaboration with associated researchers will facilitate benefits to GHGIS from some of the best knowledge and methods available for GHG measurement and analysis.

# 9.3 GHGIS System Design Considerations

### 9.3.1 System Design Tool and Trades

The capability of GHGIS to discriminate anthropogenic from natural GHG emissions and to attribute the emissions to sources in the country of origin through direct GHG observations will be determined primarily by what types of sensors are deployed, where they are deployed, how often measurements are made, and the quality of the data analysis, modeling, and inversion techniques. This will require a system design tool, an analytical tool that predicts system performance (level of uncertainty in attribution of flux levels, locations and times) as a function of system design (sensor types, locations, measurement frequency, modeling capabilities, etc.). The goal of the system design tool will be to provide robust sensor network designs that provide optimized designs for providing the required performance at minimum cost.

System design trades will be performed to determine general design guidelines for sensor placement and measurement frequency given various distributions of sources and sinks, and modeling UQ, especially considering differing geography and meteorology for countries of

interest. Some previous work on the design of sensor networks exists (Gloor et al. 2000, Patra and Maksyutov 2002, Rayner 2004).

The development of a system design tool will be an essential first step of the GHGIS design and development process. Given the unavoidable complexity of a global GHG monitoring system, it is difficult to predict how well this system can be developed to meet requirements without a system design tool. This tool will need to simulate emission sources and sinks based on current best knowledge (EDGAR, for example), propagate gases with meteorological models, and simulate measurements of gas concentrations given input sensor types, locations, and times. The analytical capability to then provide attribution to emission sources will likely be early versions of the analysis tools intended for use in the deployed GHGIS. Taking into consideration the uncertainty in the results, a determination of system performance in providing attribution of emissions can be assessed as a function of the input sensor network. Many variations in the inputs will need to be studied to determine efficient and robust sensor network designs.

A method used to predict performance of a sensor network is the OSSE methodology, in which known or simulated emissions (based on existing information on source locations and fluxes) are transported using meteorological models, and synthetic observations are inferred at hypothetical sensor locations. Inverse modeling techniques are then used to determine how well different sensor networks can estimate the emitted flux levels and source locations. The OSSE methodology provides a promising tool that can be adapted for use as a system design tool. The methodology and its utility are described in more detail in the next section.

It will be important to investigate a variety of sources, meteorological models or conditions, and sensor types and locations including ground, air, and space to understand how all these variables affect predicted system performance. General "rules of thumb" and design guidelines (e.g., Kaminski and Rayner 2008), that result from such exercises are likely to be as or more useful than analyses of optimized point designs. Constraints and unexpected influences may lead to deployment of less-than-ideal sensor networks, and quick-turnaround analyses may turn out to be more valuable than intensive high-fidelity point-design analyses. Test beds for doing so are discussed in Chapter 6 and elsewhere in this report.

It will be important to understand performance and cost trades associated with deployment of land, (possibly) sea, air, and space sensors. As discussed in Chapters 3 through 5, there are advantages and disadvantages to the various observational platforms. For instance, though satellites can provide large area coverage without needing to secure access to foreign land or airspace, satellite observations of  $CO_2$  are less precise than in situ measurements and are currently unable to detect <sup>14</sup>C for discrimination of anthropogenic from natural  $CO_2$ . On the other hand, ground-based tower measurements can provide precise measurements of GHGs, but only at a particular location and with measurements dominated by local effects (Gerbig et al. 2009) with an effective spatial extent/coverage determined by tower height. Airborne measurements provide a flexible capability for in situ and flask-based measurements for various spatial and temporal scales. Performing the trades to assess system performance to the various space/air/land/ocean elements for minimum cost will be an important part of the system design phase.

Exploiting the combined benefits of multiple sensor modalities will be a key characteristic of GHGIS. Though it is possible that general design guidelines and recommendations such as "deploy as dense of a tower network as possible with a goal of 3-km spacing" could arise from design studies, such a network would be infeasible over, say, the United States, and it is desirable instead to develop guidelines that show the benefit of combined sensor types. For instance, perhaps towers on a 30-km grid with a single satellite and regular air campaigns could provide improved performance with reduced cost over a 3-km tower grid. Though this is a simplified example, it illustrates the complexity of the design process, and the goal of GHGIS to provide integrated sensor and data solutions to provide maximum benefit for the minimum cost.

Finally, at a higher level and as discussed in various contexts above, sensor placement and measurement density will need to be determined in concert with available and anticipated modeling capabilities. Generally speaking, the more capable and reliable modeling proves to be, the fewer measurements will be required. Conversely, as discussed in Chapter 7, if the preponderant fraction of uncertainty derives from data model-dependent inversions, and if the level of those uncertainties proves to be higher than required to meet the criteria set in the Requirements Framework discussion (Chapter 2), then a recourse, as discussed in Chapter 6, is to densify measurements, combining ground, air, and space sensors, so reliance on models yields acceptably small uncertainties in the final product. That perhaps represents the most complex trade to assess at this writing and is beyond the scope of the present study.

An additional benefit of the development of the OSSE-type system design tool is that it will have dual use as a deployed system performance tool and system requirements verification tool. When a sensor network is deployed, the actual sensor types, locations, and measurement frequency can be entered to simulate performance under a variety of emission and meteorological scenarios. Since modeling is an integral part of an OSSE, such an OSSE approach can also help assess the trade between measurement density and type, and reliance on modeling. However, following the best verification that can be performed, validation of system performance will come through testing the ability of GHGIS to provide attribution for anthropogenic emissions known with high confidence.

## 9.3.2 Utility of OSSE Methodology

Data-assimilation techniques whereby global observations are incorporated into numerical models of Earth's atmosphere have become the cornerstone of numerical weather prediction (NWP) (Kalnay 2003). Data-assimilation performance for the prediction or estimation is critically dependent on the accuracy, precision, and distribution of the underlying observing system. Consequently, the design of this observing system, including the relative importance of its constituent elements and components, has been an area of significant research focus. OSSEs represent critical tools today in the design and evaluation of observing systems. The purpose of an OSSE is to quantitatively assess the impact of a set of new observations on the predicted state of a geophysical field, e.g., temperature, humidity, ozone, or the reduction in uncertainty of a physical process, e.g., sources and sinks of CO<sub>2</sub>. These systems are related to observing system experiments — also called data-denial experiments — that assess the relative importance of observations within an existing system (Hilton et al. (2009). The development of OSSEs originated in the NWP community dating back to at least the 1950s (Arnold and Dey 1986) and

are now routinely used to design and evaluate the impact of new satellite observations (Masutani et al. 2010).

These tools have been more recently applied to the construction or assessment of observing systems and instruments of trace gases such as carbon dioxide ( $CO_2$ ) and carbon monoxide (CO) to constrain estimates of sources and sinks (Rayner et al. 1996, Jones et al. 2003, Edwards et al. 2009). OSSEs are particularly important for these applications because observing systems primarily measure trace gas concentrations and not the surface fluxes and anthropogenic emissions of interest to GHGIS. As a consequence, it is difficult to develop measurement sampling, precision, and accuracy requirements that can be quantitatively traced to surface-flux accuracy requirements. OSSEs can serve as the bridge that mediates between these requirements.

The elements of an OSSE adapted for a satellite design are shown in Fig. 9-4. The reference model field, sometimes called the Nature run, is generated from a numerical model. In the case of CO<sub>2</sub>, these models are generally atmospheric-transport models forced by boundary/in-flow and initial conditions defined by carbon sources and sinks. These fields are subsequently spatio-temporally sampled, e.g., samples corresponding to the viewing of a sun-synchronous low Earth orbit satellite. For nadir-viewing satellites, radiation from the vertical distribution of the trace gas is propagated to the instrument aperture. The instrument model, which accounts for the type, e.g., Fourier-transform spectrometer [FTS] as in GOSAT, or grating spectrometer as in Atmospheric Infra-Red Sounder (AIRS) and Orbiting Carbon Observatory (OCO), precision, accuracy, and calibration of the instrument, is used to process the incoming radiation into a synthetic observation.

In many cases, such as for OCO (Crisp et al. 2004), the observations (measurements derived from the spaceborne sensor) are used to infer vertical profiles of  $CO_2$  through a retrieval algorithm (e.g., Connor et al. 2008, Kulawik et al. 2010). These profiles, along with their observation operators (Jones et al. 2003), are ingested into a data-assimilation system, which includes a transport model substantially different from the model used to generate the reference model fields, e.g., different boundary conditions and transport mechanisms. The data-assimilation system will then correct the model, e.g., surface fluxes, based on the ingested data. In the case of  $CO_2$  source and sink estimation, estimated fluxes are compared with reference fluxes used to generate the reference fluxes. If the estimated fluxes do not meet thresholds defined by those metrics, then the spatio-temporal sampling and instrument model characteristics are modified and the process is repeated. The extension to multiple instruments and platforms (including surface networks) is more or less straightforward.

This approach has been applied with varying degrees of sophistication to augmentations of surface networks (Gloor et al. 2000, Suntharalingam et al. 2003) or extensions of the network with remote sensed measurements (Rayner and O'Brien 2001) at both global and regional scales (Law et al. 2003, Carouge et al. 2010). More recently, OSSEs have been constructed to assess the impact of data from individual satellites on fluxes (Chevallier et al. 2007, Miller et al. 2007, Baker et al. 2010) and comparisons between different platforms (Hungershoefer et al. 2010). Transport errors represent a well-known challenge for accurate  $CO_2$  flux estimates (Peylin et al. 2002, Patra et al. 2003, Baker et al. 2006). As a consequence, OSSEs have incorporated transport error to assess their potential impact on flux estimates (Chevallier et al. 2010).



Figure 9-4. Satellite-based OSSE schematic. Boxes represent outputs, and ovals represent processes. The pictures are illustrative of the different outputs in the system. The blue ovals indicate processes that can be impacted by the outcome of the OSSE.

Despite their substantial use in the NWP and carbon-cycle communities, there are areas of open research in the use and characterization of OSSEs. Formal techniques for optimal placement of observations are an example. The definition of science metrics and their impact on observing systems has not been fully explored. The realism and credibility of OSSEs are best assessed through OSSE "calibration," whereby fluxes calculated with an existing observing system are compared to a simulation of that same system (Masutani et al. 2010). Differences in performance can be used to judge how reliable the OSSE results are for a future system. Nevertheless, even in this case, a new observing system may reveal processes (e.g., chemical  $CO_2$  sources) that are not incorporated in an OSSE. Consequently, to fully realize the potential of OSSEs for observing system design, a rigorous evaluation process must be developed that incorporates known uncertainties and has been tested (validated) with real observations.

The OSSE approach employed in remote sensing described above can be generalized and extended to support all sensor and sensing design, assessment modeling, and implementation in support of GHGIS.

### 9.3.3 Data Integration, Analysis, and Modeling

As discussed in the previous section, there are significant trades in sensor network designs that must be evaluated to ensure that the system meets performance, reliability, and other requirements, while minimizing cost. Similar trades must be made for data analysis and modeling tools. These considerations are not independent from the design of the sensor network, however. For example, at one extreme, the ability of GHGIS to provide attribution of anthropogenic emissions to localized sources could primarily rely on the density of the sensor network, or remote-sensing soundings. As discussed in Chapters 3 and 6, an extremely high density of sensors with continuous monitoring could potentially eliminate the need for inverse modeling and other atmospheric transport analyses. On the other hand, highly accurate and dense meteorological information along with sophisticated modeling techniques could greatly reduce both the number of required sensors as well as measurement frequency.

Trades associated with analytical/modeling techniques and the sensor network must primarily address the cost of sensor deployment and operation, access to the desired location, the measurement precision and accuracy, and uncertainties introduced by the analysis and modeling tools in producing the output. Driving needs are for low cost and high confidence in the final products. The drive for low cost will motivate the development of lower-cost sensors, but ultimately it will drive down the number of sensors that can be deployed and increase the need for careful system design, as discussed in Sec. 9.3.1. The drive for higher confidence in the GHGIS products may motivate use of a larger number of sensors, or remote-sensing sounding/measurement density, and reduce reliance on high-uncertainty modeling techniques.

The ability to determine and quantify anthropogenic GHG emission rates and attribute them to emission-source locations from measurements of GHG concentrations is difficult, as discussed in detail in Chapters 7 and elsewhere in this report. For some GHGs, the lifetime of the gas in the atmosphere can necessitate measurement relatively soon after its emission, which requires a measurement close to the source. Regardless of the lifetime of the gas in the air, however, atmospheric transport of the gas complicates the inference of where and when the gas was emitted. Reducing uncertainty in the estimated location, time, and amount of gas emitted is greatly benefited by measurements close to the source in space and its emission time. With a well-designed sensor network system, both the need to reduce the number of sensors (reduce cost) as well as the need to reduce the uncertainty in analysis and modeling outputs, improving performance, can be addressed.

To summarize, the key challenges that emerge in evaluating designs for GHGIS will be:

- 1. finding an appropriate balance between sensor network density, sensor type, and finding optimal sensor locations;
- 2. the sophistication of and new requirements imposed on the analysis and modeling tools given the sensor network design and available meteorological information; and
- 3. the upper bounds on the uncertainty in the results dictated by the requirements framework.

### 9.3.4 Design Challenges, Risks, and Mitigation

An effective design for ground-sensor placement will depend on sensor capability, local meteorology, location, strength of nearby GHG sources and sinks, and many other factors, as also discussed in Chapters 5, 6, and 7. Uncertainty in these factors will contribute to uncertainty in system performance. In addition, even if all these factors were well understood, an ideal site may turn out to be inaccessible, resulting perhaps from politics, sovereignty concerns, or denied-territory, in general, as much as from geography or the lack of a communications or energy infrastructure.

The performance of the deployed system will likely be different than designed and planned. As a consequence, robustness to changes in sensor placement or uncertainties in sensor performance must be a key attribute of the system design. Sensitivity analysis to sensor type, location, and performance will be essential to determining preferred system designs.

Ideal ground-sensor locations could be denied for non-technical reasons, but sensors may also be deployed to non-ideal locations for non-technical reasons. Perhaps existing weather sites provide ready power and communication infrastructure with minimal delays from approval processes. As discussed in Sec. 9.4.6, hours' notice may be given to decide where a given number of sensors are to be deployed. For all these reasons, sensor network design efforts should focus on general design guidelines for sensor type, distance between sensors, measurement sampling frequency, distance to known sources and sinks, placement relative to prevailing wind patterns, and other relevant factors.

The common theme in this section is that system design for direct GHG measurement networks should focus not on high-performance point designs, but instead on general design guidelines and the overall robustness of the system to uncertainties in ground-sensor placement and performance as well non-technical factors that influence access to desired/ideal deployment sites.

As discussed in Chapter 3, spaceborne sensors operate with different design considerations and constraints as regards their placement, which are largely dictated, in turn, by the chosen orbits. These have to trade distance from Earth's surface that determines revisit times over nadir points and aperture size for a given ground-pixel resolution, orbit inclination, relation to the sun (e.g., sun-synchronous, or not). For spaceborne sensors built to purpose, these choices must also be optimized and taken into consideration in a system sense. As discussed in Chapter 3, spaceborne sensors available today and planned for were all designed as science/research instruments focusing on specific goals and meeting the derived requirements, and not in support of a GHGIS.

Not least, GHGIS must address the danger that any improvement in system performance will likely be considered desirable. There is always a cost, however, and in such a complex system, cost will be a major constraint. Not only should the system be designed for the minimum cost that permits the requirements to be met as a driver, but the implementation plan must reflect this need. As long as the implemented system meets the system requirements, and therefore the users' needs, there will be no need for additional sensors or development of capability, unless the requirements change. Requirements creep for reasons other than meeting acknowledged new needs and requirements must be resisted.

### 9.3.5 Sensor Network Reliability Modeling and Analysis

The main questions to be addressed regarding GHGIS sensor network robustness and reliability are:

- Is it possible to detect errors in sensors, either as a consequence of instrument drift or manipulation/sabotage? In other words, how robust must the system be and in what ways able to detect such accidental or willful errors?
- If unreliable sensors are to be taken out of service, by how much is our ability to discriminate and attribute anthropogenic emissions impacted by the lack of one or more sensors? In other words, how must the system be designed and with what degree of redundancy to be able to withstand single-/few-sensor failure?

Sensor consistency and redundancy will generally be addressed at a global level. Because sensors measure the same physical processes, and often in a partially redundant manner, but not using the same technology (e.g., ground, vs. air, vs. space sensors), the system should be designed to reconstruct or predict the measurement at a given sensor, conditional on measurements from other sensors. Such techniques use spatial statistics to perform a "knock-one-out" analysis to ensure that sensor readings are consistent. Further, if multiple measurements are made simultaneously at the same site (e.g., concentrations of CO, CO<sub>2</sub>, NO<sub>x</sub>), the concentrations obey correlations, as discussed above in several contexts, which can be derived from a measurements time-series obtained at the same site. Systematic deviations from predictions based on the observed correlation (e.g., Liu et al. 2008) indicate an anomaly. Further, since satellite measurements may be available for the in situ sensor sites, they too may be used to identify anomalies. The difficulty lies in reconciling the point measurements of the in situ sensors with the column-and-footprint-averaged measurements by satellites; however, techniques to perform such comparisons between point and cell-averaged measurements/model predictions exist (Heald et al. 2004, Riccio et al. 2006) and may be adapted for the purpose.

The impact on the estimation of national anthropogenic emissions if/when sensors are removed from service, for one reason or another, is the logical follow-on to the reliability analysis described above. Inversions performed solely with in situ measurements are expected to display a sharp degradation in the accuracy of estimates given the sparseness of the network. Further, given the costs associated with a monitoring network, insufficient redundancy can be expected. However, inversions jointly conditioned on measurements from in situ (ground and air) and spaceborne sensors may be less sensitive to sensor failures. The difficulty lies in representation errors; i.e., while in situ measurements are point estimates, satellite measurements are gridboxaveraged, depending on their designed ground-altitude resolution, as discussed in Chapter 3. Initial analyses to reconcile measurements at different spatial scales have started (Heald et al. 2004, Pillai et al. 2009), and interim inversions of  $CO_2$  that mix satellite and in situ readings have been performed (Nassar et al. 2010). These techniques should be expanded in the future to allow the calculation of the sensitivity of emission estimates relative to the absence of sensors as well as initiate studies into network designs that reduce such sensitivities and vulnerabilities.

### 9.3.6 The Integrated Carbon Observation System (ICOS)

A partial list of US-government-funded data centers that collect and integrate data on GHGs and Earth science is given in Sec. 8.3.1. Section 8.3.2 describes existing analogous operational monitoring systems. The subsection discusses the system that is probably the best international analogy to GHGIS, the Integrated Carbon Observation System (ICOS) [www.icos-infrastructure.eu]. ICOS is a collaborative European carbon monitoring system still in development that "will integrate terrestrial and atmospheric observations" to "allow a unique regional top-down assessment of fluxes from atmospheric data, and a bottom-up assessment from ecosystem measurements and fossil fuel inventories." ICOS intends to provide a daily map of GHG ( $CO_2$ ,  $CH_4$ , CO, and radiocarbon- $CO_2$ ) sources and sinks at scales down to 10 km.

ICOS is currently in the "Construction Phase" and is intended to enter the "Operational Phase" in 2012 (Ciais et al. 2009). A prime user of the data products will be CarboEurope, a collaboration of European carbon cycle research programs. The sensor network consists primarily of over 40 planned atmospheric stations and ecosystem ground stations featuring standardized and modular sensor systems. Data collection is centralized, data products are available to researchers, and the user-friendly CarboScope provides summarized information on measured  $CO_2$  concentrations and estimated fluxes.

The primary differences between the goals of GHGIS and ICOS are related to the nature of the two systems (operational vs. research), scope, and the intended users. GHGIS products are intended for use not only by the international science and emissions-monitoring communities but also to generate additional data for US-policy purposes only, while ICOS is intended primarily for use by the European and international carbon cycle Earth-science research community. In contrast, GHGIS is envisioned as an operational system that primarily aims to serve as an emissions monitoring system, for treaty monitoring but also for other purposes, and therefore will integrate all sources of data relevant to monitoring; not only emissions, but also actions and the effects of actions related to mitigating, or increasing, anthropogenic emissions. Additionally, GHGIS will take a requirements-based system design approach in which observational platforms (land, ocean, air, space) as well as sensor types and locations will be driven by a design process for the fully integrated system.

Especially relevant to the GHGIS development is the ICOS experience with down-selecting hardware and the development of measurement and communication standards for sensor data. In addition, ICOS has taken a two-tiered approach in which some atmospheric stations contain the full suite of chosen sensors, and others only contain a subset. GHGIS may employ a similar design concept in which the high density of measurements is achieved through numerous less-capable observation systems, and reduced uncertainties achieved through meteorological and ecological characterization via a less dense but more comprehensive suite of observational systems.

As discussed throughout this report, GHGIS will benefit from interactions and collaborations with all GHG data centers, other information systems, and research programs focused on the measurement of GHGs and the assimilation of data to provide insights into anthropogenic emissions. ICOS provides a valuable analogy to many aspects of GHGIS and will undoubtedly

have many lessons to share as development continues. Importantly, aspects and elements of a future GHGIS can be made available to ICOS and vice-versa.

### 9.4 GHGIS Deployment and Integration

### 9.4.1 GHGIS Mission Operations Center (GMOC)

The required GHGIS capability to reliably deliver valuable and timely information products requires the operational integration and processing of all relevant data. As discussed above, valuable information can be provided through an all-source approach to integrating existing sensors and a variety of other information sources. The first step in implementing GHGIS should therefore be the design and implementation of GMOC to integrate existing relevant information sources, including GHG measurement data from data centers, meteorological data, and other types of proxy data (energy, infrastructure, remote sensing, etc.) useful for verifying actions taken to reduce overall anthropogenic emissions. Reliable access to data and data sharing protocols will need to be established.

An operational entity/agency will need to be identified to operate the GMOC and work closely with GMOC designers and developers to understand and implement the operational requirements. Computational and communication infrastructure will need to be implemented, and personnel trained to maintain operations for the GMOC. Operations and maintenance, data-integrity tags, and cybersecurity procedures will need to be implemented to ensure reliability, availability, and responsiveness requirements. More details regarding GMOC deployment were discussed in Chapter 8.

### 9.4.2 Sensor Deployment

As discussed throughout this report, the ability to attribute anthropogenic emissions to country and, perhaps, economic sector of origin with direct GHG measurement data, meteorological data, and analysis tools, as well as reconciliation with bottom-up inventory data, will require an extensive sensor network. If GHGIS is to reliably meet its long-term anthropogenic emission attribution requirements, the sensor network must be well designed, deployed, and managed as an operational asset, in concert and in tight integration with the modeling and data-retrieval components, as discussed throughout this report. This implies strict requirements on timely access to the data, data authentication to prevent tampering, standardized measurement techniques and data formatting, regular maintenance and testing to ensure reliability, redundancy of high-value sensors if discontinuity in measurements will compromise GHGIS performance, and version, calibration, verification, and validation traceability for the models employed.

Reliability requirements for sensor operation should be addressed through appropriate lifetime and environmental testing, determined by how quickly and at what cost the sensor asset can be repaired or replaced. Clearly, in the case of satellite assets, very strict environmental testing and reliability analyses would need to be performed, as is typical with operational satellites. Redundancy or backup systems should be planned in case of either launch failures or in-space failures from radiation effects, hypervelocity-particle impacts, or other causes.
## 9.4.3 Analysis-Tool Development

An initial data integration and analysis capability should be developed and implemented for the Phase 1 (3 years following project-development start) GHGIS, with software upgrades as new analysis capabilities are developed, tested, and certified. Testing and certification will need to ensure that the analysis, modeling, and simulation capabilities meet appropriate performance and QA standards. Early versions of data analysis capabilities should be developed, in collaboration with R&D efforts, to share funding resources as well as provide additional opportunities to test analysis tools. Upgrades will need to be managed to minimize downtime and meet appropriate availability and system reliability requirements.

## 9.4.4 System Interfaces

The system interfaces consist primarily of the communication links between GMOC and sensors, data centers, ground stations, and other information providers. In parallel with the design and deployment of GMOC, access to existing data and information sources must be approved and data-sharing agreements will need to be put in place. To the extent possible with existing sources of GHG data, standardized data formats, data QA/QC, and timeliness goals should be developed and pursued. It is unlikely, however, that operational requirements for reliability, availability, data authentication, and timeliness can be met using shared sensor assets, unless significant resources and motivation are provided to a data provider to serve as a "GHGIS data provider." More likely, other assets will be viewed as providing valuable additional data and information that augments the purpose-built operational sensors and other assets developed for GHGIS.

To the extent possible with resources provided to implement GHGIS, dedicated sensors should be deployed along with an adequate communication infrastructure to ensure that high-quality data will be reliably communicated for integration in GMOC. When data are gathered by personnel, as with air-flask retrieval and measurements, appropriate training and procedures must be developed and be in place to allow tracking and ensure traceability and that measurements are made and communicated in a reliable and timely manner.

Most importantly, the interface between the GMOC and the users must be carefully defined and maintained to ensure that users can obtain the information they need when they need it. With automated processing and dissemination of information products, appropriate communication procedures and infrastructure need to be developed and implemented. For user queries to be processed by the GMOC, a reliable software user interface needs to be developed and maintained, or GMOC analysts must be trained and available to interact with users to understand the need, perform the appropriate analysis, and communicate the results to the user in a timely manner as requests are received that are not already part of the automated GHGIS product-delivery suite. More details of the proposed GMOC CONOPS were provided in Chapter 8.

### 9.4.5 Lessons Learned from the International Monitoring System

There are analogies between GHGIS and the International Monitoring System (IMS) that are instructive and provide lessons learned that can benefit GHGIS development (Bowyer 2010). The IMS provides verification for Comprehensive Nuclear Test Ban Treaty (CTBT) support (Sullivan 1998) through the monitoring of airborne radionuclides as well as seismic,

hydroacoustic, and infrasound signals. Radionuclide detection stations are shown in Fig. 9-5. Similar to GHGIS, sensors are deployed worldwide with the goal of detection of the air constituent of interest and using meteorological data to attribute the release to a specific region of the Earth's surface. However, there are differences, given that IMS is intended to detect a single release that is well-localized in space in time, and it is not expected that the detected signal will consist of a strong background that must be discriminated against.<sup>1</sup> Given these differences, GHGIS will almost certainly need a much larger number of sensors and additional and new sensor types to help discriminate the anthropogenic signal from the natural/biogenic signal.



Figure 9-5. The locations of 79 of the 80 stations that encompass the radionuclide component of the International Monitoring System (IMS). The location of the 80<sup>th</sup> station has yet to be determined. Squares represent stations that can monitor radioactive particulate matter and xenon isotopes in the atmosphere. Circles represent stations with the ability to monitor radioactive particulate matter only.

Similar to the plan for GHGIS development, the number and location of radionuclide samplers were determined using modeling and predictions of detection probability given the location of the release, typical meteorological conditions, and location of the samplers. However, various influences and constraints led to the particular sampling network as it exists today. For instance, air-based collections were desired as part of the IMS. However, sovereignty concerns as well as cost restrictions contributed to the decision to not employ air-based sensors.

The data from IMS are sent to the International Data Centre for centralized processing and operations. These data contain the measurements as well as the state of health of the sensors. Given the potentially sensitive nature of the data and the potential motivation for the operating country to tamper with the data, IMS data are collected, stored securely, and transmitted with encryption keys over a dedicated private communications backbone.

<sup>&</sup>lt;sup>1</sup> An important exception to this is seismic sensing that takes place within the continuous background offered by the dynamic Earth.

There is another key difference between IMS and GHGIS that will be important to how sensors are deployed in foreign countries and how the data are collected. In the case of IMS, signers of the CTBT are aware of the IMS as an official monitoring system related to that treaty. If a country is willing to sign the treaty, it is assumed they are also willing to host IMS sensors in their country and agree to data authentication (encryption) as a means to ensure that the data can be trusted. This is more or less how it works, even though practice may have proven to be less than perfect. Since GHGIS is intended as a monitoring system related but independent of climate-change treaties, a country willing to sign a treaty to commit to GHG emission reductions may not necessarily be motivated to allow GHGIS sensors to be deployed in their country, limiting themselves to reliance on their declarations and considering it as an infringement of sovereign rights to be forced to accept monitoring in their territories.

It is not clear how best to address the issues of sensor placement in foreign countries and authenticating the data, but these issues will certainly need to be addressed. If GHGIS also serves as a US-controlled system, and those components are not part of an internationally recognized monitoring system for climate and GHG emissions treaties, then it will be important to provide incentives to countries if sensor placement in their country is important to the desired capability of GHGIS to attribute anthropogenic emissions. Alternatively, as a recourse, GHGIS may rely on spaceborne sensors, for which there is no denied territory, as well as downwind ground and air sensors that can provide sources of independent (top-down) data.

Since the intent of GHGIS is to provide reliable and trustworthy information products, data authentication must be provided for all sensors on which GHGIS relies to deliver its products as an operational system, including those deployed in the United States. If the choice is presented to deploy a sensor without data authentication or to not deploy it at all, the benefit of the additional data it can provide versus the lack of confidence and expense can be assessed on a case-by-case basis with reliance on the redundancy provided by surrounding sensors and independent corroborating data. Independent methods of detecting anomalies in data, perhaps through comparison to other sensor data, could provide an alternative to data encryption and make deployment worthwhile with or without data authentication.

Given the similarities between the IMS and GHGIS, it will be beneficial to maintain communications with the IMS and CTBT communities as GHGIS develops. Given the complexity of GHGIS, it is well worth applying the lessons of IMS to help create the highestperforming system with the fewest impediments and at the lowest cost possible.

## 9.4.6 When GHGIS Meets Its Requirements

A GHGIS will be a powerful but costly information system. It is important that GHGIS not become, nor be perceived as, a project that requires an endless source of funding to produce endless enhancements based on the latest science and technology. When GHGIS meets its system requirements, and therefore meets the needs of the users, then there is no further need for increasing the system performance, at least as long as customer needs do not dictate new requirements. In particular, if emissions agreements are successful and anthropogenic GHG emissions decrease, they will also decrease as a fraction of natural/biogenic fluxes, making the signal-to-"clutter" ratio more onerous, dictating tighter performance standards. In addition, there will be a need for continued sensor deployment to maintain system performance and reliability, such as when sensors fail or reach their predicted end of life. Additionally, if new science and technology allows for replacement of sensors that provide a significant reduction in operating and maintenance costs, then sensors may be replaced or even removed. Similarly, if improvements in meteorological information or analytic techniques allow for a reduction in the number of sensors while maintaining system performance, then costs can be further reduced. Again, the experience of the CTBT monitoring systems can serve as a guide.

# 9.5 Recommendations and Path Forward

### 9.5.1 Maintaining a System-Level Perspective

Global monitoring of emissions-mitigation actions taken to reduce anthropogenic GHGs and the effects of those actions will require an integrated and complex system. It is easy to get lost in the science, technology, data analysis and modeling, and UQ complexities and forget that the system must ultimately serve a specific purpose. The purpose of GHGIS is to fulfill a need for monitoring actions and the effects of actions related to reducing anthropogenic GHG emissions. While GHGIS will provide a plethora of other benefits, those should be treated as optional and should not allow a requirements creep to compromise attainment of the primary goal. To verify that GHGIS meets this need, it will be important to manage the design, development, and maintenance with a strong systems-level perspective.

The complexity of GHGIS will result in a cost-constrained system. An ideal combination of land, sea, air, and space observational platforms (with or without access to some foreign countries) will be cost-prohibitive. Every effort must be made to find the most cost-effective means to meet agreed-upon system requirements. Initially, the GHGIS development effort will most likely be capabilities-driven, with later development exploiting requirements-driven purpose-built components. Ultimately, the need is for reliable information as soon as possible at lowest cost, and, as discussed in this chapter and elsewhere in this report, this information may derive from many sources in addition to direct GHG measurements. These direct GHG measurements, in turn, may come from a variety of government, commercial, educational, and science-research entities. If data quality and assurance are to be achieved, cost-sharing across groups may lead to the highest performance for the cost. The importance of understanding uncertainties in the data and derived GHGIS products should not be underestimated, however. The information provided by GHGIS is intended to inform decisions for actions, and there is significant risk that misinformation will lead to misguided actions with economic, political, and environmental consequences.

To keep a system-level perspective, there must be an agency or group that *owns* the problem of negotiating requirements with users and funding agencies, trading cost with performance, schedule, and risk. Needs will change, funding profiles will change, and new opportunities will arise for gathering information through new science, technology, and computational capabilities. Tolerance for risk and the level of acceptable uncertainty in the information delivered may also change with time. The agency or group providing system engineering and integration support must keep track of the major risks and develop plans for allocation of resources to address these risks and maintain the performance and reliability of the system. This will require a variety of investments of both economic and political capital, and may include deployment of redundant

sensors, replacement of aging sensors, upgrading communication infrastructure, negotiating access to new geographical areas, standardization of measuring techniques, and much more. These efforts must be directed and purposeful, which will not happen without an agency or group that has clear ownership of the GHGIS system as a whole.

Though the proposed GHGIS relies heavily on the knowledge and capabilities of scientists, technologists, and engineers, it is important to understand that GHGIS is intended to be a useful tool, a source of valuable information that will inform decisions for high-consequence actions taken by US and foreign governments. If GHGIS provides fascinating scientific information and deploys state-of-the-art towers, aircraft, and satellites, yet fails to meet the end-users' needs, then it will have failed. As the proposed GHGIS is a highly complex system, the risk of failure to meet system requirements and user needs is high, and a systems engineering approach will be essential to mitigating risk and ensuring sufficient performance for the cost.

### 9.5.2 A Proposed Path Forward

GHGIS has the potential to provide significant value, both towards its stated purpose, but also for other purposes, not least for Earth science; however, there is much that will need to be accomplished. The recommended next steps can be roughly grouped into three parallel efforts:

- 1. What must be done to provide a valuable Phase 1 (3-year effort from project-development start) prototype GHGIS capability;
- 2. What should be started to begin developing the analysis tools and sensor network that will enable the Phase 2 (10-year) GHGIS capability; and
- 3. What would be helpful if developed by parallel, for-the-purpose efforts, as well as other science and technology R&D efforts (covered in the previous subsection).

In order to provide the Phase 1 (3-year deliverable from project-development start) prototype GHGIS capability, the following are recommended (not an exhaustive list):

- Identify users and needs and maintain communication as users and needs change;
- Design, develop, and deploy the GMOC;
- Negotiate access to existing GHG data, proxy data (energy, infrastructure...), and other relevant information;
- Design and develop purpose-built sensors of all kinds (land, air, space, and, possibly, sea), in anticipation of Phase 2 deployments;
- Develop a sensor (land, sea, air, space) network design and performance analysis tool;
- Develop sensor-network design guidelines and expand and augment existing sensor networks; and
- Support the basic R&D of next-generation modeling tools to decrease the fraction of the uncertainty budget that modeling is projected to contribute; and

• Develop and implement a basic data analysis capability to combine a priori information, self-reported inventory data, and GHG measurements to detect significant reporting anomalies.

The last two items may well prove to have the longest lead times of all operational deliverables, so this part of the work should begin first. In fact, as such a capability will impact a broad spectrum of science needs, present research, and operational activities, it is recommended that it begin as soon as possible, independently of the decision and timing to develop and deploy a GHGIS.

To begin the process of developing the Phase 2 (10-year deliverable) operational GHGIS capability, the following are recommended:

- Continuously track users and needs and maintain communication as users and needs change;
- Following on the basic-research modeling effort during Phase 1, invest in intensive model development for data retrieval and attribution of anthropogenic emission;
- Invest in sensor technology development and measurement capabilities to support an extensive sensor network;
- Collaborate with R&D efforts to develop and test new measurement technology and techniques, and new analysis and modeling tools;
- Deploy purpose-built sensors for GHGIS as soon as is feasible and budgets permit; and
- Implement operational integrated modeling and analysis tools in an iterative fashion, as budgets permit.

# Chapter 10. Conclusions

Supporting emissions-mitigation efforts and agreements, as well as energy- and fossil-fuel intensive national and global activities, would be facilitated by a process of *monitoring*, *reporting*, *verification*, and *validation* (MRV&V), as proposed by the study team in the February 2009 interagency meeting at DOE headquarters on monitoring emissions, forests, land-use, and carbon stocks. An operational greenhouse-gas information system (GHGIS) would be required if this approach is adopted and *validation* of national, subnational, or by economic sector anthropogenic emissions estimates is deemed a necessary element in such a regime.

While errors and uncertainties in fossil-fuel reports are unlikely to lead to the magnitude of the variances that the experience with  $SF_6$  and other halocarbon measurements indicate, as described in the Introduction, the truth is (1) we do not know the magnitude of the variances involved, and (2) the consequences of large uncertainties and errors can be high, especially if or when a monetary value is ascribed to emissions. In this event, some means of ascertaining that emissions uncertainties are within acceptable limits is indicated, as almost all previous studies on the subject have also concluded.

The present study examined existing and presently available capabilities that would be required for a future GHGIS. These include sensors and measurement technologies; data analysis and data uncertainty quantification (UQ) practices and methods; model-based data-inversion practices, methods, and their associated UQ; the need for traceable calibration, verification, and validation processes and attached metadata; differences between present science-/research-oriented needs and those that would be required for an operational GHGIS; the development, operation, and maintenance of a GHGIS missions-operations center (GMOC); and the complex systems engineering and integration that would be required to develop, operate, and evolve a future GHGIS.

All GHGIS components and the processes that lead to their output products, ranging from sensors, software, data-analysis, modeling and data-inversion methods and technologies, must adhere to a strict regimen of *calibration*, *verification*, and *validation*, as defined in this report. This adherence would need to be traceable and stand up to strict scientific and process scrutiny if it is to provide decision and policy support.

Present monitoring systems were developed to serve science and research needs. They would be heavily relied upon in any GHGIS implementation at the outset and likely continue to provide valuable contributions to GHGIS in the future. However, developing and supporting an *operational* GHGIS, if it is to serve its goals, will require a new approach and management, as well as sustained funding and other support.

Based on these and other findings, the study team concludes that *no component or capability presently available is at the level of technological maturity required for implementation in an operational GHGIS today*, but that purpose-designed and -built components could be developed for a future GHGIS.

While a future GHGIS would be purpose-designed, -developed, and -built as an operational decision- and policy-support system, its value to Earth and other science would be immense. An

example is provided by the International Monitoring System (IMS) in support of the Comprehensive Test Ban Treaty (CTBT) that enabled the remarkable increase in the understanding of Earth's interior and dynamics. This was acquired both in the course of the development of its sensors, their integration as parts of an operational system, and the analysis of the output data, as well as a consequence of the increase in the quality, density, and reliability of the data that flowed from it.

The study team finds that a future GHGIS could be developed in two phases, distinguished by different deliverables.

- 1. A Phase 1 implementation would be *capability-driven*, integrating capabilities, data, and products of existing available systems and would deliver a *prototype* GHGIS. This initial implementation would use existing data to define baselines, which could assist in the negotiation process. With adequate funding and other support, this could be delivered within 3 years, or so, from the beginning of its development effort.
- 2. A Phase 2 GHGIS would be *requirements-driven*, integrating sensors, their integration, data-analysis, and modeling designed and developed to purpose. With adequate funding and other support, this effort would deliver an *operational* GHGIS within 10 years, or so, from the beginning of the development effort.

The two phases have different deliverables and could commence concurrently, with the Phase 2 project benefitting from Phase 1 progress and products, as that advances.

The development effort would both need to be managed as a long-term *program* and *project* if it is to deliver on its expectation within allocated schedules and budgets. The need to bring several US government agencies together to achieve this goal poses its own challenges that can only be addressed if, at least in the US, a single agency is given the lead-role and -responsibility.

An important conclusion is that a future GHGIS can only be designed and developed as a *system* wherein components are developed and specified as *system components*. The development of all necessary components and their integration could be initiated pending a definition of requirements and resulting specifications following focused studies to produce these, followed by specific component-design studies in each case.

Requirements for a future GHGIS will almost certainly evolve with time, if global energy, industrial, and economic patterns evolve in a changing national/international regulatory/legal environments that reduce emissions. However, that is unlikely to occur in the near future, so a GHGIS development could start and proceed as indicated for today's environment and evolve in a spiral-development fashion as the environment in which it operates changes with time. An analogous situation and experience occurred with nuclear-detonation monitoring, which can serve as an example.

In conclusion, significant time and effort will be required to create a first operational GHGIS. Work needs to begin as soon as possible if the envisaged GHGIS is to begin to provide monitoring and decision-/policy-support during this decade.

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# Chapter 12. Definitions and Acronyms

### Α

ABLE	Atmospheric Boundary Layer Experiment
ACCMIP	Atmospheric Chemistry & Climate Model Intercomparison Project
ACG	Alaska (US) Coast Guard
ACOS	Atmospheric CO <sub>2</sub> Observations from Space (ACOS) NASA project at JPL
Actionable Information	Implies an analytical framework for decision making. An actionable position is supported by information and a level of uncertainty low enough to make a confident decision. Operationally, often requires two independent bases that support the same conclusion.
Acquisition (GMOC)	Data flow into the system
Acquisition (Sensor)	Collection of observables
ACRF	ARM Climate Research Facility
AFOLU	Agriculture, Forestry, and Other Land Use
AGAGE	Advanced Global Atmospheric Gases Experiment
ARIES	AIRS Follow-on mission concept
AIRS	Atmospheric Infra-Red Sounder
AMERIFLUX	(North) American FLUXNET
AMS	Accelerator mass spectrometry
Analyst (GMOC, External)	A person possessing the technical competence and domain familiarity to properly process and analyze greenhouse gas data
Analyst (GMOC, Internal)	A person possessing all of the qualities of an external analyst. In addition, this person possesses familiarity with GMOC software, monitors the system, evaluates data, runs models, and produces technical products.
ANNEX-1 parties	<ul> <li>(to the UNFCCC) These include the industrialized countries that were members of the OECD in 1992, plus countries with economies in transition (the EIT Parties), including the Russian Federation, the Baltic States, and several Central and Eastern European States. Specifically: Australia, Austria, Belarus*, Belgium, Bulgaria, Canada, Croatia*, Czech Republic*, Denmark, Estonia, European Union, Finland, France, Germany, Greece, Hungary, Iceland, Iteland, Italy*, Japan, Latvia, Liechtenstein*, Lithuania, Luxembourg, Malta, Monaco*, Netherlands, New Zealand, Norway, Poland, Portugal, Romania, Russian Federation*, Slovakia*, Slovenia*, Spain, Sweden, Switzerland, Turkey*, Ukraine*, United Kingdom of Great Britain and Northern Ireland, United States of America.</li> <li>* Denotes a party for which there is a specific COP and/or CMP decision. http://unfccc.int/parties_and_observers/parties/annex_i/items/2774.php</li> </ul>

AOS	Atmospheric Observing Systems
AQUA	NASA spacecraft (hosts AIRS, TES, and other instruments)
Archive	Long-term data storage
ARCTAS	Arctic Research of the Composition of the Troposphere from Aircraft and Satellites
ARM	(DOE) Atmospheric Radiation Measurement (sites/laboratories)
AROC	Area under the Receiver Operating Characteristic Curve
ASCENDS	Active Sensing of $CO_2$ Emissions over Nights, Days, and Seasons. Earth Decadal Survey space mission
ASC	Advanced Simulation & Computing (DOE/NNSA program)
ASCI	Accelerated Strategic Computing Initiative (DOE/NNSA program)
A-SCOPE	Advanced Space Carbon and Climate Observation of Planet Earth. ESA Candidate mission concept under the Earth Explorer Opportunity Missions program. Uses active laser for sensing
ASP	Atmospheric Science Program (DOE-SC)
ASTER	Advanced Spaceborne Thermal Emission and Reflection Radiometer) is an imaging instrument flying on Terra, a satellite launched in December 1999 as part of NASA's Earth Observing System (EOS)
Attribution	Determination of what country, location, or modality (anthropogenic vs. natural/biogenic) is responsible for observed emissions
Automated/Automatic	Operations performed by software or processes that do not require human intervention
Availability	The degree to which a system or component is operational and accessible when required for use. This is often expressed as a probability. http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=00159342
В	
Baseline	Year or other reference used to measure changes in emissions, or emissions mitigations
BAU	Business-as-usual (path)
BER	Office of Biological and Environmental Research (DOE-SC)
BMA	Bayesian Model Averaging

#### С

<sup>13</sup> C	carbon 13 (isotope)
<sup>14</sup> C	carbon 14, radiocarbon (isotope)
CALNEX	California Nexus (of air quality and climate change)
CAMS	Center for Accelerator Mass Spectrometry (LLNL)
CARB	California Air Resources Board
CarbonSat	Carbon Monitoring Satellite. One of two ESA Candidate mission concepts for launch in 2018 under the Earth Explorer Opportunity Missions (EE-8) program.
CarbonTracker	A CO <sub>2</sub> model-retrieval system (developed by ESRL)
CARES	Carbonaceous Aerosols and Radiative Effects Study
CARIBIC	Civil Aircraft for the Regular Investigation of the Atmosphere Based on an Instrument Container
CASA	Carnegie-Ames-Stanford Approach biosphere model
CCGG	Carbon Cycle Greenhouse Gases
CCMVal	Chemistry-Climate Model Validation Activity
CDIAC	Carbon Dioxide Information Analysis Center, operated by ORNL for the US DOE. Includes the World Data Center for Atmospheric Trace Gases
CEM	Continuous Emission Monitoring
CESM	Community Earth System Model (developed by NCAR and DOE)
CEQ	Council on Environmental Quality (The White House)
CGO	Cape Grim Observatory (Southern Hemisphere)
CH <sub>4</sub>	methane
CITE	Chemical Instrumentation Test and Evaluation experiments
C-LAMP	Carbon Land Model Intercomparison Project
CN	Carbon Nitrogen model (NCAR)
СО	carbon monoxide
$CO_2$	carbon dioxide
CO <sub>2</sub> e	Carbon dioxide equivalent (per GWP, cf. Table 1-1)
Composite Product	A compilation of complementary products

CONOPS	Concept of Operations; describes the characteristics of a proposed system from the system user's point of view
Continuous data	Data that arrive as they become available or delivered. These data do not have a specified retrieval time defined, but instead stream in, as needed.
CONTRAIL	Comprehensive Observation Network for Trace gases by AirLiner
CrIS	Cross-track Infrared Sounder
CTBT	Comprehensive Test Ban Treaty
CRDS	Cavity Ring-Down Spectroscopy/Spectrometer
CSIRO	Commonwealth Scientific and Industrial Research Organisation (Australia)
CTBT	Comprehensive Test Ban Treaty
CV&V	Calibration, verification, and calibration (cf. Chapter 1 and Appendix B)
D	
DAAC	Distributed Active Archive Center
DAKOTA	Design Analysis Kit for Optimization and Terascale Applications (SNL- developed software package)
Data Processing	Operations performed on data, either by software or an analyst
Decision	A commitment of resources utilizing a known uncertainty that is irrevocable or revocable only at some cost
Derived Product	A product that is the result of analyzing and processing data (e.g., running models, creating trends, etc.)
DESDynI	Deformation, Ecosystem, Structure and Dynamics of Ice. Earth Decadal Survey space mission
Discrimination	Differentiating between one type of source, or another, e.g., anthropogenic vs. natural/biogenic greenhouse-gas sources
DNS	Direct Numerical Simulation: best effort to solve the exact (differential) equations of motion with no modeling, or parameterizations
DOE	(United States) Department of Energy
DOE-SC	Department of Energy Office of Science
E	
ECMWF	European Centre for Medium-Range Weather Forecasts
ECV(s)	Essential Climate Variable(s)

EEA	European Environmental Agency (EEA) that also maintains the Emissions Database for Global Atmospheric Research (EDGAR)
EIA	(US DOE) Energy Information Administration
EIT Parties	(Nations with) economies in transition
Emission Factor	Ratio of chemical emitted to fuel burned in a combustion process
Emissions	Materials (gases, particles, vapors, chemical compounds, etc.) discharged from smokestacks, chimneys, tailpipes, etc. http://cdiac.ornl.gov/pns/glossary.html
EOS	Earth Observing System
EPA	(US) Environmental Protection Agency
ESA	European Space Agency
ESRL	(NOAA) Earth System Research Laboratory
EU	European Union
EU ETS	European Union Greenhouse Gas Emissions Trading Scheme
F	
FC(s)	Fluorocarbon(s)
FIA	Forest Inventory Analysis
Flexibility	The ease with which a system or component can be modified for use in applications or environments other than those for which it was specifically designed. http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=00159342
FLUXNET	Flux Network (for CO2, water, energy, and methane)
FOV	Field of view
FTIR	Fourier Transform Infrared Spectroscopy
FTS	Fourier Transform Spectroscopy/Spectrometer
FPAR	Fraction of absorbed Photosynthetically Active Radiation
G	
GASP	Global Atmospheric Sampling Program (NASA)
GAW	Global Atmospheric Watch
gC	grams carbon
gCeq	grams carbon equivalent
GC&E	Global Change & Energy

GC-FID	Gas Chromatography Flame Ionization Detector
GCHN	Global Historical Climatology Network
GCM	General Circulation Model
GCMS	Gas-Chromatography Mass Spectrometry
GCOS	Global Climate Observing System
GCP	Global Carbon Project
GDP	Gross domestic product
GEO	Geosynchronous Earth Orbit
GeoFTS	(Proposed) geosynchronous FTS mission
GEOS	Goddard Earth Observing System Model (NASA)
GEOS-chem	A CTM developed at Harvard
GE WEX	Global Energy and Water Cycle Experiment
GE OSS/GEOSS	Global Earth Observation System of Systems
GFDL	Geophysical Fluid Dynamics Laboratory (NOAA)
GHG	Greenhouse gas. In the context of GHGIS, this refers to the key gases often referenced by the IPCC: F-gases, carbon dioxide, methane, and nitrous oxide.

See Introduction (Chapter 1) of this report for a detailed discussion. Image below provides the basis for the gases listed above. N<sub>2</sub>O F-gase 60 b) a) CH 14.3 49.0 50 44.7 GtCO<sub>2</sub>-eq / yr 0 0 0 0 39.4 35.6 CO<sub>2</sub> (deforest decay of biomass, 17.3% s, etc) CO<sub>2</sub> (other) 2.8% c) Energy supply 25.9% Forest 17.49 10 0 Agriculture 13.5% 1970 1980 1990 2000 2004 CO2 from deforestation, decay and peat CO2 from fossil fuel use and other sources Industry 19.4% tial and cial buildings CH4 from agriculture, waste and energy N2O from agriculture and others comm 7.9%

GHGIS	Greenhouse-gas information system (defined in this report)
GIM	Geospatial Inversion Method

GISS Goddard Institute for Space Studies (NASA)

This image is Figure 2-1 from the figures listing for this publication: http://www.ipcc.ch/publications\_and\_data/publications\_ipcc\_fourth\_assessment\_repo rt\_synthesis\_report.htm.

GMAO	Global Modeling and Assimilation Office (NASA)
GMOC	GHGIS Missions Operations Center
GNIP	Global Network Isotopes in Precipitation
GOSAT	Greenhouse gases Observing Satellite (JAXA)
GtC	gigatons of carbon
GTE	Global Tropospheric Experiment
GWP	Global Warming Potential cf. Table 1-1 and related discussion)
н	
HadCM	Hadley Centre Coupled Model (UKMO)
HFC(s)	Hydrofluorocarbon(s)
HDFn	Hierarchical Data Format <i>n</i>
HIPPO	HIAPER Pole-to-Pole Observations
HYSPLIT	Hybrid Single Particle Lagrangian Integrated Trajectory model (NOAA)
I	
IAGOS	In-Service Aircraft for the Global Observing System
IAEA	International Atomic Energy Agency
IASI-A	Infrared Atmospheric Sounding Interferometer-A, built by CNES and scheduled to be launched in 2012 on the METOP-A satellite
IASI-B	Infrared Atmospheric Sounding Interferometer-B, built by CNES and scheduled to be launched in 2012 on the METOP-B satellite
IASI-C	Infrared Atmospheric Sounding Interferometer-C, built by CNES and scheduled to be launched in 2016 on the METOP-C satellite
IBUKI	JAXA greenhouse-gas monitoring satellite
ICOS	Integrated Carbon Observation System
IEA	International Energy Agency
IGBP	International Geosphere-Biosphere Program
IGCO	Integrated Global Carbon Observation System
IKONOS	Commercial Earth observation satellite, providing panchromatic and multispectral imaging. Launched in 1999, owned and operated by GeoEye (US – formerly OrbImage)

IMPACT	Integrated Massively Parallel Atmospheric Chemical Transport model (DOE)
IMPACTER	IMPACT Emission Retrieval system (DOE)
IMPROVE	Interagency Monitoring for Protection of Visual Environments
IMS	International Monitoring System (supports the CTBT)
INFLUX	Indianapolis Flux Experiment
Integrity	The degree to which a system or component prevents unauthorized access to, or modification of, computer programs or data. http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=00159342
Inventories	Listing of greenhouse-gas emissions sources and sinks for which a country is accountable
IOC-UNESCO	Intergovernmental Oceanographic Commission (UNESCO)
IPCC	Intergovernmental Panel on Climate Change
IPSL	Institute Pierre Simon Laplace (Paris, France)
IR	Infrared
IRMS	Isotope ratio mass spectrometry
J	
JAL	Japan Airlines
JASON	US government consulting group
JAXA	Japan Aerospace Exploration Agency
JPL	Jet Propulsion Laboratory (NASA), California Institute of Technology
JPSS	Joint Polar Satellite System
к	
KOMPSAT-2	KOrean MultiPurpose SATellite. A very-high-resolution imaging satellite owned by the Korean Aerospace Research Institute (KARI)
L	
LAI	Leaf Area Index
LANL	(DOE) Los Alamos National Laboratory
LANL LANDSAT	(DOE) Los Alamos National Laboratory A series of Earth-observing satellite missions jointly managed by NASA and the US Geological Survey (Department of the Interior). First launch, 1972.

LBL, LBNL	(DOE) Lawrence Berkeley (National) Laboratory
LEO	Low Earth Orbit
LIDAR	Light Detection and Ranging (or Laser Radar)
LLNL	(DOE) Lawrence Livermore National Laboratory
LNG	liquid natural gas
LTAN	Local Time of Ascending Node
LULUC	Land-use/land-use change
М	
MAGICC	Measurement of Atmospheric Gases Important to Climate Change
MATCH	Model of Atmospheric Transport and Chemistry (a CTM developed at NCAR)
mb	millibar (unit of pressure)
MCI	Mid-Continent Intensive
MEDEA	US Government consulting group
Metadata	Data describing data
MEO	Medium (altitude) Earth Orbit
MicroCarb	CNES Mission concept to monitor CO <sub>2</sub> in the atmosphere
Mid-Trop	Middle Tropospheric (altitude)
MILAGRO	Megacities Impacts on Regional and Global Environment
MM5	Mesoscale Model version 5 (Penn State/NCAR)
MOC	Mission Operations Center
MODIS	Moderate resolution Infrared Sounder
Monitor	Observe and check the progress or quality of (something) over a period of time; keep under systematic review. Maintain regular surveillance over.
MOZAIC	Measurement of Ozone and Water Vapor by Airbus In-Service Aircraft
MOZART	Model of Ozone And Related Tracers (a CTM developed at NCAR)
MRI	Meteorological Research Institute (Japan)
MRV	Monitoring, reporting, and verification
MRV&V	Monitoring, reporting, verification, and validation
Mt	Mega ton = $10^6$ tons

Ν

$N_2O$	nitrous oxide
NACP	North American Carbon Program
NAS	National Academy of Sciences
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research
NDIRS	Non-dispersive infrared spectroscopy
NDVI	Normalized Difference Vegetation Index
NEC	National Economic Council (The White House)
NEE	Net Ecosystem Exchange
NEON	National Ecological Observing Network
NH	Northern hemisphere
NIES	National Institute for Environmental Studies (Japan)
NIST	National Institute of Standards and Technology
NNSA	(DOE) National Nuclear Security Administration
NO <sub>x</sub>	Oxides of nitrogen, e.g., NO and NO <sub>2</sub>
NOAA	National Oceanic and Atmospheric Administration
NOGAPS	Navy Operational Global Atmospheric Prediction System
NPP	NPOESS Preparatory Project
NPOESS	National Polar-orbiting Operational Environmental Satellite System
NRC	National Research Council
NSF	National Science Foundation
NxOy	Oxides of nitrogen with one, or more, nitrogen atoms, e.g., NO, NO <sub>2</sub> , N <sub>2</sub> O, N <sub>2</sub> O <sub>4</sub> , N <sub>2</sub> O <sub>5</sub> , etc.
NWS	National Weather Service (NOAA)

0	
0C0	Orbiting Carbon Observatory; first NASA spacecraft/instrument of this type that failed at launch (February 2009)
OCO-2	Orbiting Carbon Observatory 2. NASA spacecraft scheduled for launch on February 2013
OCO-WF	Orbiting Carbon Observatory – Wide Field
OECD	Organization for Economic Cooperation and Development
O&M	Operations and maintenance
OMI	Ozone Monitoring Instrument
OPMS	Ozone Mapping and Profiling Suite
Operational	In the context of GHGIS, an operational system is comprised of high reliability and traceability, verified and validated components (algorithms/models/tools), automated processing pipelines, offline processing capabilities, secure system guaranteeing data/product integrity, and historical tracking to support reanalysis and reprocessing.
Operational	Pertaining to a system or component that is ready for use in its intended environment, or pertaining to a system or component that is installed in its intended environment. Pertaining to the environment in which a system or component is intended to be used. http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=00159342
Operator	A class of users with a thorough understanding of the system for which that user is responsible; one who operates a system.
OrbView	A commercial constellation of global imaging satellites owned and operated by GeoEye (US)
ORCHIDEE	ORganizing Carbon and Hydrology In Dynamic EcosystEms (IPSL)
ORNL	Oak Ridge National Laboratory
OSC	(US DOE) Office of Science
OSSE	Observation Systems Simulation Experiment
OSTP	Office of Science and Technology Policy (of the US President)
Р	
PanFTS	Panchromatic Fourier Transform Spectrometer
Parameter	In the context of GHGIS, this could be an aggregated representation of collected data. As an example, concentration is a parameter, but models use values such as an average of concentrations. This leads to decisions involving the appropriate level of discretization to apply to concentrations.

PBL	Planetary Boundary Layer
PCMDI	Program for Climate Model Diagnosis and Intercomparison (DOE)
PCP	Programmable compressor package
PEM	Pacific Exploratory Missions
PFCs	Perfluorocarbon(s)
PFP	Programmable flask package
Pg	petagram (or gigaton, Gt)
Pipeline	A software or hardware design technique in which the output of one process serves as input to a second, the output of the second process servers as input to a third, and so on, often with simultaneity within a single cycle time. http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=00159342
PNNL	Pacific Northwest National Laboratory (DOE)
ppb	parts per billion
ppbv	parts per billion by volume
PPPI	Pre-Planned Product Improvement
ppm	parts per million
ppmm	parts per million by mass
ppmv	parts per million by volume
PTR-MS	Proton Transfer Reaction Mass Spectrometry
Pre-Sentinel-5	Sentinel-5 precursor mission. ESA satellite with an UV-NIR payload planned to provide gap fill climate data between ENVISAT and Sentinel-5 (2013–2019/2020)
Processing	A sequence of steps performed for a given purpose. http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=00159342
Product	Some output of the system
Provenance	Descriptive methodology to trace data and operations through a complex process
Q	
QA	Quality Assurance
Quality (Data)	The degree to which data meet specified requirements or customer needs or expectations (e.g., data are non-spurious; data come from a sensor that is functioning properly). http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=00159342

Quality (System)	The degree to which the system meets specified requirements or customer needs or expectations. http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=00159342
Quality Control (QC)	A procedure or set of procedures intended to ensure that a manufactured product or performed service adheres to a defined set of quality criteria or meets the requirements of the client or customer. http://whatis.techtarget.com/definition/0,,sid9_gci1127382,00.html
QuickBird	Commercial Earth Observing Satellite operated by DigitalGlobe (US), Launched in 2001
R	
RAMS	Regional Atmospheric Modeling System (CSU)
RapidEye	Commercial Optical imaging satellite constellation (5 satellites) owned and operated by RapidEye AG (Brandenburg an der Havel, Germany)
Raw data	Unanalyzed, unprocessed data
Real-Time	Pertaining to a system or mode of operation in which computation is performed during the actual time that an external process occurs, in order that the computation results can be used to control, monitor, or respond in a timely manner to the external process. http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=00159342
Reliability (System)	The ability of a system or component to perform its required functions under stated conditions for a specified period of time. http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=00159342
RHGDP	Real Historical Gross Domestic Product
ROIC	Read-Out Integrated Circuit
ROC	Receiver Operating Characteristic (curve)
S	
SA	Sensitivity Analysis
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY (ESA)
Sectoral	(attribution). Attribution of emissions, or other related activities to a particular economic sector, e.g., transportation, concrete or steel production, power generation, etc.
Sensitivity Analysis	Computation of the effect of changes in input values or assumptions on the output
Separatrix	Dividing line/criterion
SCR	Signal-to-clutter ratio

SF <sub>6</sub>	Sulfur hexafluoride, a gas with a very high GWP (cf. Table 1-1) that is inert, hardly soluble in water, with very small natural sources. It is widely used in the electric grid network as a spark-arrestor (dielectric) gas, an inert gas in casting magnesium, as a space filler for double-pane windows, and also used in the semiconductor industry.
SiB	Simple Biosphere model
SIO	Scripps Institution of Oceanography (UCSD)
SMAP	Soil Moisture Active/Passive (Earth Decadal Survey mission and NASA space mission of record)
SNL	Sandia National Laboratories (DOE)
SNR	signal-to-noise ratio
SO <sub>2</sub>	sulfur dioxide – typically co-emitted with fossil-fuel combustion.
SOA(s)	Secondary Organic Aerosol(s)
SODAR	Sonic Detection and Ranging
SPOT	Satellite Pour l'Observation de la Terre (CNES Optical Observation Satellite)
State of Health	Provides information on the operational status of the station and the quality of the raw monitoring data transmitted from the station. These are supplementary data provided by sensors connected to, or associated with, equipment and instrumentation at the station. http://www.ctbto.org/glossary/?letter=s&cHash=5c9e417f18
STC	Supplemental type certification
STILT	Stochastic Time-Inverted Lagrangian Transport model
SWAP	Size, Weight, and Power (payload specifications)
т	
TCCON	Total Carbon Column Observing Network
TEA	Target-Elevation Angle
TES	Thermal Emission Spectrometer (instrument on board the EOS-Aura spacecraft)
TM5	Tracer Model version 5 (developed by several institutes in Europe)
TOMS	Total Ozone Mapping Spectrometer (space sensor)

Traceability	The degree to which a relationship can be established between two or more products of the development process, especially products having a predecessor-successor or master-subordinate relationship to one another; for example, the degree to which the requirements and design of a given software component match. The degree to which each element in a software development product establishes its reasons for existing; for example, the degree to which each element in a bubble chart references the requirements that in satisfies. http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=00159342
TRACE-A	Transport and Chemistry near the Equator in the Atlantic experiments
TRACE-P	Transport and Chemistry Evolution over the Pacific
TRANSCOM	The Atmospheric Tracer Transport Model Intercomparison Project
U	
UAV	Unpiloted Air Vehicle
UCSD	University of California at San Diego
UKMO	United Kingdom Met Office
Uncertainty Analysis	Computation of the total uncertainty induced in the output by quantified uncertainty in the inputs and models, and the attributes of the relative importance of the input uncertainties in terms of their contributions. Morgan, M.G., and M. Henrion 1990 Uncertainty: A Guide to Dealing with Uncertainty in Quantitative Risk and Policy Analysis (Cambridge University Desce), p. 20
Uncertainty	The quantitative characterization of uncertainties in applications
Quantification (UQ)	also providing a metric for uncertainty reduction
UNFP	United Nations Environment Programme
UNESCO	United Nations Educational, Scientific and Cultural Organization
UNFCCC	United Nations Framework Convention on Climate Change
UQ	Uncertainty Quantification
USDA	US Department of Agriculture
USFS	US Forest Service
USGEO	US Group on Earth Observations
UT/LS	Upper Troposphere or Lower Stratosphere

#### V

Validation (model)	Confirmation that a model represents reality to an acceptable, or adequate level of fidelity (e.g., are the right equations being solved?). See Section 1.8 and Appendix C for a full discussion.
Validation (software/ algorithm/system)	The process of evaluation a system or component during or at the end of the development process to assess whether it satisfies the specified requirements (e.g., does the system perform as required when tested against its intended environment?). See Section 1.8 and Appendix C for a full discussion. http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=00159342
Verification (model)	Confirmation that the mathematical equations employed by the model are solved self-consistently and correctly. See Section 1.8 and Appendix C for a full discussion.
Verification (software/ algorithm/system)	The process of evaluating a system or component to determine whether the products at a given phase satisfy (are consistent with) the requirements imposed at the start of that phase. See Section 1.8 and Appendix C for a full discussion. http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=00159342
VIIRS	Visible/Infrared Imager/Radiometer Suite
VNIR	Visible and near-IR parts of the spectrum
Verification (treaty)	Assessment of compliance against treaty terms or requirements, e.g., adherence to obligations and reporting processes
VOC(s)	Volatile Organic Compound(s)
w	
WMO	World Meteorological Organization
WRF	Weather Research and Forecasting model
WRI	World Resources Institute

## Appendix A. Bottom-up Emissions Inventories – Attribution by Time, Space, Economic Sector

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Disturbance of the natural, global cycling of carbon among the atmosphere, biosphere, and hydrosphere has been and is driven by human activities that release carbon from geologic deposits of fossil fuels and that change the amount of carbon contained in plants, plant debris, and soils. Carbon is released to the atmosphere in both cases, principally as carbon dioxide (CO<sub>2</sub>) but also as methane (CH<sub>4</sub>). While it remains a scientific challenge to understand and quantify the impact of human actions on the carbon stores of the biosphere, it seems straightforward in principle, and perhaps in fact, to inventory the amount of carbon released from the oxidation of fossil fuels. Because of the economic importance of fossil-fuel consumption, records have long been maintained on at least a portion of the fossil fuel that is produced and traded.  $CO_2$  is also released to the atmosphere when limestone (CaCO<sub>3</sub>) is calcined to produce cement or other industrial products, but the emphasis in this appendix is on the far larger amount of carbon released from fossil-fuel oxidation. Emphasis here is also on  $CO_2$ , the dominant infrared-absorbing gas responsible for human impact on the Earth's energy balance.

Although the completeness and quality of the data are extremely variable around the word, and the uncertainty often large, there are considerable data on how much fossil fuel is produced and traded. Most of these data are at the scale of countries and years. Fossil-fuel data exist mostly in terms of the physical units of production and trade - mass or volume - but it is possible to approximate the amount of carbon involved. For coal and natural gas there is a strong correlation between the energy content of the fuel and the carbon content, and because there is primary interest in the energy content, it is generally possible to estimate the carbon content even when the carbon content is infrequently measured. For liquid fuels there is strong correlation between the carbon content and both the energy content and the density so it is again generally possible to make reasonable estimates of the carbon content. Because CO<sub>2</sub> is the equilibrium product of fossil-fuel combustion, the amount of CO<sub>2</sub> emitted can, in principle, be estimated from the carbon content of the fuel and the fraction of fuel that is oxidized during use. Historically there was considerable fuel left unoxidized from, for example, coal-fired locomotives, and now a large fraction of fossil fuel is used for non-fuel purposes like lubricants, solvents, and synthetic materials. In general, the amount left unoxidized from fuel uses has been decreasing with time while the amount used for non-fuel purposes has been increasing with time. Most so-called "bottom-up" inventories of CO2 emissions - inventories based on ground-level estimates of emission processes - are based on data on energy consumption and are at the scale of countries and years, the scale at which most energy data are maintained.

Estimates of  $CO_2$  emissions to the atmosphere at the global scale thus rely on estimates of how much fuel is consumed, our understanding of average fuel chemistry, and estimates of the fraction of fuel consumption that results in actual oxidation of the fuel. Estimates at the country scale call on national data on fuel production, consumption, and trade. To estimate  $CO_2$  emissions at finer spatial and temporal scales encounters a variety of additional data and

accounting challenges. In general, "the task of high resolution emission models is the allocation of annual national totals to small spatial and temporal scales" (Thiruchittampalam et al. 2010).

Emissions of CO<sub>2</sub>, of course, occur at the place and time that fossil fuels are actually oxidized and this is only partially reflected by economic data on fuel production, consumption, and trade. Actual consumption within a given space and time can be estimated from "apparent consumption," which is equal to production plus imports minus the total of exports, decreases in stocks on hand, and bunker fuels – where bunker fuels are those fuels loaded for trading between regions. Consumption can also be estimated with surveys of fuel users, sales data, physical measurements of fuel delivered to a specific combustion process, or models of fuel-consuming processes. In all of these approaches there are inherent accounting problems and uncertainties, which can be illustrated with two examples. For an automobile, there are inherent challenges and uncertainties in the sales data, but even then the fuel is not oxidized at the time and place of the final sale, and fuel purchasers may drive across the boundaries of statistical regions (e.g., country, state, county, company, ...) to purchase fuel that is slightly less expensive. Similarly, a coal-fired power plant may purchase fuel as opportunity or economics permit, but oxidize it in response to the instantaneous demand for power. All fuel streams have some physical heterogeneity and for many the flow rate can vary widely over short time intervals.

The sources, magnitude, and nature of uncertainty will change as the spatial and temporal scale of bottom-up emissions inventories change. In general we expect that uncertainty will increase as the temporal and spatial scale decrease – the exception to this may be for large point sources of emissions where it becomes practical to install monitoring equipment that can continuously measure emissions. Even for continuous emissions monitoring systems – such as those at large power plants in the United States – there are challenges in measuring the  $CO_2$  content and flow rate of turbulent exhaust gas streams (see, for example, Ackerman and Sundquist 2008; see also Pétron et al. 2008).

Still, there are important reasons to want bottom-up inventories at a variety of time and space scales. In the text that follows we characterize briefly efforts to inventory emissions by country, by some sort of global spatial grid, by month, by state, and by space and time scales that approach kilometers and hours. Some of these have been pursued to produce global coverage, others for specific national or other purpose, some as a one-time view, and some with continuous coverage. Times lags for providing estimates can vary from the minutes required to run computer models to the 2+ years required to compile national surveys. We note that the spatial distribution of emissions includes three dimensions because the dispersal and potential measurement of emissions will differ for high-altitude emissions from aircraft or the higher injection level of emissions that emerge from tall stacks or at elevated temperatures.

There are currently four organizations that produce systematic, global, annual estimates of  $CO_2$  emissions from fossil-fuel consumption: the Carbon Dioxide Information Analysis Center (Boden et al. 2010), the International Energy Agency (IEA 2010), the Energy Information Administration of the US Department of Energy (US DOE 2010), and a joint effort of the Joint Research Center of the European Commission and the Netherlands Environmental Assessment Agency called EDGAR (Emissions Database for Global Atmospheric Research, van Aardene et al. 2010). In general these estimates agree with each other, for both global and national emissions, and with national estimates produced by the major developed countries, within about

 $\pm$  5%. See, for example, IEA (2010), Macknick (2009), Marland et al. (1999, 2007, 2009), and Ciais et al. (2009) for developed countries. Differences can be much larger for developing countries with less commitment to data collection and reporting.

These compilations start with energy data from different sources, but ultimately all of the energy data come from national or corporate reporting. Energy statistics compiled by the IEA and the United Nations Statistics Office, for example, are now collected from countries with a common and shared survey form. Nonetheless the various international statistics are subject to differences in emphases, categories, unit conversions, and processing within the host organizations. The international statistics compilers are also left to fill in the blanks when nations provide incomplete data or do not respond at all (a common occurrence in Africa, for example).

The first efforts to distribute CO<sub>2</sub> emissions within countries searched for proxy data that would reflect the internal distribution of energy use within countries and focused on population density to represent the spatial distribution, but stuck with annual sums. Recognizing that large point sources of emissions from power plants and refineries are not distributed identically to population and that differences such as those related to climate and urbanization lead to significantly different patterns of energy consumption, population density nonetheless was adopted to give an indication of within-country distribution of energy use that could be used in a consistent way across all countries. Subsequent analyses on the United States, where there is considerable data at the sub-country level of states and the sub-annual level of months (Blasing et al. 2005a, 2005b, and 2007) show that there are variations within the United States, in per capita emissions, that reach an order of magnitude; and yet population still seems a useful proxy when there no other consistent data are available on which to distribute emissions within countries. The pattern of distribution within a country can be useful, but the uncertainty can be quite large for a given point. As noted by Oda and Maksyutov (2010), "population statistics provide only diffuse approximations of the spatial distribution of potential sources."

Both the Carbon Dioxide Information Analysis Center (CDIAC) (Andres et al. 1996) and EDGAR (van Aardene et al. 2010) used data on population density to derive estimates of global emissions on a 1° latitude  $\times$  1° longitude grid. EDGAR now goes a step further in trying to distribute some emissions from international bunker fuels along the primary routes of international commerce while the CDIAC gridded data sum to something less than the global total because of the omission of the small fraction (order of 4%) of emissions that come from bunker fuels. In its most recent releases, EDGAR now uses data for large point sources to help distribute emissions within countries and, as of 2009, estimates emissions on a  $0.1^{\circ} \times 0.1^{\circ}$  degree grid. To the extent that distribution is based on population density it, of course, depends on the population data set selected and the year for which the population data were compiled. Data for population density are not available for all years and preparing gridded time series data sets will rely on the availability and choice of data sets. As in many of the comparisons one might undertake, some care is required in comparing gridded data because treatment of components such as emissions from cement manufacture, natural-gas flaring, and non-fuel uses of hydrocarbons are not uniform. Data from large point sources are typically based on capacity and/or annual load and the user is challenged to ensure first that the location is correct and then to estimate accurately the appropriate fraction of operating capacity and the distribution of this fraction with time. Bringing a power plant down for maintenance, for example, can have a very large impact on the temporal profile of emissions at that particular location and on the

distribution of emissions across a region if the load is increased at other generators to make up for the loss at the facility in maintenance.

As noted, the estimated distribution of emissions within some large countries can be improved with energy data at the level of states and provinces, but where these data are available it is still mostly annual data. The finest temporal scale at which real data on energy consumption are widely available is monthly, and monthly data tend still to be available in only a few countries and over only short time spans, and not necessarily for all fuels. Andres et al. (2010) have recently constructed a global data set of emissions by month but this required extensive mathematical analysis to complete and extend time-series data and to establish proxies for places where there were no energy data to work from. Gregg et al. (2009) were able to estimate emissions over North America by both state and month.

Other efforts to distribute emissions at a scale finer than national have now focused on satellite observations of night lights as a proxy for the density of energy consumption and thus of CO<sub>2</sub> emissions. In the case of Oda and Maksyutov (2010), night-lights data are supplemented with data from large point sources. As for the use of data on population density, a problem with the data on large point sources is the limited amount of data available, i.e., for only a few recent years. Oda and Maksyutov (2010) emphasize that night-lights data correlate with human activity best in developed countries and that the data do not indicate temporal variability. Oda and Maksyutov include emissions from fuel ethanol and biodiesel but do not include international bunker fuels or natural gas flaring. Rayner et al. (2010) use an assimilation system to combine night-lights data with data on population density and they believe that, at least for the one region they tested (the United States), the result is superior to using population density alone. They are not able to examine the temporal variation of emissions and write that "we are unlikely to find proxies for the temporal variation in overall source so we will be forced to impose temporal structures derived from intensive observations at a few points." Rayner et al. (2010) do not include emissions from gas flares, bunker fuels, or cement manufacture. The lack of an independently generated measure of emissions from fossil-fuel consumption at relevant spatial and temporal scales makes objective comparisons of the different distributions problematic.

There are now at least two ongoing efforts to provide high-resolution emissions estimates by identifying "indicators, which are capable of describing the spatial pattern of the emissions sources." (Thiruchittampalam et al. 2010, see also Gurney et al. 2009, Pregger et al. 2007). These include details on point, line, and area sources such as the locations and capacities of power plants and industrial facilities, the locations and traffic volumes of roads, the location of residential areas, etc. To refine temporal resolution, sector-specific time profiles are used – monthly, weekly, and hourly. The process is very demanding of location and fuel-specific data. Estimates for Germany and Western Europe have been prepared at the University of Stuttgart and the Vulcan project has prepared a high-resolution data set for the United States.

The Vulcan project (www.purdue.edu/eas/carbon/vulcan) has quantified emissions for the United States at the scale of 100 km<sup>2</sup> and hours. The Vulcan effort is one that did not start by disaggregating US national emissions data, but it succeeded in achieving similar numeric totals by aggregating up from sectoral, census, and proxy data and using air-pollution models. It is process-level and fuel-specific (48 fuels). Although aspirations are global, the data demands are very high and to date the inventory is limited to the continental United States and to year 2002.

The Vulcan system is able to utilize detailed data from continuous monitoring at power plants. Gurney et al. (2009) provide a useful perspective by suggesting that uncertainty could be "as high as 16% at the state level and 50% at the county level."

In comparing different existing data sets on  $CO_2$  emissions it is clear that there are very different approaches but that these are often in response to different needs and goals. Rayner et al. (2010) are explicit that their need is for a globally homogeneous product and that many of the intensive data sources used for some regional or national inventories are not available globally. Their interest is in generating the structure of global emissions over the longest possible time series. Dealing with the uncertainty at a point is quite different from being concerned with global patterns. A large uncertainty at one point may be of great importance for monitoring treaty compliance but of little importance if it merely represents small spatial error in a scientific modeling framework. Different objectives are reflected in that some inventories report emissions by sector whereas others focus on emissions by fuel. Studies of mitigation strategies will likely prefer the former while studies of carbon isotopes will likely prefer the latter. The challenges and uncertainties of finer spatial and temporal scales are quite different, but can be linked. Proxy data will be important and fine temporal scales will almost necessarily rely on models of the emissions generating processes. Independent atmospheric measurements will provide important constraints and cross-checks.

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## Appendix B. Surface Fluxes from Concentrations

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A gas-species concentration field in the atmosphere is governed by the fluid dynamic equations, augmented by surface and volume sources and sinks – the latter if the gas-species is produced or destroyed chemically, photochemically, etc. In particular, the transport equation for a gas-species  $\alpha$ , away from the surface, is given by

$$\frac{\partial}{\partial t}\rho Y_{\alpha} + \nabla \cdot \rho \mathbf{u} Y_{\alpha} = \omega_{\alpha}, \qquad (B-1a)$$

where  $\rho = \rho(\mathbf{x},t)$  is the atmospheric density field [kg/m<sup>3</sup>],  $Y_{\alpha}(\mathbf{x},t)$  is the  $\alpha$ -species mass-fraction field, such that  $\rho Y_{\alpha} = \rho_{\alpha}$  is the  $\alpha$ -species density field [ $\alpha$ -species-kg/m<sup>3</sup>],  $\mathbf{u}(\mathbf{x},t)$  is the flow velocity vector field [m/s], and  $\omega_{\alpha}(\mathbf{x},t)$  is the net (volume) source/sink strength, i.e.,  $\alpha$ -species kg/(m<sup>3</sup>·s), by chemical reactions, photolysis or photosynthesis, etc.

The  $\alpha$ -species transport equation is expressed in terms of its *mass*-fraction field,  $Y_{\alpha}(\mathbf{x},t)$ , i.e., kg of  $\alpha$ -species per kg of atmosphere, and not the mole-fraction field,  $X_{\alpha}(\mathbf{x},t)$ , that may be what is measured. The equation may also be expressed in terms of the mole-fraction field, but, if it is to remain exact but in that form, is complex for a variable-composition atmosphere. The contribution of molecular diffusion to  $\alpha$ -species fluxes at the scales of interest is negligible and was omitted from Eq. B-1a (see Dimotakis 2005, for example, for a more detailed discussion).

Equation B-1a is *linear* in the  $\alpha$ -species mass-fraction  $Y_{\alpha}$ . Also, subtracting any constant from it, such as the previous year's value,  $Y_{\alpha 0}$ , leaves the equation unaltered,

$$\frac{\partial}{\partial t}\rho(Y_{\alpha} - Y_{\alpha 0}) + \nabla \cdot \rho \mathbf{u}(Y_{\alpha} - Y_{\alpha 0}) = \omega_{\alpha}.$$
(B-1b)

Integrating over a (fixed) cell volume  $V_c$  [m<sup>3</sup>], as indicated by the cell denoted by solid edges in Figure B-1, with a bottom (ground) bounding surface of area  $A_0$  [m<sup>2</sup>], four vertical surfaces ( $A_i$ , i = 1,4) and a top surface  $A_5$ , then yields

$$S_{\alpha} = \int_{A_0} s_{\alpha} dS = \dot{m}_{\alpha} + \left\{ \sum_{i=1,5} \int_{A_i} \right\} \rho(Y_{\alpha} - Y_{\alpha 0}) \mathbf{u} \cdot d\mathbf{S} - \Omega_{\alpha} .$$
(B-2)

In this expression,  $S_{\alpha}$  [kg/s] is the total  $\alpha$ -species ground-surface flux of interest over the gridcell ground-surface area  $A_0$ , from natural and anthropogenic sources combined, with  $s_{\alpha}(x,y;t)$  the time-dependent surface flux field [kg/(m<sup>2</sup>·s)] with x and y the coordinates along the ground surface,  $m_{\alpha}$  the time-rate of change of the total  $\alpha$ -species mass in  $V_c$ , the braces add the flux

<sup>&</sup>lt;sup>1</sup> Paul Dimotakis served as JPL's Chief Technologist at the beginning of this effort. He has since returned to his position as a full-time member of the Caltech faculty, continuing his association with JPL as a Senior Research Scientist.

contribution over the surface integrals of the five bounding surfaces of  $V_c$  in the atmosphere (four vertical sides plus the top), and  $\Omega_{\alpha}$  is the  $\alpha$ -species net source in the grid-cell volume  $V_c$ .

Equation B-2 can be summarized by summing the vertical- and top-surface fluxes to produce the total out-bound and in-bound flux from and into the grid-cell volume  $V_c$ , i.e.,

$$S_{\alpha} = \dot{m}_{\alpha} + \mathcal{F}_{\alpha, \text{out}} - \mathcal{F}_{\alpha, \text{in}} - \Omega_{\alpha} . \tag{B-3}$$

In other words, the total  $\alpha$ -species grid-cell ground-surface flux,  $S_{\alpha}$ , i.e., the flux contributed through the grid-cell bottom area,  $A_0$  [m<sup>2</sup>], is equal to the rate of increase in the  $\alpha$ -species mass accumulating in  $V_c$ ,  $\dot{m}_{\alpha}$  [kg/s], plus the difference between the outgoing and incoming  $\alpha$ -species flux through the facets in the air, less any net production by volume sources.



Figure B-1. Schematic of grid-cell volume  $V_c$  over urban terrain, showing the ground-level surface  $(A_0)$ , the four vertical facets  $(A_1, ..., A_4)$ , and the top surface  $(A_5)$ , as well as the wind field, u(x,t), in blue and the surface-flux field,  $f_a(x,y;t)$  in red. Indicated grid cells are aligned with the compass directions. Imagery (Google Earth, 2 April 2011) is of Pasadena, CA, with the San Gabriel Mountains to the north (top).

Importantly, if the top facet of grid-cell volume is above the day-time planetary boundary layer ceiling, typically less than 2.5 km above the surface, then the surface-emissions distribution,  $s_{\alpha}(x,y;t)$ , and their total  $S_{\alpha}$ , will not contribute any net flux through the top surface,  $A_5$ , that sees only background concentration levels and, as a consequence,  $A_5$  will not enter in the tally, if over reasonably flat terrain or other circumstances that can create updrafts up to such an altitude.

Three major challenges are manifest in these expressions:

1. For carbon dioxide (CO<sub>2</sub>), its addition to  $V_c$  above the present-day background concentration of  $X_{CO2,0} \cong 380$  ppmv (parts per million by volume), or  $Y_{CO2,0} \cong 580$  pmmm (parts per million by mass), is a small fraction of  $Y_{\alpha 0}$ , i.e.,  $(Y_{\alpha} - Y_{\alpha 0}) \ll Y_{\alpha 0}$ , so the flux from ground-level by emissions is a small part of the background flux entering and

exiting  $V_{c}$ . The calculation must then deal with differences between large numbers so even small errors in either can dominate the quantity of interest increasing its uncertainty.

If the mole fraction above background that comprises the signal, i.e.,  $\Delta X_{\text{CO2}} = (X_{\text{CO2}} - X_{\text{CO2,0}})$ , must be known to within, say, 5%, and emissions sources have increased the local mole fraction by  $\Delta X_{\text{CO2}} \approx 10$  ppmv above  $X_{\text{CO2,0}}$ , which may be typical in an urban environment,  $X_{\text{CO2}}$  must be measured to a precision<sup>2</sup> no less than 0.5 ppmv.

- 2. This challenge is compounded by the amplitude of the anthropogenic contribution to surface fluxes that is 6 to 8% of the (averaged) total natural/biogenic contributed by Earth's land area (e.g., Figure B-2).
- 3. If the wind field is not solved as part of the same model/code that processes concentration data, it must be provided by other means. A fractional uncertainty in the wind field,  $\mathbf{u}(\mathbf{x},t)$ , translates into the same fractional uncertainty in  $S_{\alpha}$ . Both  $|\mathbf{u}(\mathbf{x},t)|$  and  $(Y_{\alpha} Y_{\alpha 0})$  are at the same level of significance (linear) in Eq. B-2. For a sufficiently tall grid-cell volume, negligible volume sources/sinks ( $\Omega_{\alpha} = 0$ ), and an approximately uniform wind-field speed,  $\langle |\mathbf{u}(\mathbf{x},t)| \rangle_{V_c} = U$ , the total surface emissions flux over the grid-cell bottom (ground-surface) area  $A_0$  can be approximated by at steady state ( $\dot{m}_{\alpha} = 0$ ),

$$\mathcal{S}_{\alpha} \simeq \left[ \left\langle \varrho(Y_{\alpha} - Y_{\alpha 0}) \right\rangle_{\text{in}} - \left\langle \varrho(Y_{\alpha} - Y_{\alpha 0}) \right\rangle_{\text{out}} \right] U A_{\perp} \,. \tag{B-4}$$

In this expression,  $\langle \varrho(Y_{\alpha} - Y_{\alpha 0}) \rangle_{in}$  and  $\langle \varrho(Y_{\alpha} - Y_{\alpha 0}) \rangle_{out}$  denote the atmospheric density times the  $\alpha$ -species mass fraction over its background/reference value, averaged over the windward- and leeward-facing facets, respectively, and  $A_{\perp}$  denotes the projection of the grid-cell area in the direction perpendicular to the wind vector. As measurements of GHG concentrations improve by densifying the sensor network or improving measurement accuracy/precision, or both, uncertainties in resolved wind-field data will likely dominate the surface-flux uncertainty budget.

It may appear that too many quantities must be provided as input to Eq. B-2 through B-4 for a solution of the ground flux  $S_{\alpha}$ . However, these quantities are not independently provided to each grid-cell. Considering grid-cell volumes adjacent to  $V_c$ , i.e., to its north, east (right), south, west (left), and on top, it can be seen that the flux out of the east facet of the grid-cell to the west (left cell with dashed edges), is the flux through the west facet of  $V_c$  of area  $A_4$  (cf. Figure B-1). Similarly for the other  $V_c$  facets. Fluxes in the air must be inverted as part of a system of equations to infer ground fluxes. Of greater challenge is the estimation of  $\dot{m}_{\alpha}$  when there are transients in the total  $\alpha$ -species mass in  $V_c$  that only time-dependent data can help specify.<sup>3</sup>

The data inversion and attribution part of the analysis must contend with differences between large numbers to estimate surface fluxes, and, further, must attempt to attribute a small part of

<sup>&</sup>lt;sup>2</sup> *Precision* rather than *accuracy* is required here because common-mode errors will cancel when using *differences* in measured quantities in the conservation equations.

<sup>&</sup>lt;sup>3</sup> There can be transient increases (or decreases) in  $\alpha$ -species mass in a grid-cell volume, such as from emissions that produce an *accumulation* of  $\alpha$ -species in  $V_c$ , e.g., an increase in the average  $Y_\alpha$  in  $V_c$ , because a power plant has begun emitting and the pocket of air with the excess concentration has not reached the  $V_c$  bounding surfaces, or because the overall density  $\rho(\mathbf{x},t)$  is increasing in  $V_c$  because the temperature is falling, or some combination of such effects (however,  $m_\alpha = 0$  at steady state).

that difference to anthropogenic fluxes with acceptably small uncertainties. Equation B-4 provides the basis for direct estimation from concentration measurement data (coupled with provided wind-field data), with uncertainties traceable to measurement accuracy and resolution (Chapter 6) and wind-field uncertainty, while various methods for implicit integrated data-inversion analyses are discussed in Chapter 7.

In today's measurement-poor environment, data density (space-time sampling frequency) is an important consideration. Generally, one can have no more independent pieces of output information than the input data allow, or one has an underdetermined system. Ideally, one prefers to have more information degrees of freedom in the data in than the data out to allow for some optimization, such cost-function minimization, to provide a best fit. In an important example in Chapter 7 on modeling, samples measured at several locations downwind were used to infer the location of a *single* source (Algeciras), discriminating between priors based on this assumption (see Figure 7-4 and related discussion).

Prior models of natural/biogenic and anthropogenic surface-emission distributions are employed that cover large patches of land. They are denoted as  $s_{pr}$ , or  $s_{\alpha,pr}$  (or  $S_{\alpha,pr}$  depending on whether the distribution within a cell is resolved or not) in Chapters 1 and 7. Models run forward in time and invert concentration data from various sources, seeking agreement between measured concentration data and upwind surface fluxes, in the sense of Eqs. B-1 through B-4. In this approach, emissions are estimated in terms of factors that multiply prior patch-emissions models,  $s_{pr}$ , as required to produce a balance of the  $\alpha$ -species flux in the volume  $V_c$  over that patch and as discussed in Chapter 7. For these techniques to be reliable, the dependence of the results on particular choices of prior source distributions needs to be weak, i.e., driven by measurement data and less by prior assumptions. As discussed in Chapter 7, this is not the case today.

Providing surface-emissions estimates for every pixel in a global grid would require as many pieces of information from measurement (and other) data as there are pixels. Even if the spatial resolution of this grid was  $(100 \text{ km})^2$ , i.e., ~ 1° latitude × 1° longitude, it would require ~ 64,000 pieces of information over Earth's surface. Approximately 20,000 pieces of information would be required at the same grid resolution, if emissions were to be estimated over the total land surface only. As discussed in Appendix A, in its most recent releases, the Emissions Database for Global Atmospheric Research (EDGAR) uses data for large point sources to help distribute emissions within countries and, as of 2009, provides estimates of emissions on a refined grid of  $0.1^{\circ} \times 0.1^{\circ}$  (~ 10 × 10 km<sup>2</sup>), increases the number of pixels by two orders of magnitude. Fortunately, a large fraction of Earth's land surface does not host significant anthropogenic emissions sources as a result of land type, land use, and other considerations (Figure B-2).


Figure B-2. Composite image of Earth's land mass from space (Mercator projection). Graphic courtesy of NOAA/USGS/MODIS.



Figure B-3. Population density map. Courtesy of NASA (http://veimages.gsfc.nasa.gov/116/pop\_density.jpg), 20 May 1999.

A second parsing and prioritization into global and national areas of interest to the Greenhouse Gas Information System (GHGIS) derives from population density. That is often used as a surrogate (factor) in modeling (local) energy production and fossil-fuel use (cf. discussions in Chapter 7 and Appendix A).<sup>4</sup> This is depicted in Figure B-3, based on 1999 data, and illustrates global population-density inhomogeneity.

<sup>&</sup>lt;sup>4</sup> Population density can be used as a surrogate after national/regional adjustments for per-capita energy/fossil-fuel use.



Figure B-4. Night lights, as seen from space. Courtesy of NASA (http://visibleearth.nasa.gov), 23 January 2000 data.

Similar inferences can be drawn from images of night lights from space (e.g., Oda and Maksyutov 2010), as illustrated in Figure B-4. The similarities, but also differences, between the distributions indicated in Figures B-3 and B-4 are quite revealing and important for GHGIS and other contexts. They also indicate the sense in which population and night lights can serve as surrogates for energy use, albeit scaled by various factors. Finally, Figures B-3 and B-4 attest to the great inhomogeneity of land use, as well as energy use per unit area, per capita, etc.

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# Appendix C. Calibration, Verification, and Validation

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This appendix discusses the *calibration*, *verification*, and *validation* (CV&V) concepts, as they apply to the Greenhouse Gas Information System (GHGIS) elements described in Chapter 1 and referred to throughout this report.

## C.1 Calibration

A few examples may be helpful in assessing the role of calibration as it applies to the GHGIS components, and to clarify the concept.

#### C.1.1 Sensor Calibration

Consider a temperature sensor that is part of an in situ ground sensor that measures a particular greenhouse gas (GHG) concentration, say, carbon dioxide (CO<sub>2</sub>). If a thermocouple is used as the transducer in a thermometer needed to augment the measurement, it may have a stated accuracy of  $\Delta T = \pm 2$  K in the temperature range of interest from its manufacturer, if assembled and connected to the signal amplifier and data-acquisition system per manufacturer instructions and specifications. However, most of this uncertainty derives from manufacturing variations (impurities in the metals welded to form the thermocouple junction), extraneous bimetallic contacts in the wiring between the thermocouple junction and the input to the signal amplifier that may not be balanced or not exposed to matched temperatures along the thermocouple signal chain, or variations in gain and offsets in the signal amplifier chain and digital-to-analog (D/A) converter. These extraneous potential sources of error need not invalidate the fundamental dependence of the thermocouple sensor output voltage on, and its linear response to, temperature, so a calibration that sets two calibration constants, e.g., an offset voltage  $(V_0)$  and thermocouple sensor system sensitivity s = dT/dV, i.e., the temperature difference per unit output voltage change (kelvin per volt), can yield accuracies of  $\Delta T = \pm 0.10$ -0.15 K. This is at least possible in a laboratory environment, if a suitable calibration against (NIST-traceable) standards is made part of the measurement process, e.g., if it is performed just before and right after every temperature measurement recorded to ensure that extraneous effects have been accounted for and that the measurement itself was not compromised. However, if the order-of-magnitude reduction in measurement uncertainty described above is to be relied upon, the thermocouple-based temperature measurement to estimate the GHG concentration (mole-fraction) for GHGIS purposes<sup>2</sup> must be accompanied by calibration-data tagging and tracking. This is so that if the

<sup>&</sup>lt;sup>1</sup> Paul Dimotakis served as JPL's Chief Technologist at the beginning of this effort. He has since returned to his position as a full-time member of the Caltech faculty, continuing his association with JPL as a Senior Research Scientist.

<sup>&</sup>lt;sup>2</sup> In the case of CO<sub>2</sub>, for example, some in situ sensors described elsewhere in the report measure the total number of CO<sub>2</sub> molecules in a particular volume (e.g., optical cavity interior). Converting that measurement to a CO<sub>2</sub> mole fraction ( $X_{CO2}$ ) to an accuracy of 0.1 to 0.2 ppmv that some of these sensors are capable of requires accompanying

data are questioned, a concurrent but independent, or even subsequent, calibration (if drift with respect to time is not an issue) becomes part of the uncertainty quantification (UQ) of the resulting temperature data. Further discussion on this topic is included in Chapter 6.

The example above describes a simple sensor (a thermocouple-based thermometer) that produces a single output measurement that (mostly) depends, in turn, on the quantity measured. Spaceborne remote sensors, such as the National Aeronautics and Space Administration (NASA) AIRS and OCO remote sensors discussed in Chapter 3, are instruments whose output is a complex function not only of the measured quantity, say,  $X_{CO2}$  that is averaged over a particular horizontal ground pixel, vertical sampling kernel, and integration time, but of other quantities and environmental parameters that must also be estimated if they are to yield a measurement of the desired quantity (cf. Chapter 3 and Appendix E). Calibration of such instruments requires the quantification of the dispersive relation,<sup>3</sup> i.e., where (on which pixel) each wavelength ( $\lambda$ ) lands on the detector array and its uncertainty, and the quantification of the detector response (e.g., nV/photon for each  $\lambda$ ) for each pixel and its uncertainty. For a spaceborne sensor to be qualified for flight, these calibration steps must be performed on the ground, before launch, in appropriate thermal-vacuum chambers that simulate the space environment.

The calibration results become part of the remote-sensing measurement data analysis archive. However, regardless of the care and quality of engineering implemented on the spacecraft, differences between the ground testing environment and the (changing) space environment (e.g., entering in and coming out of eclipse, depending on orbit), as well as drifts with time as components age under exposure to space radiation, require continuous on-board calibration, equivalent to (but more complex than) the before-and-after calibration steps described in the simple thermocouple-based thermometer example above. In the case of AIRS, slow drifts (low-frequency noise) in the mercury-cadmium-telluride (HgCdTe) detector are addressed by a calibration step *after every spatial sweep*, using an on-board, National Institute of Standards and Technology (NIST)-traceable black-body source, whose emission spectrum was also calibrated before launch. The per-sweep calibration data that derive from this procedure become part of the data-analysis sequence and metadata, and, along with the data-retrieval process that leads to the AIRS sensing accuracy for CO<sub>2</sub> of 1 to 2 ppmv that was established by *calibration*, in concert with *verification* and *validation* steps described below.

The importance of tracking and maintaining calibration information that accompanies all sensor data cannot be overemphasized. The following example, based again on the AIRS instrument discussed above, illustrates the case.

Following the 2002 launch of NASA's AQUA spacecraft that hosts the AIRS and other Earthobserving instruments, and during the in-space sensor-calibration phases, it was noted that, *at times*, the instrument returned anomalous results that could not be reconciled with the data uncertainty bounds previously established. After some effort, the anomalous readings were correlated with times when the spacecraft trajectory took it over the Sahara and, to a lesser extent, the Australian desert (cf. Figure B-2). It was assessed that very slightly higher thermal

measurements of temperature and pressure to convert the measurement, if the accuracy is to stay within the in situ instrument uncertainty budget for the  $X_{CO2}$  measurement/estimation.

<sup>&</sup>lt;sup>3</sup> Both the AIRS and OCO instruments rely on grating (as opposed to Fourier-transform) spectrometers.

loads from infrared (IR) emissions from the two hot deserts resulted in an estimated *sub-micron* dimensional deformation of the spectrometer frame. The on-board calibration provision and the fact that the measured spectrum comprises molecular (IR) emissions that provide absolute wavelength fiducials (photon frequency, or wavenumber  $k = \text{cm}/\lambda_0$ , with  $\lambda_0$  denoting the photon wavelength in vacuum, to be more precise), allowed the small effect to be included as a systematic and quantifiable correction in the data-analysis sequence. The low uncertainty levels established the rest of the time were then found to also extend to times corresponding to overdesert passages of the spacecraft.<sup>4</sup>

Spaceborne sensors pose particular challenges since, once launched, they are inaccessible and must include in their design, implementation, and operation the means to accommodate and compensate, to the extent possible, for potentially unexpected effects in a systematic and quantifiable manner. This, of course, is not always possible, and efforts made for such provisions contribute to the cost of spacecraft. Such complications typically contribute to the time delay between successful orbit insertion and when reliable data retrievals derive from the space sensor. They must be taken into account in designing and planning for an operational GHGIS, as discussed in Chapter 3 and elsewhere in this report. Continuing post-launch health-monitoring, calibration, and validation of space sensors using air and ground sensors becomes important in this context.

### C.1.2 Data Analysis and Retrieval Calibration

Measurements are seldom of (just) the quantities needed. Measurement data need to be analyzed to estimate the specific quantities of interest, along with their uncertainties. Calibration is also often needed to quantify the results.

Returning to the in situ CO<sub>2</sub> concentration-sensor example, an issue with transmitting and using such concentration data is the assignment of the estimated measurement volume and shape,  $V_{\rm m}(t)$ , of the parcel of air convected past the sensor and sampled, over which the  $X_{\rm CO2}(t)$  mole fraction was averaged to produce  $\langle X_{\rm CO2}(t) \rangle_{Vm(t)}$ , as also discussed in Chapter 5. If the measurement is a flask-type measurement from a ground sensor, mounted on a land tower at a fixed location (e.g., latitude, longitude, and sensor aspirating opening altitude above ground), the size and shape of  $V_{\rm m}(t)$  will depend on the vector wind field during the measurement time interval,  $\tau_{\rm m}$ , centered at  $t_0$ , i.e., the interval  $t_0 - \tau_{\rm m}/2 \leq t \leq t_0 + \tau_{\rm m}/2$ , as depicted in Figure C-1.

The in situ measurement of the average  $X_{CO2}(t)$  over the volume  $V_m(t)$ , i.e.,  $\langle X_{CO2}(t) \rangle_{Vm(t)}$ , will likely be assigned to the (centered) measurement time,  $t_0$ . However, the data must be accompanied by other quantities, such as sufficient wind-field data needed to estimate  $V_m(t)$  – not just its size – during the measurement averaging time interval,  $t_0 - t_m/2 \leq t \leq t_0 + \tau_m/2$ , as well as possibly other quantities, such as the temperature (and pressure) history during the sampling time, T(t) and p(t), as noted above. The data analysis that accompanies the CO<sub>2</sub> mole fraction measurement must include a convective estimate of  $V_m(t)$  and must, itself, also be calibrated by comparing the data analysis results with a known  $V_m(t)$ . To illustrate the point, if the measurement is taken during a windy day and in situ sensor is exposed to a wind speed of, say, 10 m/s (~ 20 knots), and the sampling time interval is  $\tau = 1$  min (time to fill a flask), the

<sup>&</sup>lt;sup>4</sup> This account is based on a private communication with H. (George) Aumann and M. Chahine of Caltech/JPL.

streamwise extent of  $V_{\rm m}(t)$  would be 0.6 km, which is not necessarily small when compared with local CO<sub>2</sub> concentration-gradient length scales.

This simple arithmetic assumes that the wind vector has not (substantially) changed direction during  $\tau_m$ ; otherwise, more complicated wind-field data would be required to estimate the sampling volume associated with the particular measurement that may well not be available. Whether this represents a serious shortcoming or not can be assessed only through a system calibration that takes the data analysis and how the data are used into account. In particular, since land towers are, for the most part, under the terrestrial planetary boundary layer (PBL) ceiling during daytime hours, the wind field in the PBL will be turbulent and intermittent, producing a complex  $V_m(t)$  more likely to resemble the one depicted in Figure C-1, rather than a linear tube implied by the steady 10 m/s wind-speed example above.



Figure C-1. Schematic of a sampled air-parcel volume,  $V_m(t)$ , shaded in blue, over which the measurement is made, convected past a tower-mounted in situ ground sensor at the location indicated by the cross-hairs by the wind field at the time  $t_0$ , during the sampling time interval  $(t_0 - \tau_m/2, t_0 + \tau_m/2)$ .

The flow in the daytime PBL is typically unstably stratified and, when it is, is dominated by upwelling drafts of (positively) buoyant plumes responsible for considerable homogenization under the PBL ceiling, but also downwelling drafts that bring upper-layer air in which the concentration of  $CO_2$  is uncorrelated with surface-emissions sources. In this case, it is possible that the appropriate  $V_m(t)$  for a particular measurement sample may not even contain air that originated near the emissions source.

Attributing a CO<sub>2</sub> concentration measurement during daytime hours is a complex proposition whose data analysis and calibration remain research topics at this writing. In contrast, the night-time PBL is typically stable (the ground is cooler) and one expects atmospheric waves, as in any stably stratified flow, rather than a collection of upwelling and downwelling plumes. As a consequence, attribution at night is a simpler proposition, and while careful calibration procedures can provide important information to help the data analysis and attribution to sources later in the GHGIS processing sequence, the challenges are fundamental and real. Calibration, in this case, may require a complex test-bed environment in which source locations and their emissions fluxes are known and are surrounded by a suite of ground, air, and space sensors, so establishing what is needed, at a minimum, for correct attribution can be assessed. Such test beds are proposed and described elsewhere in this report.

The examples above illustrate that while the location of in situ sensors may be well known, their measurements can sample significant air-parcel volumes that must be quantified themselves, perhaps using additional measurements that must themselves be *calibrated*, and processes to allow complete and correct data analysis. In particular, they cannot always be considered as representing *point measurements*, in either space or time.

The data analysis for in situ measurements recorded from an airborne platform face similar challenges, except that, in that case, the air speed convecting the sampling volume past the sensor input is dominated by that of the aircraft. At a cruising altitude of 35 kft, for example, an aircraft moves at about Mach = 0.8 or so, or at speeds in the range of 200 to 240 m/s. A similar measurement of an air sample acquired over a minute would then be a measurement that samples an airtube volume,  $V_m(t)$ , that is approximately 12 km long.<sup>5</sup> The corresponding issues for remote-sensing measurements and atmospheric sampling from space (Chapter 3 and Appendix E), or high-flying aircraft (Appendix H), are more complex yet and beyond the illustration purposes of the brief discussion offered here.

#### C.1.3 Sensor and Subsystem Operating Software Calibration

As implied in the introductory definition, calibration extends to sensor and subsystem operating software. By way of a previous example, software that operates a spaceborne instrument will include adjustable constants, such as an instrument's dispersion relation vs. wavelength, and the wavelength-dependent sensitivity of each pixel in the instrument's detector, along with real-time analysis of the raw data to produce the downlink bit stream. Such constants and the ensuing analysis incorporate the results of pre- and post-launch calibration processes, as discussed above. Instrument-operating software calibration would then check whether the results of the calibration were correctly incorporated in the integrated hardware-software system, i.e., whether it can reproduce the calibration results.

#### C.1.4 Calibration of Data Quality Assurance/Quality Control and UQ Processes and Methodologies

Data quality assurance/quality control (QA/QC) and UQ processes can set uncertainty bounds on the compiled and reconciled data. As discussed in Chapter 6, this part of the data-analysis process will need to reconcile measurement data from disparate sources, from sensors that measure GHG concentrations and other auxiliary quantities on different grids, with different accuracies/uncertainties, and with different sampling volumes  $V_m(t)$ . The challenge is illustrated by the need to compare and combine data from ground, air, space, and, possibly, sea sensors.

The large range of spatial and temporal scales will almost certainly be the result of serious undersampling of the GHG concentration and other fields. Satisfying the Nyquist sampling criterion, for example, will almost always prove infeasible. While there are approaches and methods for handling undersampled field data, they require additional (explicit or implicit) assumptions. Calibration of those assumptions and approaches will be needed through comparison with measurement data to check the correctness of the methods employed. This could be done, for example, by withholding randomly selected independent data from the input data stream and comparing predicted values with the excluded data values. Variances would need

<sup>&</sup>lt;sup>5</sup> Fortunately,  $CO_2$  concentration fields are nearly uniform at aircraft cruising altitudes, so even though  $V_m(t)$ , in this case, is of much greater extent, this is not likely to present GHGIS with an issue. More important, however, as noted in Chapter 4 and in the discussion on the PBL above, is that a concentration measurement significantly above the PBL is not readily attributable to surface emissions sources because of the complex stratified and unstratified mixing environment in the lower troposphere, the jet stream aloft, and complex inter-layer fluxes.

to statistically fall within the estimated uncertainty bounds to calibrate (and validate, as discussed below) the data UQ process and the resulting data UQ values.

#### C.1.5 Modeling and Data-Inversion Code Calibration

As the discussion on modeling above and in Chapter 7 suggests, *calibration* of codes can, and must be, performed to determine values for adjustable parameters that best fit the data. The two important caveats above apply, however, namely that for parameterizations employed that are not physics-based, while adjusting available parameters will always increase goodness of fit, the applicability of the resulting code (with parameters, resulting in uncertainties that are difficult to quantify in different environments. The challenge is particularly acute because the interest in GHGIS is near the surface, with transport in the unstably or stably stratified PBL (for day or night transport, respectively), for which adequate general parameterizations are not available, at least during daytime hours where energy and industrial productions peak, along with attendant fossil-fuel emissions.

A parenthesis is opened here to provide an example that will help with calibration, as it applies to modeling. The example describes a common parameterization and illustrates the point. The subgrid-scale (SGS) flux,  $\mathbf{j}_{\alpha}$ , of some species  $\alpha$  (say, CO<sub>2</sub>) is often modeled as proportional (scaled) with the gradient  $\nabla c_{\alpha}$  of its concentration  $c_{\alpha}$ , i.e.,

$$\mathbf{j}_{\alpha} = -\mathcal{D} \, \nabla c_{\alpha} \,. \tag{C-1}$$

The diffusivity,  $\mathcal{D}$ , in this context, is accepted as a proportionality that is either constant, or modeled as a function of local flow properties, and called the "*eddy*, or *effective*, *diffusivity*," or,  $\mathcal{D}_{eff}$ , to be used in place of  $\mathcal{D}$ . The model embodied in Eq. C-1, with some effective diffusivity,  $\mathcal{D}_{eff}$ , is referred to as the "gradient-transport" model for species transport and is inspired by the (correct) relation for molecular diffusion fluxes, but with the (actual) molecular diffusivity,  $\mathcal{D}$ . One can measure the (subgrid vector) flux of a particular species by measuring (subgrid) flow vector velocity fluctuations and the concentration of the species of interest, as well the (subgrid vector) species concentration gradient. If the proposed parameterization were valid, the ratio of the (magnitudes) of the two vectors would be found to be in a fixed ratio that could be determined by calibration, *and* the two vectors would always be aligned.

For several reasons, reality does not support either part of this hypothesis for macroscopic species transport in turbulent flow.

In the molecular-diffusion case, species are transported and diffuse by molecular collisions that occur on (mean-free-path) spatial scales much smaller than the macroscopic transport scales of interest, rendering the diffusive-flux model exact in the limit, with the molecular diffusivity,  $\mathcal{D}$ , a well-defined *thermodynamic* (flow-independent) quantity that is (and must be) positive definite (otherwise entropy-production from spontaneous mixing processes would be negative). The molecular diffusivity,  $\mathcal{D}$ , can be measured, or calculated *ab initio* in simple cases, e.g., from the kinetic theory for gases. In the atmosphere, eddies responsible for species (and other) transport span the full extent of the spatial scales across which SGS fluxes must be estimated, invalidating

the hypothesis and the attendant parameterization. In fact, species-transport fluxes can often be *counter*-gradient ( $\mathcal{D}_{eff}$  negative at times); flow and small-scale eddies are driven by other dynamics and are agnostic about the concentration gradients of passive species they transport, but can be correlated with them in stratified or atmospheric flows, for example. While subgrideddies span only a single grid cell, it is the transport across that cell that would need to be parameterized and the same difficulties (and objections) obtain.<sup>6</sup>

A calibration of a numerical code with such parameterizations can be undertaken by comparing numerical-code results and predictions with data, and adjusting the values of parameters, such as  $\mathcal{D}_{eff}$ , to produce a best fit. However, if the approximations and parameterizations do not represent an acceptable approximation of physics/reality, even matching data (typically, select and undersampled data) in a particular instance and environment, does not necessarily imply that values set for the various adjustable parameters will yield simulation results that can capture different realizations.

An example is offered by the dynamics of the PBL discussed above. A parameter fit to daytime data, for example, would not yield a numerical code likely to be successful in capturing night-time transport. Perhaps one might rely on different day and night parameterizations, or models, relying on different calibrations for each.<sup>7</sup>

While the fundamental challenges are clear, they can only be assessed, in turn, by calibration and attempts at validation. Specifically, a particular parameterization may be difficult to *verify*, i.e., assessed to be implemented consistently in the code, and *validate*, i.e., agree with reality in all environments in which the code will be used. However, it may be that, for GHGIS purposes, uncertainties in the results of the data inversion using the calibrated numerical code may be dominated by other uncertainties, e.g., uncertainties in the convecting wind field that may typically be provided as an input to the transport modeling, and which may not be computed itself as part of the model. In other words, while the validity of a particular parameterization may be questionable, the *sensitivity* of the results to it may be low, and, as a consequence, the variance from reality resulting from the particular parameterization may not be material to the adequacy of the source attributions in a GHGIS product and will set lower bounds to the uncertainty of the corresponding GHGIS inversion and product. Whether this is a concern, or not, can only be established by comparing results with reality in controlled experiments, such as those described as part of proposed test-bed efforts elsewhere in the report. While success there may not guarantee success in general, failure would be definitive.

In the context of modeling, modeling UQ, and data-inversion and attribution steps in the GHGIS top-down-data processing sequence, calibration options include withholding information on

<sup>&</sup>lt;sup>6</sup> The discussion in this parenthetical paragraph derives from theoretical, experimental, and numerical-simulation work conducted by P. Dimotakis and his research group on turbulent transport and mixing over the years. A more detailed discussion on this technical topic is beyond the purposes of the present report.

<sup>&</sup>lt;sup>7</sup> Then there are the sunrise and sunset hours, during which stratification is approximately neutral as PBL stability reverses, that cannot be parameterized/modeled by either daytime or night-time parameter settings. Sunrise and sunset are important with high correlations (positive and negative) in energy and industrial production, with differences that are hebdomadal (weekly) in the transportation and industrial sectors, seasonal for space heating and cooling, related to daylight-savings time changes, etc. A moment's reflection helps gauge the considerable challenges that simple parameterizations are called upon to address.

some direct concentration measurements and reliable information on surface fluxes (natural and anthropogenic) to calibrate the integrated model-dependent results. Such steps will add confidence and provide independent, or semi-independent, confirmation of uncertainty levels in the results.

#### C.1.6 Calibration of GHGIS Products and Reports

Beyond calibration of sensors that yield measurement data; the consequent data analysis; the reconciliation and assignment of data UQ; and modeling, modeling UQ, and data-inversions that will attribute concentration measurements to natural and anthropogenic surface sources, also discriminating between the two, calibration issues will arise when the final data fusion and integration occurs as part of the GHGHIS Mission Operations Center (GMOC) operations, as discussed in Chapter 8. Again, as with data fusion, data UQ, and modeling and modeling UQ, calibration can be realized by either comparing with withheld direct measurement data or with high-confidence bottom-up data. It should be noted, however, that a decision is required as to whether to utilize comparisons with bottom-up data to tune the GHGIS top-down data-processing sequence, or rely on the GHGIS data and exploit the detection of variances to assess the validity of bottom-up data sets. Quite likely, such decisions can and will be made on a case-by-case basis, as alluded to in Section 1.1.4.

## C.2 Verification

To recapitulate and summarize, the concept for verification entails internal consistency in the implementation. Below is a brief discussion on how that applies to the various GHGIS components listed above. Significantly, as will emerge from this brief discussion, successful verification need not imply that the component is delivering what it is designed to deliver; the design could be in error.

#### C.2.1 Sensor Verification

Sensor verification means that the sensors were built and fielded as designed. This represents a design verification step, often to be carried out by people other than those who designed, built, and tested the sensors, i.e., that they were built and implemented per plan. In the case of spaceborne sensors, for example, this step is carried out by a mission-assurance team and precedes the actual pre-launch testing. While the prelaunch subsequent testing may reveal issues that were not identified and bring the sensor subsystem back to qualify the implantation, if not the design, sensor verification takes place without regard to test data.

#### C.2.2 Data Analysis and Retrieval Verification

Again, this is a task aimed to assure that the data analysis and retrieval is in accord with the designed and agreed-upon process.

#### C.2.3 Sensor and Subsystem Operating Software Verification

With the number of lines of code increasing exponentially with time, software verification is emerging as a discipline into itself. Aided by formal-logic methods, the intent is to verify that the lines of code that operate a system or subsystem perform the logic and sequential-logic tasks intended. Again, this does not guarantee that the software will perform as intended, only that it performs as specified. The implied caveat is that if the software specifications are in error, even successful verification that, in the ideal case, may catch all software "bugs" and other coding errors will not catch software specification errors, since the verification step, in this case, is to assure that what the software delivers is per specification.

#### C.2.4 Verification of Data QA/QC and UQ Processes and Methodologies

As with data analysis and retrieval, this is a task assures that data QA/QC processes and tags are per specifications. Verification of data UQ presents a different challenge, especially when it comes to fusion and reconciliation of data collected with different sensors, sensing modalities, spatial and temporal resolution, precision and accuracy, etc., but, again, the intent of this step in the GHGIS sequence is to provide a check that it is, and has proceeded, per plan.

### C.2.5 Modeling and Data-Inversion Code Verification

In the context of the simple example of gradient transport discussed above, it would be possible to implement Eq. C-1 numerically correctly in the code and to have the implementation converge and pass all consistency tests that are employed and are consistent with Eq. C-1 and all the other equations used. Such a code would then be found to be *verified*. It should be acknowledged here, however, that modeling and data-inversion code verification represents one of the greatest challenges in the context of GHGIS, at least when considering the present state of the art in these capabilities.

Verification, in this context, means not only that the code is correct, i.e., bug-free, but that the *numerical and algorithmic implementation* of the hydrodynamic differential equations and physics models employed is also correct. Those equations describe and model a complex environment. The challenge can be appreciated by noting that the equations describe the chaotic turbulent-flow environment of high Reynolds number flow that can be stably or unstably stratified, and is coupled with complex processes of evaporation and condensation that lower or raise temperature, injecting energy and buoyancy forces that, in turn, alter momentum fluxes.

The complexity of this system and the high (modal) dimensionality of its possible realizations are such that it would be impossible, perhaps in principle, to *prove* correctness. Specifically, when the set of all possibilities is very large, perhaps infinite, proving correctness would require exercising all possibilities to check that the model/code delivers solutions of what the equations it "solves" represent. Not only does the size of that set preclude the option, but what the "right answers" are, in each case, is not known. Basically, it is not possible to prove the model "right" in the *verification* sense discussed above. This is a generic issue in the verification of computational fluid dynamics and multi-physics codes, as they apply to the environment that needs to be modeled in support of GHGIS.

What is accepted as verification, in practice, is testing for consistency and correctness in a more restricted sense: subjecting the code to a finite number of well-defined tests. To be sure, passing those does not prove the model/code "right." However, failing *any one* of them fails verification will prove the code "wrong" by this criterion. The discussion will return to this point below.

Tests that can be applied are of several kinds. One set targets checks that the (discrete) numerical implementation of the (continuous) differential equations in the code leads to convergence that is realized at the expected rate. For example, if the code is designed and expected to be second-order-accurate in time and space, cutting the grid resolution by 1/2 should decrease residual errors by 1/4. For a code that converges in this sense, one expects convergence to acceptable accuracy after successive subdivisions of the grid size in each direction, e.g., going from  $[\Delta x, \Delta y, \Delta z; \Delta t]$  to  $[\Delta x/2, \Delta y/2, \Delta z/2; \Delta t/2]$ , with an attendant increase in computation burden, as discussed above. If the code does not (or is not expected to) converge, either at this rate, or not at all, the code's results are subject to an implicit parameterization traceable to grid resolution. Of course, convergence is a necessary condition. If attained, it does not prove, by itself, that the result that the code has converged to is correct.

This challenge can be addressed through *calibration* of the model and its results, wherein, for example, at each grid resolution employed, one calibrates *all* adjustable constants (as a function of resolution). However, in accord with the distinction made in the discussion on the definitions of CV&V above, this approach would lead to a *calibrated* but not a *verified* model, and the caveats discussed in the context of calibration would apply.<sup>8</sup>

Models/codes can be subjected to a second set of *verification* tests to check that model/code solutions meet the requirements that the equations of motion also meet. By way of example, code results must conserve mass, linear and angular momentum, energy, and, possibly, other invariants, to the order and accuracy of the grid resolution employed. In this context, again, if code results observe these conservation constraints they need not be right. However, if they do not, they are "wrong," again, by the criteria of verification.

Other tests employed for *verification* is checks that a model/code reproduces solutions to specific (usually, simple) problems for which we have incontrovertible detailed solutions, either analytically, or via high-resolution large-scale direct numerical simulation (DNS), or by any other means, *with expected convergence rates*.

Presently employed atmospheric-transport codes do not (and cannot be expected to) converge as the grid is refined. However, they either are, or can be, calibrated, in the sense described above. Many can also fail the other two classes of tests.<sup>9</sup> As a consequence, models, or codes, that fail these tests cannot be *verified* in the sense described above.

<sup>&</sup>lt;sup>8</sup> A code's grid resolution can be an adjustable parameter. By and large, atmospheric transport models available today do not converge as grid resolution increases, for reasons beyond the purposes of the present discussion.

<sup>&</sup>lt;sup>9</sup> Ascertaining that a code conserves mass (locally, not just overall) the simplest but most important of the conserved quantities, is not as straightforward as it may seem and typically requires the implementation of methods that assure conservation by construction in the discrete numerics. Failure to conserve mass leads to failure to conserve momentum, which is (mass) density times flow velocity  $\mathbf{u}(\mathbf{x},t)$ , etc. Recent formulations of climate models conserve mass. However, (many) regional models do not.

#### C.2.6 Verification of GHGIS Products and Reports

Verification of GHGIS products and reports will rely on audits that will be carried out by a team, or teams, that are independent of and do not report to the hierarchy that produced these products. Part of the GHGIS product QA/QC process, product and report verification, will assure that GHGIS results are self-consistent and per agreed-upon processes.

## C.3 Validation

Successful validation documents that a component that was calibrated and verified returns an output that agrees with reality, to within required uncertainty, i.e., that variances with reality are lower than those acceptable.

#### C.3.1 Sensor Validation

A sensor whose design, implementation, and operating software have been verified and calibrated can be validated by testing its output data through measurements of known samples across its validity domain that are separate from those used to perform the calibration. Successful validation then requires agreement to within specified uncertainty bound maxima, without any further adjustments to calibration constants, internal data-analysis software and processes, etc. If these are found to be necessary, one needs to return to the calibration stage and reassess sensor verification, before attempting validation anew. The validation process must establish the uncertainty of the reference data used to validate the sensor, which must be lower than that of the sensor being validated.

### C.3.2 Data Analysis and Retrieval Validation

Data analysis and retrieval validation can be performed in a variety of ways. In its simplest form, it can be applied to the analysis of measurement data derived from well-documented test beds, comparing retrieved and attributed fluxes to known (directly measured) fluxes. The proposed Four Corners test bed, discussed in Chapters 5 and 6 and Appendix F, would be an important example. A more challenging validation, however, would involve estimated attributions in well-documented environments that contribute a more-complex mixture of natural/biogenic and anthropogenic emissions. Establishing a correct and reliable validation process, in such cases, represents a challenge in its own right.

### C.3.3 Sensor and Subsystem Operating Software Validation

Sensor and subsystem operating software validation is undertaken to assure that the codes that may have been checked to be consistent with the logic and other functions they are intended to perform, and be bug-free, for example, actually deliver their intended products. Software may have been correctly written to perform the tasks specified, but the specifications of these tasks may be in error and the goals are not achieved. This can only be assessed using a validation step that, independently of the calibration and verification parts of the process, determines that the intended measurements, as processed by the sensor and operating software, are correct. As above, comparisons with reality and intended ends must rely on data and tests that are independent of any used in the calibration steps.

#### C.3.4 Validation of Data QA/QC and UQ Processes and Methodologies

Validation of data QA/QC and UQ processes and methodologies can be performed using statistical methods (see Chapter 2 for a partial discussion) to ascertain that independent measurement data fall within estimated probability density functions and implied uncertainties around transmitted data values.

#### C.3.5 Modeling and Data-Inversion Code Validation

Validation of a model/code is a check that, ideally, can only be performed following successful verification and perhaps presents the greatest challenge. In practice, since, as discussed above and in Chapter 1, verification can never be complete, a code will be deemed to have been verified in the restricted sense discussed above before it is subjected to validation tests. In its purest form, validation is indistinguishable from performing a large number of *predictions*, i.e., offering solutions without the benefit of any data derived from the reality modeled, and without the benefit of any adjustments in its parameters. If parameters are adjusted as a result of comparisons with reality, the model/code reverts to one that has been *calibrated*, but not *validated*.

*Valid* theories, or models, target a certain *domain of validity* that must be established and within which they must be *predictive*.<sup>10</sup> Models needed for GHGIS data analysis, even within their necessary domain of validity, must correctly envelop Earth's atmospheric dynamics. The large number of occurrences that an atmospheric-transport model must predict correctly renders validation, in principle, an (almost) unbounded task.<sup>11</sup>

Fortunately for the purposes of GHGIS, validation need only encompass correct predictions of attribution to surface sources, based on concentration measurements. *Correct*, here, means predictions that agree with reality within the uncertainty bounds of the data themselves (cf. discussion in Chapter 6) and, if that is satisfied, not least, within the uncertainty bounds set by

<sup>&</sup>lt;sup>10</sup> Newton's "Laws" apply adequately when the speed of light is not approached in matters where Galilean invariance is expected (independence of the results from the relative speeds of frames of reference that leads to the Special Theory of Relativity), when the invariance between gravity and frame acceleration does not influence the dynamics (leads to the General Theory of Relativity), and when great precision is not required. These three criteria define Newton's Laws domain of validity. Precision space navigation, for example, that can place a spacecraft within a few hundred meters from a bull's eye at the right time, for insertion into a Mars-capture orbit, ~ 700 ×  $10^6$  km from Earth, i.e., an *accumulated* uncertainty in the spacecraft trajectory and its determination of less than  $1:10^6$ , requires incorporation of Einstein's Special and General theories of relativity in the spacecraft navigation toolkits. In this case, it is the precision requirement of the application that breaches the boundaries of the domain of validity of Newton's Laws, and not (solely) the (relative) speeds that may be high, but do not approach that of light in an absolute sense.

<sup>&</sup>lt;sup>11</sup> As Aristotle (implicitly, in his discussion on proofs, their types, and completeness) and more recently and explicitly Ernst Mach (of the eponymous flow number) would say, empirical generalizations and theories are provisional. At best, they can claim consistency with a limited number of occurrences that have actually been experienced, whereas a much larger, perhaps infinite, number of different occurrences is possible (e.g., Hickey 2010).

the GHGIS requirements (cf. discussion in Chapter 2), i.e., that the added uncertainty still allows the overall UQ estimates to remain below acceptable thresholds.

Most of today's models/codes that describe atmospheric transport cannot be *verified* in the sense defined and described above, and, as a consequence, can only be *calibrated*, but not *validated*. The importance and level of scrutiny that GHGIS models, inversions, and products must be able to sustain suggests that the modeling systems employed must accept the full rigor the calibration, verification, and validation processes discussed here. This presents a great challenge for the proposed GHGIS and leads to the recommendation in Chapter 7 that a program to develop next-generation atmospheric-transport models that can be both verified and validated, with complete understanding and traceability of uncertainties, should be undertaken. The span of the benefits that would ensue from the development of such a capability far exceeds the specific domain of interest of the proposed GHGIS and should be initiated as soon as possible.

Conversely, however, a code that has only been *calibrated* may suffice, if its domain of validity is such that it envelops the range of reality that must be captured. Most weather models fall in this category and have evolved into extremely useful *forecasting* tools.

### C.3.6 Validation of GHGIS Products and Reports

Validation of GHGIS reports will require proof of correctness of integrated GHGIS products of anthropogenic emissions allocated to required domains (national, subnational, or economic sectors, and perhaps sectors of other activities), within required uncertainty bounds. Such a validation could be performed via a number of comparisons:

- 1. comparisons with independent test-bed data, i.e., data that were not used to develop the GHGIS product being validated, as described and proposed elsewhere in this report;
- 2. comparisons of bottom-up emissions source data whose uncertainty is lower than that of the GHGIS product based on top-down measurement data; and
- 3. comparisons with other similar products, independently generated, such as those of European programs that track emissions and are described elsewhere in this report.

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# Appendix D. GHGIS Detection Scenarios in Terms of Receiver-Operating Characteristic (ROC) Curves

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The central, long-term function of GHGIS is to measure and validate country-level GHG emissions. Using top-down components, GHGIS targets the independent validation of claims or declarations made by countries of interest. In order to do so, GHGIS must be able to distinguish between declared or "target" emissions and actual emissions when the two differ (that is, GHGIS must be able to detect "departures" from target emissions). The required accuracy for GHGIS to do this depends on the magnitude of the departure that we wish to detect, as well as how quickly and with what degree of confidence we wish to detect it. In order to estimate the required accuracy of GHGIS, we laid out a simple "target" emissions profile and four departure trajectories for a hypothetical industrialized country, "Midlandia" with emissions of 100 Mt  $CO_2e$  in the year 2010. These trajectories were discussed in detail in Chapter 2. An illustration of the emissions scenarios is reproduced here for reference (Figure D-1).

We considered the simple detection problem where Midlandia has committed to the "Target" emissions trajectory but actually follows the "BAU" (Business as Usual) trajectory. In the first year covered by the treaty, there is a 3% discrepancy between target and actual emissions. We assumed that GHGIS measures total annual GHG emissions with a Gaussian uncertainty distribution characterized by a relative 95% (1.96  $\sigma$ ) confidence interval. Figure D-2 illustrates the detection problem at the end of the first year, assuming a measurement uncertainty of ±5%. The probability distribution of measurements one would expect to make if Midlandia's emissions are on target (the "noise" distribution) overlaps substantially with the distribution of measurements one would expect to make if Midlandia's emissions distribution). As with most signal-detection systems, a "decision-threshold" must be designated, above which action is triggered, if GHGIS reports emissions above this threshold. While the measurement error is a technical characteristic of the measurement system, the decision threshold and the value of the GHGIS information depend on the policy context in which the system operates.

If the consequences of a positive reading (i.e., a reading that Midlandia is off-target) are mild, for example triggering further investigation, we may wish to set the decision-threshold low. This makes it more likely that we will catch a departure when it occurs. The trade-off is that we will get more false-positives. If the consequences are severe, for example issuing sanctions against Midlandia for its violation, then we would wish to set the decision threshold high in order to limit false accusations and perhaps to make the decision credible to third parties. In order to propose accuracy requirements for GHGIS in Chapter 2, it was necessary to make some assumptions about the desired performance of the system and choose an appropriate decision threshold. Here we show the decision threshold trade-off more explicitly.

Figure D-3 shows the trade-off between the True Positive Rate (TPR) and False Positive Rate (FPR) for the BAU scenario and a GHGIS measurement uncertainty of  $\pm 20\%$ . Three curves

represent the detection problem after 2, 4, and 7 years of measurements. In signal-detection parlance, these are known as Receiver-Operator Characteristic (ROC) curves.



Figure D-1. (also Fig 2-1 in Chapter 2). Potential emissions trajectories for the hypothetical country Midlandia. According to an emissions reduction agreement, "Target" emissions drop by 2% per year, relative to the baseline year 2010, achieving a 20% reduction by 2020 and an 80% reduction by 2050. If no mitigation actions are taken, Midlandia follows the BAU path, increasing emissions by 1% per year. Each scenario is described in detail in Chapter 2.





Figure D-2. Example detection problem. Distribution of measured values given compliance (at emissions = 98, the "target") and noncompliance (at emissions = 101, "actual") with a measurement uncertainty of  $\pm 5\%$  and a decision threshold of 95% confidence (5% false-positive rate).

By varying the decision threshold, the performance (TPR and FPR) characterized by any point on the curve can be achieved. However, for a given FPR one can only achieve a higher TPR than the one on the curve by making technical improvements to GHGIS or by waiting longer for subsequent measurements. Note that, in Chapter 2, we essentially chose the point on each curve corresponding to the 5% FPR.



Figure D-3. ROC curves for the Business as Usual (BAU) scenario with ±20% measurement precision.

The area under the ROC curve (AROC) is a metric of performance for a measurement system that is independent of the decision threshold. An AROC of 1 corresponds to a perfect measurement system and an AROC of 0.5 indicates performance no better than chance. The AROC for each curve in the BAU detection scenario is shown in Fig. D-3. Figures D-4 and D-5 show the ROC curves and AROC values for the "partial mitigation" and "inflated baseline" scenarios and selected accuracies of GHGIS.

As an alternative to the set of arguments laid out in Chapter 2, a future analysis could set the performance requirements of GHGIS in terms of AROC rather than probability of detection. Such an analysis would require additional knowledge of the policy context in which GHGIS is to be used.



Figure D-4. ROC curve for the "inflated baseline" scenario with ±20% measurement precision.



Figure D-5. ROC curve for the "partial mitigation" scenario with  $\pm 10\%$  measurement precision.

# Appendix E. IR Sampling Kernels

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Passive infrared (IR) sounding can provide vertical-profile information of temperature (e.g., Chahine 1968, 1977), concentration (mixing ratio) of select gases, and potentially of other quantities. Exploiting this feature in the case of gases, the Atmospheric Infra-Red Sounder (AIRS) has included mid-tropospheric data products of carbon dioxide (CO<sub>2</sub>) mixing ratio since September 2002 with a demonstrated accuracy of 1 to 2 ppm globally (Chahine et al. 2008).

AIRS is a cross-track ("whisk-broom") scanning grating spectrometer covering the spectral range from 3.74  $\mu$ m to 15.4  $\mu$ m with 2,378 channels, with a nominal spectral resolving power of  $\lambda/\delta\lambda = 1200$ . The AIRS and its companion instrument, the Advanced Microwave Sounding Unit (AMSU), have been flying since May 2002 on a sun-synchronous, near-polar orbit on the National Aeronautics and Space Administration (NASA) Aqua satellite (Aumann et al. 2003). AIRS and AMSU were designed, built, and launched to support improved meteorology.

AIRS and AMSU data are simultaneously analyzed to eliminate the effects of clouds (Susskind et al. 2006) to produce "Level 2" products that include the "cloud-cleared" IR radiances, the retrieved profiles of atmospheric temperature versus pressure, T(p), water vapor H<sub>2</sub>O(p), ozone O<sub>3</sub>(p) and surface emission at a nominal spatial resolution at nadir of 45 km. The Level 2 products provide input to the retrieval of the vertically weighted CO<sub>2</sub> mixing ratio at three layers in the atmosphere. An AIRS-only algorithm that provides Level 2 products has been developed and is in place in anticipation of the AMSU instrument end of life.

In 2010,  $CO_2$  products were pursued for two additional vertical layers: one in the stratosphere with a peak sensitivity around 25 km (30 mb) and one near the surface with a peak sensitivity around 2.2 km (775 mb), as shown in Figure E-1.

The retrieval algorithm used is the same for all layers (Chahine et al. 2005) with changes primarily in the spectral channels selected and the quality controls applied. The basic concept attributes received radiative energy incident on the spaceborne instrument aperture as a superposition of thermal emission at each wavelength/wavenumber, from each atmospheric level at a pressure p, as moderated by atmospheric transmission between the emitting atmospheric layer through the intervening atmosphere between that layer and the instrument aperture (see also Pierrehumbert 2011).

Physically, radiances at highly absorbing (low-transmissivity) wavenumbers cannot penetrate the atmosphere to any depth and will preferentially return radiance to the instrument aperture from the upper atmospheric layers. Moderately absorbed radiation penetrates deeper, while high-transmissivity radiation can reach the surface or near the surface.

Quantitatively, the upward radiance can be estimated by assuming that each layer emits in thermal-radiative equilibrium as moderated by transmittance through the layers above it (e.g., Chahine 1968, Rodgers 2000, Pierrehumbert 2011),

$$I(\nu) = E_0(\nu, T_0) \int_0^{\infty} \frac{\partial \tau(\nu, z)}{\partial z} dz + \int_0^{\infty} B[\nu, T(z)] \frac{\partial \tau(\nu, z)}{\partial z} dz$$
  
$$= E_0(\nu, T_0) \tau_0(\nu) + \int_{\ln(p_0)}^{-\infty} B[\nu, T(\ln p)] \frac{\partial \tau(\nu, \ln p)}{\partial \ln p} d\ln p \qquad (E-1)$$

where v is the radiation frequency (wavenumber, or wavelengths per cm),  $E_0(v, T_0)$  is the surface emission at v and at a surface-temperature  $T_0$ ,  $\tau_0(v)$  is the transmittance from the surface to space at v; B(v, T) in the integrands is the Planck (black-body) function;  $\tau(v,z)$  or  $\tau(v,lnp)$  is the transmittance at the wavenumber v and at the altitude z or pressure-altitude  $\ln(p)$ ; and T(z) or  $T(\ln p)$  is the temperature profile versus altitude or pressure-altitude. The second form of the equation offers the preferred implementation with  $\ln(p)$  serving as a surrogate for altitude with a broader generality.



Figure E-1. Thermal IR weighting functions (kernels) averaged over selected channels show sensitivity to stratosphere, mid-troposphere, and lower-troposphere (near-surface) layer. The horizontal axis is in the variables used in Eq. E-1. Reproduced from Figure 3-4 (to appear in Pagano et al. 2011) and included here for completeness.

Implicit in Eq. E-1 is a full model of the atmosphere's profile, such as T(z) or  $T(\ln p)$ , its composition vs. altitude, the density profile  $\rho[p,T(\ln p)]$  given by the equation of state, etc., to allow the transmittance function to be estimated at each wavenumber. Much of the information required for the required data retrieval comes from the spectral data itself, as described in the references cited above. At each vertical level, the yield and accuracy can be determined by comparisons of data-retrieval results to other, preferably direct, observational data.

While not of direct interest in assessing surface emissions and related phenomena that are the focus of the current study, stratospheric  $CO_2$  concentration can help determine the "age" of air in the stratosphere. Since  $CO_2$  sources and sinks are near-surface, one can exploit the chemical stability of  $CO_2$  to allow a parcel of air to be related to previously generated and transported tropospheric  $CO_2$ , at lower mixing ratios (e.g., air-parcel "age"), as a form of Lagrangian (age) marker (Morgenstern et al. 2010). Further, vertical-profile information contributes to the understanding of tropospheric-stratospheric exchanges responsible for vertical leakage of tropospheric  $CO_2$  that may need to be accounted for in global  $CO_2$  flux budget estimations. By way of example, such information could track changes in the Brewer-Dobson circulation between the upper troposphere and the lower stratosphere and trend them throughout the lifetime of the AIRS mission.

Lower Troposphere  $CO_2$  mixing-ratio retrievals are the ones of direct interest to this study; however, they are less mature and under early development at this writing. The mid-troposphere data are available for the entire mission at the Goddard Earth Sciences Data and Information Services Center (GES DISC): http://disc.sci.gsfc.nasa.gov/AIRS/data-holdings/. Links are provided there for the Level 2 and Level 3  $CO_2$  products, and all other AIRS data products.

The CO<sub>2</sub> retrieval method is based on a post-processing algorithm applied after the AIRS Level 2 product generation. The CO<sub>2</sub> solution is obtained by an iterative process that minimizes the RMS difference (i.e., residuals) between cloud-cleared radiances and radiances computed from the retrieved Level 2 profiles for a number of selected CO<sub>2</sub> channels in the  $v \approx 15$ -µm band. The method is based on the total differential of multi-variable functions. At a stationary point (extremum, e.g., a minimum), the first partial derivatives of the function with respect to each unknown variable must vanish. Since the goal of all retrieval methods is to minimize the residual difference in a least-squares sense between measured and computed spectra, we can write an expression for the radiance residual,

$$G^{(n)}(\mathbf{X}) = \sum_{\nu} \left[\Theta_{\mathrm{M}}(\mathbf{X},\nu) - \Theta_{\mathrm{C}}^{(n)}(\mathbf{X},\nu)\right]^{2}, \qquad (\text{E-2})$$

where  $G^{(n)}(\mathbf{X})$  represents the value on a hypersurface (akin to a cost function) in the space of the vector variable  $\mathbf{X} = [X_1, X_2, X_3, X_4, X_5]$  that we wish to minimize.

The components of **X** express the dependence of the detected radiance on the various unknown parameters:  $X_1$  represents CO<sub>2</sub>,  $X_2 = T(p)$ ,  $X_3 = O_3$ ,  $X_4 = H_2O$ , and  $X_5 =$  surface emission that is only important when retrieving the Lower Troposphere channel.  $\Theta_M(\mathbf{X}, v)$  is the measured brightness temperature at frequency v (after eliminating cloud effects),  $\Theta_C^{(n)}(\mathbf{X}, v)$  is the computed brightness temperature based on the retrieval model, and n is the iteration order. Minimizing  $G(\mathbf{X})$ , bringing the forward model in near-agreement with observations, can be achieved by finding the local minimum on the multi-dimensional surface, i.e., finding the *N*-dimensional point where each of the partial derivatives vanishes, i.e.,

$$\frac{\partial G}{\partial X_i} = 0, \quad i = 1, \dots, \ N = 5; \tag{E-3}$$

where the component variables of  $\mathbf{X} = [X_i, i = 1, ..., 5]$ , are approximated as linearly independent in the Radiative Transfer Algorithm (RTE) used to compute  $\Theta_C^{(n)}(\mathbf{X}, \nu)$ . Equation E-3 provides the necessary and sufficient condition for an extremum of  $G(\mathbf{X})$ . Ascertaining that the extremum is a (local) *minimum* (and not a maximum) can be achieved with an a posteriori check that any variation in any of the  $X_i$  from the extremum leads to increases in  $G(\mathbf{X})$ . The minimum is sought by a method akin to that of steepest descents wherein variations in each of the components are required to produce decreases in  $G(\mathbf{X})$ , until a minimum is attained. This yields a solution for  $\mathbf{X}$ and each of the component variables, including the CO<sub>2</sub> mixing fraction.

The dependence of  $G(\mathbf{X})$  on component values in Eq. E-3 for the lower-troposphere channel is illustrated in Fig. E-2, calculated from a forward model as a function of latitude, leading to a solution that with a well-defined minimum in the five-dimensional space. For real radiance measurements, the radius of curvature for each of the near-parabolas scales uncertainties in the retrieved values.



Figure E-2. The multi-D Gaussian surface at the minimum for each of the variables:  $CO_2$ , temperature, water vapor, ozone, and surface emission. The simulations relied on AIRS Level 2 retrieval products, for latitudes from 77N to 87S, and AIRS  $CO_2$  lower-troposphere frequencies (Chahine et al. 2011).

Potential caveats include the assumed  $X_i$  independence, the completeness of the variable set, that the minimum found may not be global, that the non-commutative averaging of variations of the variables within data pixels does not lead to significant errors, etc. In particular, each data pixel averages the spectrally resolved radiance that is contributed to by the various physical parameters whose values are being retrieved. However, the average radiance corresponding to the spatially variable parameter values need not be the same as the radiance corresponding to the average radiance, i.e., averaging in this case is not commutative.

Data from a particular spectrum band may not lead to zeros in all partial derivatives, as required by the condition expressed in Eq. E-3, in which case, the sounding data are discarded as not yielding a solution. Added quality controls are applied during the retrieval including: the radiance residual (Eq. E-2) should decrease from one iteration to the next and homogeneity of a  $2 \times 2$  set of spatially adjacent retrievals (clusters) must agree within 2 ppm, in a root-meansquare sense. The resulting data products achieve a yield over 15,000 mid-tropospheric CO<sub>2</sub> retrievals per 24-hour period (Fig. E-3), i.e., almost a <sup>1</sup>/<sub>4</sub> of all possible soundings, with a horizontal footprint of  $100 \times 100$  km<sup>2</sup> each and an accuracy better than 2 ppm. Similar results have recently been obtained for the stratosphere, presented here as preliminary, pending validation (Fig. E-4).



Figure E-3. Sample AIRS mid-tropospheric  $CO_2$  retrieval yield (July 2003). Left Panel: Typical daily yield at 1°× 1°spatial resolution. Right Panel: Typical monthly accumulation yield at 1°× 1°spatial resolution. NASA AIRS data.

The relative sensitivities of  $CO_2$  retrievals in the three layers are given in Table E-1 and are based on a quantitative analysis using the forward radiative transfer calculations. Results show that sensitivities to the atmospheric constituents and to temperature differ for the three layers. The atmospheric temperature used is derived from the AIRS Level 2 product and shown (Chahine et al. 2006) to be accurate to 1 K/km in the troposphere, i.e., radiosonde accuracy. For this reason, the expectation is that the success in the mid-troposphere retrievals will be matched with those in the stratosphere.



Figure E-4. Measured and model stratospheric  $CO_2$  for January 2003 (M. Chanine and the NASA AIRS project team, unpublished data, personal communication). Left Panel: AIRS-retrieved stratospheric  $CO_2$ , with 30 hPa GPH contours overlaid. Color-bar range: 360 to 380 ppm. Right Panel: GEOS-Chem stratospheric  $CO_2$  with AIRS stratospheric weighting function applied. Expanded color-bar range 368 to 372 ppm. The measurements indicate a larger variance in  $CO_2$  concentration than is accounted for by the model.

The contribution to the Lower Troposphere radiance by the CO<sub>2</sub> mixing fraction also depends on surface emission that contributes to the upwelling radiance at the high-transmittance wavenumbers selected for that vertical sampling kernel. A summary of the sensitivity of the three sampling kernels discussed to the most-important variables discussed in the text is listed in Table E-1. Differences in sensitivity to the CO<sub>2</sub> mixing fraction are largely attributable to differences in the (temperature) lapse rate (K/km) in the three regions. The ratio  $\Delta G/\Delta CO_2$  (last row in Table 1) quantifies this, representing the sensitivity of the observed spectra to changes in the CO<sub>2</sub> mixing ratio. It is a function of the atmospheric temperature lapse rate, which is 7 K/km in the midtroposphere, 1.5 K/km in the stratosphere and 10 K/km near the surface. As can be seen and as is expected, surface emission plays no role in the stratospheric band and a very weak role in the mid-tropospheric band because of the limited atmospheric transmission at the corresponding spectral bands (cf. Fig. E-1).

	Stratosphere (30km)	Mid-troposphere (10km)	Lower Troposphere (2.2km)	
	17 CO <sub>2</sub> channels:	7 $CO_2$ channels: 13 $CO_2$ channels:		
	$650 \text{ cm}^{-1} \le v \le 680 \text{ cm}^{-1}$	$700 \text{ cm}^{-1} \le v \le 722 \text{ cm}^{-1}$	$730 \text{ cm}^{-1} \le v \le 745 \text{ cm}^{-1}$	
<i>T</i> ( <i>p</i> ) Very strong		Strong	Strong	
O <sub>3</sub>	Weak	Strong	Medium	
H <sub>2</sub> O	No impact	Medium	Medium	
Surface emission $(T_0, \varepsilon_0)$	No impact	Very weak	Medium	
$\Delta G/\Delta CO_2$ ~0.2		~0.4	~0.5	

Table E-1. Factors affecting passive-IR  $CO_2$  retrievals with the three sampling kernels (Fig. E-1). Altitudes in parentheses indicate the centroid heights for the set of spectral channels.

See also discussion in the related JASON report (2011). An informal presentation of the first Lower Troposphere  $CO_2$  retrievals was made recently (Chahine et al. 2011).

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# Appendix F. Four Corners Test Bed – GHG Attribution, Verification, and Validation (AV&V)

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Monitoring national CO<sub>2</sub> emissions from afar is challenging because of CO<sub>2</sub>'s variable and large background (390 ppm) and dilution of emissions by atmospheric transport (WMO 2007), as discussed in Chapters 1 and 7, and Appendix B. Quantification of anthropogenic CO<sub>2</sub> emissions that are 2-3% of natural CO<sub>2</sub> fluxes in amplitude globally (cf. Chapter 1 and Appendix B) and attributing them to particular locations is a daunting task. The National Academies released an emissions verification study that prioritizes accelerated research to address this challenge (NRC 2010a). Current verification approaches are in situ and CO<sub>2</sub>-centric (Marquis 2008). Spaceborne sensors have not yet provided near-surface measurements of CO<sub>2</sub> with the required accuracy.<sup>1</sup> To address this challenge there is an opportunity to develop an approach using measurements of co-emitted pollutants (carbon monoxide [CO], nitrogen dioxide [NO<sub>2</sub>], sulfur dioxide [SO<sub>2</sub>], and <sup>13</sup>CO<sub>2</sub>, among others) to derive CO<sub>2</sub> emissions as part of the Four-Corners test-bed project.

The emission ratio (ER) of Species X ( $ER_X = X/CO_2$ ) depends on fuel composition and combustion process. These vary by sector (transportation, power generation, etc.) and by nation, and, as also discussed at various places elsewhere this report, they can provide an important almost-independent component to help quantify anthropogenic CO<sub>2</sub> emissions (Ryerson 2001, T. Ryerson 2010, unpublished data; M.K. Dubey 2010 analysis of EPA data ). See Table F-1. Their much-lower background levels, large fractional contribution from energy activities, and the ability to measure them precisely make them sensitive probes to attribute sources, especially when ERs of multiple species are used concurrently. These attributes will also provide a validation test bed for satellites that can measure signature pollutants and co-emitted species, such as CO (cf. Chapters 3, 5, and 6, and 7, and Appendix E), NO<sub>2</sub> (Richter 2005; and Chapters 3, 5, and 6), etc.

Sector-ER	<b>Power-Coal</b>	Power-Gas	Transport	Bio-mass	Biology
СО	~0.5	~0.5	~20	~100	0
$NO_x$	~1	~1	~5	~1	0
$SO_2$	~2	~0	~0.1	~0	0
$\delta^{13}$ CO <sub>2</sub>	-24	-40	-30	-27	-26

Table F-1. ER =X/CO<sub>2</sub> in ppb/ppm by sector,  $\delta^{13}CO_2$  is in per mill relative to a global standard.

The Four Corners test bed supports the development and implementation of techniques to utilize observations of signatures species to derive regional and source-specific baselines, determine

<sup>&</sup>lt;sup>1</sup> As discussed in Chapter 3 and Appendix E, 1-2 ppmv accuracies for  $CO_2$  have been demonstrated by the spaceborne AIRS instrument for the IR mid-tropospheric channel. Data retrievals for near-surface channels that would be needed for surface-flux attribution are under development but not validated as yet (Appendix E).

trends, and infer  $CO_2$  fluxes in an important test environment where anthropogenic sources and signal-to-background ratios are more easily attributed and well known, as discussed below.

In particular, the Four-Corners test bed,

- 1. enables validation (as defined in Chapter 1 and Appendix C) that the natural background and anthropogenic-enhanced  $CO_2$  abundances, trends, and fluxes can be deduced from observations of signature gases and <sup>14/13</sup>CO<sub>2</sub>,
- 2. supports demonstrations that ratios of individual signature gas and  $CO_2$  concentration contributions from individual sectors or facilities can be attributed, and
- 3. supports validation that atmospheric CO<sub>2</sub> concentrations can be retrieved by the Japanese GOSAT,<sup>2</sup> and NASA's AIRS near-surface channel, and the anticipated Orbiting Carbon Observatory (OCO-2)<sup>3</sup> satellite.

The Four Corners, NM, locale contributes significant emissions of  $CO_2$  and signature gases from two large, distinctively different, power plants (different emission profiles) in an isolated location, an urban center, thousands of oil and gas wells, and little surrounding vegetation or other natural contributions to GHG emissions. As a consequence, the Four Corners test bed provides a valuable experimental and developmental facility for the quantitative determination of greenhouse gas (GHG) fluxes from various natural and anthropogenic sources using multi-scale multi-species atmospheric observations that can span ground, airborne, and satellite platforms and measurement scales.

GHGs and signature emissions are measured in the stacks by real-time Continuous Emissions Monitoring Systems  $(\text{CEMS})^4$  and actual emissions (or "ground truth") are known along with power production, making the site ideal to assess top-down validation methods (comparisons and blind tests of multiple approaches) and also for data and model uncertainty quantification (UQ) validation. In addition, the test bed enables not only the development and validation of techniques that attribute atmospheric concentration measurements of associated "signature" gases, aerosols, and isotopomers (e.g.,  ${}^{14}\text{CO}_2$ ,  ${}^{13}\text{CO}_2$ ) co-emitted in distinctive ratios by different fuels, combustion, and biological processes, but also leaks from gas wells that can be used for source attribution.

A core site at the San Juan substation, New Mexico, was recently instrumented with a highresolution solar tracking Fourier Transform Spectrometer (FTS) for large-scale (10- to 100-km) columnar GHG and pollution monitoring as well as key in situ measurements. The region has several disaggregated networks to monitor air quality, acid deposition, visibility, and carbon dioxide (CO<sub>2</sub>) that could be expanded and integrated, as indicated by the GHGIS systems analysis (Chapter 9). The FTS is portable and can measure atmospheric column abundances of major GHGs<sup>5</sup> and is part of the Total Column Carbon Observing Network (TCCON)<sup>6</sup>. It is possible to expand and develop additional infrastructure that builds upon the existing networks

<sup>&</sup>lt;sup>2</sup> See http://www.jaxa.jp/projects/sat/gosat/index\_e.html

<sup>&</sup>lt;sup>3</sup> See http://oco.jpl.nasa.gov/

<sup>&</sup>lt;sup>4</sup> See http://www.epa.gov/ttn/emc/cem.html

<sup>&</sup>lt;sup>5</sup> Such as CO<sub>2</sub>, methane [CH<sub>4</sub>], *nitrous oxide* [N<sub>2</sub>O]), co-emitted pollutants (CO, NO<sub>2</sub>, SO<sub>2</sub>, ozone [O<sub>3</sub>], aerosols. See Table 1-1 in Chapter 1.

<sup>&</sup>lt;sup>6</sup> See https://tccon-wiki.caltech.edu/Sites/Four\_Corners

so instruments can monitor meteorological fields and atmospheric composition from the air and ground, with sufficient resolution to allow inversions (Fig. F-1).<sup>7</sup> Further, LANL has agreements with Japan to point their GHG monitoring satellite (GOSAT) over the region for validation and plans to use the National Aeronautics and Space Administration (NASA) OCO-2 in a similar manner. Future data analysis and retrievals based on AIRS near-surface channels could also be used, albeit at lower spatial resolution (cf. Chapters 1, 3, and Appendix E). Minimal air traffic in the region makes routine monitoring by aircraft, unmanned aerial vehicles, and balloons feasible cf. Chapter 4). The ability to point GOSAT, OCO-2, and other and future satellites at the site for extended soundings supports calibration and validation.



Figure F-1. (left) The vegetation map of the Four Corners Region (brown-arid, green-forest, bright green-grass), with population density (pink). The red dots are the current measurement sites that the effort is building upon starting with the San Juan Substation FTS site with the New Mexico Environment Department (NMED). (right) All large  $CO_2$  point sources in the region showing the neighboring San Juan (NW) Four Corners (SE) power plants, the roads, and the current sites in red.

# F.1 Multi-Scale Signature Attribution at Four Corners

The test bed relies on existing infrastructure and has developed additional infrastructure for observations to validate signature-based CO<sub>2</sub> attribution science exploiting Four Corners' rich but tractable mix of power plant, urban, and oil/gas production emissions (Fig. F-1). The instrument suite, including the existing solar FTS and in situ ground sensors, enables measurement of meteorological fields, signature pollutants, GHGs, <sup>14</sup>CO<sub>2</sub>, and <sup>13</sup>CO<sub>2</sub> distributions simultaneously over point to 10 km scales,<sup>8</sup> and if supplemented with additional FTSs and airborne in situ and remote sensors (Chapter 4 and Appendix H, respectively), would enable measurement over 100 km scales.

<sup>&</sup>lt;sup>7</sup> Such infrastructure would include transportable containers (with power, environmental control, sampling systems, launch sites, and soundings) and core instrumentation (met station, wind profilers, FTS, SODARS, LIDARS).

<sup>&</sup>lt;sup>8</sup> This refers to the point-sampling as from a fixed sensor. See discussion in Appendix B for a discussion of the sampled volume of air,  $V_m(t)$ .

Satellites can be tasked to perform retrievals for which ground-truth is available. Detailed multiscale chemical transport models can be adapted to analyze the multi-component data. This test bed could become a long-term validation site dedicated to air-quality and quantitative GHG monitoring.

Establishing signature- $CO_2$  relations from multi-perspective observations requires unraveling the effects of complex chemistry and transport dynamics. This demands validation in well-documented conditions of manageable complexity, before such tools are used to develop baselines and monitor trends in more-complex environments of anthropogenic and natural GHG sources. The semi-arid ecology in the region hosts a weak natural carbon cycle, facilitating the goal of attribution to anthropogenic sector-specific sources.

The Four Corners and San Juan power plants together produce 4 GW of power. They comprise the largest point source of net  $CO_2$  and  $NO_x$  in North America, emitting ~29 Mton/yr and 72 kton/yr respectively. The Four Corners plant produces much more  $NO_x$  than the San Juan power plant (even though the energy,  $CO_2$  outputs, and coal used, are similar) because the Four Corners plant is on Indian land and not subject to stringent Environmental Protection Agency (EPA) regulations. This difference offers an opportunity to test discrimination and attribution methods.

The dispersed  $CO_2$  urban emissions comprise a small fraction (<10%) of total emissions but vary significantly. Emissions and leaks from thousands of oil/gas wells are unknown. These attributes make the site an ideal test bed to:

- 1. determine the signature (NO<sub>2</sub>, CO, SO<sub>2</sub>,  $^{13/14}$ CO<sub>2</sub>) baseline, estimating the CO<sub>2</sub> baseline from signature baselines, discerning trends, and comparing the signature-derived baseline with direct CO<sub>2</sub> observations;
- 2. estimate how accurately signatures and CO<sub>2</sub> increases can be used to determine source fluxes;
- 3. understand how to accurately discriminate the high- $NO_x$ and low- $NO_x$  plumes, resolve urban emissions using signatures, quantify the  $CH_4$  and  $CO_2$  emissions from oil and gas wells; and
- 4. establish the ability to attribute as resolution and distance from sources increase.

The  $CO_2$  signal at Four Corners is a challenge for current satellites. Its  $NO_2$  plume, however, was recently resolved (detected) by Kim (2009) from space (Fig. F-2). Models indicate a 5 ppm enrichment in the column  $CO_2$  above the regional background (Peters 2007). This large  $CO_2$  signal is of the same order as that observed at Caltech with the solar FTS and modeled by WRF (Wunch 2009; Dubey 2009, AGU). Detecting this with GOSAT and OCO-2 is a challenge that the test bed provides.



Figure F-2. Column CO<sub>2</sub> from SCHIAMACHY (ESA).

The Four Corners ground site can be instrumented with in situ and remote sensors, including upwind and downwind FTSs and a network of meteorological sensors for continuous long-term monitoring (it already has one FTS and key in situ sensors). The GOSAT satellite, with its moderate-resolution FTS designed to measure CO<sub>2</sub> and CH<sub>4</sub>, will be targeted at the site weekly. Overpasses by other satellites that monitor NO<sub>2</sub> and CO can be analyzed. Coordinated field campaigns with in situ and remote sensors will interrogate the power plants' plume, along with regional dynamics and chemistry (Dubey 2011 EGU paper, Vienna; Costigan and Dubey 2011 AMS paper, Seattle). Multi-scale chemistry-transport models can be developed to analyze the field observations. Forward modeling using the plants' reported emissions can be compared with observations to test the validity of approaches employed (Andrejchuk 2008, Steinwart 2009, Vijayaraghavan 2009). Inverse modeling using far-field observations can be used to infer sources.

**Status:** LANL has partnered with the New Mexico Environment Department (NMED) to instrument the San Juan Substation site with a trailer that houses a solar tracking FTS for columnar GHG and signature measurements that is part of the Total Column Carbon Observing Network<sup>6</sup>. The sites depicted in Figs. F-3 and F-4 are also being augmented with meteorological sensors and a separate trailer for multiple in situ GHG and signature sensors with ports for remote sensing (CO<sub>2</sub> LIDARs, etc.). See Abshire (2010). The site is located in between the two power plants, as shown in Fig. F-4 and F-5, and is powered and fenced with video-cams and wireless communication for remote operation and data downloads.



Figure F-3. The location of the FTS site relative to the Four Corners and San Juan sites.



Figure F-4. The container, the operational FTS, and the in situ Picarro- $CO_2$ - $CH_4$  instrument.

The test bed is beginning to collect both in situ and remote spectra for GHGs to determine the variability and baselines for validation. LANL has developed partnerships with NMED, EPA, the National Center for Atmospheric Research (NCAR), the United States Department of Agriculture (USDA), and the United States Forest Service (USFS) to utilize the sites in the region and they are prepared to develop the infrastructure. The ability to compare observations to "ground truth" in a relatively uncomplicated environment could be a valuable first step before deploying new instrumentation to more complex natural and urban environments.

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# Appendix G. INFLUX (The Indianapolis Flux Experiment)

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# G.1 Introduction

In September 2010, a collaborative research team led by researchers at Purdue University, Penn State University, Arizona State University, the University of Colorado, and the National Oceanic and Atmospheric Administration Earth Systems Research Laboratory (NOAA/ESRL) began a suite of intensive measurements using towers and aircraft to quantify emissions of carbon dioxide (CO<sub>2</sub>) and methane (CH<sub>4</sub>) from the city-wide Indianapolis emissions plume. This intensive is funded for two years of measurements and a shorter 'synthesis' phase. Indianapolis, a medium sized city with ~3.4MtC-yr<sup>-1</sup> CO<sub>2,ff</sub> emissions, was chosen because of its comparative isolation relative to other anthropogenic GHG sources, in combination with relatively flat local topography. Indianapolis is the first US city to have a detailed, building-level bottom-up inventory emissions estimate (http://www.purdue.edu/climate/hestia/), which lends itself to such a top-down bottom-up synthesis experiment.

These measurements will be used in combination with bottom-up inventories to evaluate the current best methodological approaches, and associated uncertainties, for quantifying urban greenhouse gas (GHG) emission fluxes from atmospheric measurements. At present the core measurements will be made from twelve (12) ground-based towers. Using cavity-ring down spectroscopy, CO<sub>2</sub> will be measured continuously at all towers and CH<sub>4</sub> and CO will be analyzed at a subset of the towers. Using programmable flask packages, time-integrated flask samples at 6 of these towers will be analyzed for <sup>14</sup>CO<sub>2</sub>, CO<sub>2</sub>, CH<sub>4</sub>, CO, and a suite of halo- and hydrocarbons (see Tables 5.2 and 5.3). The additional trace-gas measurements will be utilized to explore and elucidate tracer-tracer relations and to enable source attribution of the measured CO<sub>2</sub> and CH<sub>4</sub> plumes. Additional measurements will be taken during 40 light-aircraft flights over the Indianapolis metropolitan area. The aircraft will perform both across-plume transects and vertical profiles to define free-troposphere concentrations. In addition to basic meteorological measurements continuous measurements of CO<sub>2</sub>, CO, CH<sub>4</sub> will be made on the aircraft and augmented with the collection of discrete whole air samples for subsequent isotope and trace gas analyses. These measurements along with building-level analysis of fuel usage will enable this first high spatial and temporal resolution assessment of GHG emissions for an urban environment, and thus provide a baseline dataset for other measurement systems and analysis techniques, such as airborne or space-based remote sensing technology.

Mesoscale atmospheric models utilizing data assimilation can provide high-resolution regional atmospheric transport reanalyses (see Chapter 7). These transport models can be combined with GHG boundary conditions from global reanalyses of these gases to provide a framework for analyzing an urban GHG measurement network. Atmospheric tracers such as <sup>14</sup>CO<sub>2</sub> and CO can help to deconvolute fossil-fuel-derived CO<sub>2</sub> from other CO<sub>2</sub> sources (e.g., Graven et al. 2009;

Levin et al. 2003; Turnbull et al. 2006, 2009; Vogel et al. 2010). Fossil-fuel-derived CO<sub>2</sub> is entirely devoid of the radioactive isotope <sup>14</sup>C, because of its extreme age, whereas other sources of CO<sub>2</sub> (oceans and terrestrial biosphere) have <sup>14</sup>C content close to that of the atmosphere (cf. caveat in Chapter 7, Footnote 4, page 7-30, however). Thus the addition of <sup>14</sup>C-free fossil-fuel CO<sub>2</sub> lowers the <sup>14</sup>C content of atmospheric CO<sub>2</sub>, and these additions can be quantified in atmospheric samples (Keeling 1979, Tans et al. 1979, Stuiver and Quay 1981). Fossil-fuel-derived CO<sub>2</sub> is also correlated with CO, though the emissions ratio varies over space and time. A combination of flask-based <sup>14</sup>CO<sub>2</sub> and continuous CO measurements provides a basis for isolating fossil-fuel-derived CO<sub>2</sub> with high spatial and temporal resolution (c.f. Vogel et al. 2010 and references therein). Thus while the elements exist for constructing atmospheric estimates of urban GHG emissions at high spatial and temporal resolution, this type of experiment has yet to be conducted.

The primary goal of this research effort is to use highly accurate and precise tower-based and aircraft-based measurements of  $CO_2$  (and  $CH_4$ ), along with  $^{14}CO_2$  and CO measurements, to test atmospheric budget estimates of fossil fuel emissions, and compare these to the high-quality Hestia (http://www.purdue.edu/climate/hestia/) data product, thus quantifying the methodological uncertainties and biases present in the atmospheric methods and the bottom-up inventory. The planned measurements will enable not only assessment of the methods used and their uncertainties, but will also reveal much about the temporal characteristics of fluxes, covering diurnal, weekly, and seasonal variability in fluxes.

### G.2 Methods

#### G.2.1 Tower-Based Measurements

Continuous ground measurements of CO<sub>2</sub>, CO, and CH<sub>4</sub> and discrete flask measurements of <sup>14</sup>CO<sub>2</sub>, CO<sub>2</sub>, CH<sub>4</sub>, and CO, stable isotopes in CO<sub>2</sub>, and a suite of halocarbons and hydrocarbons will be conducted from medium height (75 m to 150 m) cell phone towers that are distributed around the Indianapolis metropolitan area. Twelve towers will be instrumented (Figure G.1). At present, only two towers will host the entire suite of trace-gas measurements. Three will include CO<sub>2</sub>, CO, and flask measurements. Three will conduct CO<sub>2</sub> and CH<sub>4</sub> measurements. Four additional sites will measure CO<sub>2</sub> only. Each tower has been selected based on prevailing winds and the likelihood of capturing measureable signals downwind of Indianapolis and at the same time capturing background signals with corresponding towers on the upwind side of the city. All measurements will be routinely calibrated using standard gases traceable to World Meteorological Organization (WMO) standards. The flask and continuous measurements of  $^{14}$ CO<sub>2</sub>, CO<sub>2</sub>, and CO will be used in combination to obtain high-resolution fossil-fuel CO<sub>2</sub> estimates. The additional species measured will aid in identifying specific fossil-fuel sources, and will also be used to examine emission ratios for these other species. Towers are being instrumented during the fall and winter of 2010-2011, and are planned to be in operation for approximately two years.



Figure G-1. General map of the Indianapolis area showing the locations of idealized (STILT back trajectory chosen) tower locations (colored push pins). Site 1, located in Mooresville, is upwind and will provide a 'local background' site. Site 2, located on the east side of the city, will capture the urban plume when the wind is aligned in the predominant vector (a northwest wind).

#### G.2.2 Aircraft Measurements

Over the next two years, more than 40 fights of the Airborne Laboratory for Atmospheric Research (ALAR, http://www.chem.purdue.edu/shepson/alar.html) will take place, during which high-precision and accuracy measurements of CO<sub>2</sub> and CH<sub>4</sub> will be conducted, along with flask samples that will be analyzed for <sup>14</sup>CO<sub>2</sub>, CO<sub>2</sub>, CH<sub>4</sub>, CO, stable isotopes in CO<sub>2</sub>, and a suite of halocarbons and hydrocarbons, to assist with source attribution. Comparison of the in-flight CRDS measurements of  $CO_2$  and  $CH_4$  with the NOAA/ESRL flask measurements of these gases (traceable back to WMO standards) will ensure reliable data, with known uncertainties. The ALAR wind probe enables determination of local 3D winds, which, along with temperature profiles that provide boundary-layer height measurement, can be used for eddy-covariance, or mass-balance-based determination of fluxes. The advantage of deploying light aircraft is that the cost is minimal and the flight plan can be quite flexible. Two recent studies done in recent collaboration between the NOAA/ESRL carbon-cycle group aircraft project (http://www.esrl.noaa.gov/gmd/ccgg/aircraft/index.html) and Purdue vielded two different successful approaches to sampling urban plumes (e.g., Mays et al. 2009 and Turnbull et al. 2010). These data also provide an effective independent test of the regional reanalyses of both meteorological conditions and atmospheric GHG concentrations that will be created with our mesoscale modeling system.

#### G.2.3 Emissions Data Product

The Hestia Project provides fossil-fuel  $CO_2$  emissions down to the building/street level every hour utilizing a bottom-up, process-driven approach that draws from Vulcan (http://www.purdue.edu/eas/carbon/vulcan/index.php, the US national emissions data product). Hestia has been demonstrated using the city of Indianapolis as a test case (Figure G.2). The approach leverages a variety of data sources and model constructs to estimate emissions in a comprehensive, methodologically consistent manner.

The approach is scalable and transferrable to other urban locations in the United States and provides considerable source detail including categorization by vehicle type, building type, and fuel consumed, among others. While high-quality data (fuel use, transportation data, etc.) is also available for most other industrialized nations from which to generate high-quality emissions inventories, the data quality is much less certain for most developing nations. Even in industrialized nations with high-quality data bases, such high-resolution inventory estimates have not been evaluated using independent methods. The ability to match such highly resolved, bottom-up inventories with atmospheric budget estimates has not yet been demonstrated. This project aims to conduct such a demonstration.



Figure G-2. An example of the bottom-up, building resolution, emissions estimate from the Hestia project.

#### G.2.4 Atmospheric Inversions

The atmospheric inversion techniques developed for regional experiments in the southeast of France and the US Mid-continental Intensive regional study will be used to infer anthropogenic GHG emissions from the study region (c.f. nacarbon.nacp/mci.htm). The inversion system utilizes the Weather Research and Forecast (WRF) model (Skamarock et al. 2008) for creating atmospheric transport fields, the Lagrangian Particle Dispersion Model (LPDM) to estimate the areas influencing each tower observation, and a Bayesian matrix inversion to solve for spatially resolved emissions. The WRF model has the ability to employ a range of plausible descriptions boundary-layer parameterization, cloud-convection of atmospheric processes (e.g., parameterization) important to the transport of GHGs, the ability to simulate the transport of multiple passive tracers simultaneously, a well-developed data assimilation module suited to the production of a transport reanalysis closely fitted to regional observations, and the ability to run a nested simulation with a more coarsely resolved, large-scale flow interacting with a more highly resolved regional mesh. For INFLUX, we will run a nested grid with ~10 km horizontal resolution encompassing a significant portion of the eastern United States, with a finer mesh (~1 km to 2 km horizontal resolution) for the ~50 km radius around Indianapolis. The model will be run in reanalysis mode, including ingestion of the available surface meteorological observations available in the Indianapolis region, and utilizing National Centers for Environmental Prediction (NCEP) reanalysis at the continental scale. Boundary conditions for CO<sub>2</sub> will be taken from NOAA's CarbonTracker system (Peters et al. 2005) and NOAA's continental network of airborne CO<sub>2</sub> profiles (www.esrl.noaa.gov/gmd/ccgg/aircraft/index.html). Estimates of fossil-fuel and biogenic CO<sub>2</sub> fluxes and anthropogenic CH<sub>4</sub> emissions will be constructed from a multi-species inversion including CH<sub>4</sub>, CO<sub>2</sub>, and CO (calibrated to represent fossil CO<sub>2</sub> using <sup>14</sup>CO<sub>2</sub>). Fluxes will be estimates at 1 km to 2 km spatial resolution and for weekly time intervals. Data removal experiments and multiple atmospheric transport schemes will be applied to test the robustness of the inverse flux estimates. The ALAR airborne data will be utilized for independent evaluation of the modeled GHG mixing ratio fields. Inversion results will be compared to Hestia estimates. The combination of the globally unique atmospheric data and high-resolution Hestia emissions inventory should provide an unparalleled opportunity to test the ability of atmospheric inversions to estimate urban GHG emissions.

## G.3 Opportunities for Collaboration

The INFLUX study represents an important opportunity to test our ability to infer urban GHG emissions using both in situ and remote measurement methods. At present, INFLUX does not include a remote-sensing component. Additional in situ measurements and expanding the <sup>14</sup>C analyses are needed. We also anticipate that atmospheric transport will be a primary source of uncertainty in our final inversion results, and note that enhanced regional atmospheric sampling will improve our ability to evaluate WRF reanalyses of regional transport. To that end we suggest four primary areas of potential collaboration and investment in the INFLUX experiment, roughly in order of priority. We emphasize that field measurements are being deployed now, and will operate for approximately 2 years; thus the suggested observational collaborations are timesensitive.

#### G.3.1 Atmospheric GHG Remote Sensing

The most likely area for which INFLUX can benefit remote sensing studies is to test the ability of atmospheric remote sensing assets to either infer urban GHG emissions or to evaluate the atmospheric inversion schemes by providing GHG data not utilized in the regional inversions. This is an area of considerable interest and highly relevant to the upcoming OCO-2 and ASCENDS satellite missions. We recommend deploying airborne or ground-based CO<sub>2</sub> remote sensing technology as part of the INFLUX experiment. This could include Fourier transform infrared spectroscopy (FTIR) column remote sensing, LIDAR CO<sub>2</sub> column remote sensing, or existing space-based (e.g., GOSAT) remote sensing assets. Deployments of any of these assets over a time period of a few to several weeks, perhaps at contrasting times of year (summer, winter), would enable substantive testing of the utility of these data. (Contacts: K. Davis and P. Shepson)

#### G.3.2 Remote Sensing of Atmospheric Transport

Ground-based, long-term (many months to full experiment duration) remote sensing of boundary layer properties and lower tropospheric winds using, for example, boundary layer radar or LIDAR would provide an excellent means of evaluating the quality of our regional atmospheric transport fields. Airborne remote sensing would provide valuable shorter-term experiments, also with the goal of evaluating and potentially improving WRF reanalyses. (Contacts: K. Davis and C. Sweeney)

#### G.3.3 Remote Sensing of the Land Surface

Enhanced remote sensing of the regional land surface (e.g., AVIRIS overflights) would benefit our effort to characterize regional emissions using inventory methods. (Contact: K. Gurney)

#### G.3.4 Alternative Atmospheric Inversion Schemes

The data base created by this experiment will provide a unique test bed for urban atmospheric inversion methods. Additional groups interested in experimenting with regional inversion approaches are welcome to collaborate. All project data will be available to the research community as soon as basic data processing and quality analyses are complete. (Contacts: K. Davis, N. Miles, C. Sweeney)

#### G.3.5 In Situ Instrumentation and Analyses

The INFLUX project includes both continuous (cavity-ring down spectroscopy) and discrete, flask based analyses of CO<sub>2</sub>, CO, CH<sub>4</sub>, and from only flasks <sup>14</sup>CO<sub>2</sub> and a suite of halocarbons. At present the operating procedure for tower-based flask measurements is to only collect when the wind direction is consistent and we are able to constrain both the upstream (background) and downstream (urban) plume. A total of 200 <sup>14</sup>C analyses are currently planned. Additional instrumentation and analyses (e.g., other tracers such as VOCs, SOAs, related combustion products, column profiles) will increase the richness of the observational data-set. Increasing the frequency and spatial distribution of <sup>14</sup>C analyses would afford us the ability to better define the

tracer-tracer relationships and  $CO_2$  attribution. In the context of the inversions, increased data density will allow nested data-model experimentation. (Contacts: C. Sweeney and J. Turnbull)

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# Appendix H. Airborne Remote Sensing of Greenhouse Gases

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# H.1 Introduction

As discussed in Chapter 4, airborne in situ sampling provides the most detailed information currently available on the horizontal and vertical distribution of atmospheric greenhouse gas (GHG) concentrations. The methods for aircraft in situ sampling of carbon dioxide (CO<sub>2</sub>), methane (CH<sub>4</sub>), nitrous oxide (N<sub>2</sub>O), and other GHGs are mature and directly traceable to reference standards for atmospheric gas concentrations. Numerous flight-proven, validated research instruments exist and have been used in campaigns ranging in scope from local (Mays et al. 2009) to regional (Carouge et al. 2010) to continental (TRACE-P, NACP) to global (HIPPO). Operational in situ sampling has also been performed on regular commercial airline flights (CONTRAIL, MOZAIC, CARIBIC). Recently, commercially available continuous in situ sensors have been developed that have high precision (e.g., 0.05 to 0.07 ppm for CO<sub>2</sub>) and long-term stability (absolute accuracy better than 0.1 ppm for CO<sub>2</sub>) rivaling the best research instruments (Crosson 2008, Chen et al. 2010). Additionally, novel low-cost air sampling methods may lead to the proliferation of accurate in situ profile sampling (Karion et al. 2010).

Compared to in situ detection, space and airborne *remote* sensing of GHG concentrations is not as precise. Space and airborne *remote* sensing of GHG concentrations both have application in a national system. Here, we highlight airborne remote sensing from three major classes of instruments: nadir-viewing spectrometers, nadir-viewing LIDAR systems, and balloon-borne solar-occultation instruments. The detection capabilities, uncertainties, and limitations of each technique are summarized. We emphasize systems for which peer-reviewed reports and validated results are available and provide a limited assessment of what capabilities will be available in the 2010–2020 time frame.

### H.2 Nadir-Viewing Remote Sensing Spectrometers

Airborne nadir-viewing thermal-emission remote sensing is mature and has been used for decades to observe spectrally resolved IR radiances. Numerous flight-proven, validated research instruments exist including the High-resolution Interferometer Sounder (HIS) (Revercomb et al. 1988), the Scanning High-resolution Interferometer Sounder (S-HIS) (Tobin et al. 2006), the Airborne Emission Sounder (AES) (Worden et al. 1997), the aircraft demonstrator for NASA's Tropospheric Emission Spectrometer (TES), the airborne demonstrators for the Japanese IMG (Shimota et al. 1999) and IASI (Té et al. 2002), and the National Polar-Orbiting Operational Environmental Satellite System (NPOESS) Airborne Sounder Testbed-Interferometer (NAST-I) (Smith et al. 1999). These instruments were developed to measure accurate, spectrally resolved thermal IR radiances, primarily to deliver temperature and water-vapor profiles. The potential for retrieving GHGs and other trace gases from nadir-viewing, high-resolution IR sounders was

noted (Chedin et al. 2003, Zhou et al. 2005) and successful retrievals of  $CO_2$  from AIRS, TES, and IASI have all been performed, as also discussed in Chapter 3 and Appendix C.

Careful selection of the spectral microwindows used in trace-gas retrievals is essential (Dudhia et al. 2002, Worden et al. 2004). This is especially true for  $CO_2$  retrievals where the  $CO_2$  information content in the spectra is not easily separated from uncertainties in the temperature profile determination (Chedin et al. 2003). See also Appendix C.

An important example of the kind of data that can be produced from airborne, nadir-viewing, high-resolution thermal IR sounders are the CO profiles determined from NAST-I spectra (Zhou et al. 2007). Those measurements indicate a vertical mean difference between NAST-I CO retrievals and in situ CO measurements that is < 5 ppbv and their standard deviation is < 22 ppbv. The mean difference illustrates the bias caused by differences in vertical resolution and absolute accuracy between retrievals and in situ observations. In contrast, the STDE illustrates the residual random error caused by these differences. Here, NAST-I averaging kernels and a priori information are not applied to in situ data to make the in situ data vertical resolution the same (i.e., the retrieval equivalent). Therefore, the different vertical resolution associated with these two datasets affects the outcome of the comparison. These statistics reveal the difference between the retrievals using a passive ultraspectral remote sensor and in situ observations. As a consequence, these results reveal how well the retrieval can capture tropospheric CO vertical features.

The comparison reveals several critical factors that influence the retrieved CO profile. The CO first-guess profile (or a priori condition) plays a major role in the estimated CO profile accuracy. The terrestrial boundary layer (TBL), or planetary boundary layer (PBL), CO accuracy, mainly determined by the first guess (or a priori information), affects the free tropospheric CO retrieval. However, CO variations in the free troposphere can still be captured while variations in the CO amount in the TBL are not retrieved very well. Thus, it is a challenge to obtain accurate CO profiles (especially in the TBL) from remote sounders such as NAST-I.

Recently, Roberts et al. (2010) demonstrated that the strong absorption signals attributable to  $CH_4$  in the short-wave IR could be used to map  $CH_4$  emissions using hyperspectral imagers, such as the airborne visible/IR imaging spectrometer (AVIRIS) (Vane et al. 1993, Green et al. 1998). A multistep  $CH_4$ -detection algorithm was developed in which the average residual between 2248 and 2298 nm showed high sensitivity to  $CH_4$ , with minimal sensitivity to water vapor or surface albedo. Roberts et al. conclude that AVIRIS is capable of mapping  $CH_4$  at low concentrations over a wide range of surface albedos. Given the high spatial resolution and broad swath that AVIRIS provides, this study suggest the possibility for accurate mapping of  $CH_4$  emissions for extended sources (urban areas, industrial facilities, wetlands, landfills, pipelines, etc.) as well as, possibly, for the detection of leakage from sequestration sites, depending, of course, on leakage levels.

The literature contains information on two airborne instruments developed for high-resolution (spectral) measurements of reflected sunlight in the near IR, even though such measurements provide excellent sensitivity for detection of total-column CO<sub>2</sub>, CH<sub>4</sub>, CO, and other GHGs.

The Japanese GOSAT project deployed the Tsukuba engineering model of their Fourier Transform Spectrometer (FTS) on small aircraft over Australia and Siberia in 2007 (Suto et al. 2008, Kuze and Suto 2009) before installing it on Mt. Tsukuba for downlooking measurements of an adjacent rice field (Yoshida et al. 2010). The Tsukuba instrument operates in three near-IR bands (12,800-13,200 cm<sup>-1</sup>, 5800-6400 cm<sup>-1</sup>, and 4700-5200 cm<sup>-1</sup>) with a ~ 0.25 cm<sup>-1</sup> resolution in each band. The field of view is fixed at 15.8 mrad, corresponding to a 240 m circular field of view from an altitude of 15 km. High signal-to-noise spectra were recorded (Figure H-1). However, there has been no report of CO<sub>2</sub> or CH<sub>4</sub> retrievals from these spectra.



Figure H-1. Spectra recorded by the Tsukuba FTS during its 2007 flight campaigns. Top panel: 12,900 to 13,200 cm<sup>-1</sup> region showing strong absorptions in the  $O_2$  A-band. Middle panel: 5800 to 6400 cm<sup>-1</sup> region showing absorptions from  $CH_4$  and  $CO_2$ . Bottom panel: 4700 to 5200 cm<sup>-1</sup> spectral region showing strong absorptions from  $CO_2$  (Suto et al. 2008). Graphic reproduced with permission from the author.

NASA recently funded the Carbon in Arctic Reservoirs Vulnerability Experiment (CARVE) as part of its Earth Ventures (EV-1) aircraft investigations. CARVE will acquire a build-to-print version of the Tsukuba FTS with an optics modification to convert the 4700-5200 cm<sup>-1</sup> channel to cover the 4000-4400 cm<sup>-1</sup> range for detection of CH<sub>4</sub> and CO. This instrument will be delivered in late 2011. Preliminary calculations indicate signal-to-noise levels in excess of 500 in all channels for a 4 s integration time over land scenes with albedos of 30%, corresponding to a CO<sub>2</sub> retrieval precision that is anticipated to be ~ 1 ppm or better, for individual retrievals. This performance is considerably better than that of the GOSAT satellite instrument as a consequence

of reduced surface scene heterogeneity and cloud/aerosol interference as a consequence of its smaller field of view.

The Methane Airborne Mapper (MAMAP) developed by the University of Bremen measures reflected and scattered solar radiation in the short-wave IR (SWIR) and near-IR (NIR) parts of the spectrum at moderate spectral resolution (Bovensmann et al. 2010, Gerilowski et al. 2011). The SWIR channel yields measurements of atmospheric absorption bands of CH<sub>4</sub> and CO<sub>2</sub> in the spectral range 1.59-1.69  $\mu$ m, at a spectral resolution of 0.82 nm. The NIR channel around 0.76  $\mu$ m measures the atmospheric O<sub>2</sub> A-band absorption with a resolution of 0.46 nm. MAMAP was designed for flexible operation aboard a variety of airborne platforms (e.g., Cessna 207, Cessna Caravan, and AWI Polar-5 aircraft). Tests demonstrate that the instrument is able to measure and retrieve CH<sub>4</sub>/CO<sub>2</sub> profile scaling-factor ratios (PSFRs) with precisions of ~0.33% (with 0.148 s exposure times), corresponding to a single-exposure SNR in the range of 1600. This is in good agreement with model simulations where shot noise, dark noise, and detector readout noise are the main contributors (Gerilowski et al. 2011). See Figure H-2.



Figure H-2. Normalized MAMAP  $CO_2/CH_4$  profile scaling factor ratio (PSFR) retrieved from measurements acquired over the Schwarze Pumpe power plant near Berlin in eastern Germany. Right: Photo automatically taken during the flight over the power plant (top), dimensionless  $CO_2$  profile scaling factors (middle), and dimensionless  $CH_4$  profile scaling factors (bottom). All values shown in a given map as part of the flight have been scaled with a constant factor such that the scaled values of the whole flight are close to unity (green). The data have been smoothed using a seven point moving average. Gaps are due to (data) quality filtering. The  $CO_2$  output of the power plant was 26 t/min during the overflights (Gerilowski et al. 2011).

At an altitude of 4500 m, MAMAP reaches an average single-readout precision of the retrieved  $CH_4/CO_2$  PSF ratios in the range of ~1.1% (for a 0.058 s exposure time) over land targets with homogeneous radiance distribution. Assuming that changes in concentration only occur in the  $CH_4$  column below the aircraft, this corresponds to a 0.73%  $CH_4$  total-column variation. For airborne measurements over targets with inhomogeneous surface radiance, the instrument achieves a single-readout precision of the retrieved PSF ratios of 2.8% (at 0.058 s exposure time) for land (LIH) and 2.74% (at 1 s exposure time) for water (WIH). Assuming changes in the  $CO_2$  column as constant and that  $CH_4$  changes occur only below the aircraft altitude (4500 m), this corresponds to single-readout total-column precisions of 1.9% for land (albedo/SSR ~0.18) and 2.5% for water (albedo/SSR ~0.01).

The demonstrated instrument precision of ~1% total column at the high spatial resolution enables  $CH_4$  emissions from strong local sources to be quantified. Such local sources comprise geological sources such as dry seeps and mud volcanoes, the destabilization of shallow gas hydrates, anthropogenic emissions from landfills with organic waste, and fugitive emissions from oil and gas industry (i.e., well drilling and abandoned gas wells, oil sand tailings settling basins, emissions from gas and oil processing, and gas compression and transport). In addition, strong local CO<sub>2</sub> sources such as coal-fired power plants and direct and sub-areal emissions from volcanoes can be measured and characterized. Measurements of emissions from strong and large areal sources such as rice paddies, tropical, and Siberia wetlands, will become feasible for periods of large emissions but requires appropriate weather conditions, flight patterns, and data averaging strategies, and, of course, airspace access.

Simulations of CarbonSat space-based observations based on the performance of the MAMAP instrument lead to the conclusion that power plant  $CO_2$  emissions can be both detected and quantified. The estimated  $CO_2$  emission uncertainty is in the range 0.5 to 5 MtCO<sub>2</sub>/year (1 $\sigma$ ) for single power plant overpasses, which is about 2–20% of the emission of a large power plant (Bovensmann et al. 2010).

## H.3 Balloon-Borne Solar Occultation

Balloon-borne solar occultation remote sensing is mature and has been used for decades to return profiles of GHGs and other atmospheric trace gases in the stratosphere and upper troposphere (5 to 45 km) (Toon 1991, Camy-Peyret 1995). Table H-1 and Figure H-3 from Toon et al. (1999) compare the results of MkIV profile retrievals with those from in situ instruments aboard the NASA ER-2 during the 1997 POLARIS campaign in Alaska (Toon et al. 1999). Agreement is very good. Detection precisions vary from 5% to 20%, depending on the molecule, with vertical resolution of ~2 km and a horizontal resolution of ~350 km. Excellent results are obtained for CH<sub>4</sub> and N<sub>2</sub>O. Sulfur hexafluoride (SF<sub>6</sub>), chlorofluorocarbons (CFC), and (other) hydrocarbons are retrieved with lower precision.

Gas	MkIV Accuracy	ER-2 Accuracy	Bias: ER-2/	Bias: ER-2/	Bias: ER-2/	
	%	%	MkIV(z)	$MkIV(N_2O)$	MkIV(N2O)	
N₂O	5	3	1 03± 05	(1.03±.00)	$(1.00\pm00)$	
01	6	5	0.98±.06	1.12±.17	098±14	
CO	5	10	0.98±.30	$0.83 \pm 35$	1 11±.36	
CH₄	5	5	0.98±.03	0 96± 01	0.98±.01	
H <sub>2</sub> O	6	10	$125\pm 61$	$1.08 \pm 71$	1.25±.99*	
NOy	15	10	1.00±10	1 15±.09	1.03±.08	
NOx	10	10	0.85±.15	0.98±.22	0 87±.21	
HCI	5	10	0 97±.07	1 05±.06	0.99±.06	
CINO <sub>3</sub>	15	20	0.71±.10	0 96±.20	078±.12	
CCL	10	3	081±09	0.79±.07	$0.85 \pm 08^{+} *$	
CChF	10	2	101±13	0 92±.07	$101 \pm 08$	
CCl <sub>2</sub> FCC	IF <sub>2</sub> 20	3	0.91±.07	0 88±.06	$0.89 \pm 05^+$	
CCl <sub>2</sub> F <sub>2</sub>	10	2	1 00± 06	0 96± 04	0 99± 03	
SF <sub>6</sub>	10	5	0.87±.06	0 85±06	0.86±.05**	
CHCIF <sub>2</sub>	15	5	0.96±03	0.91±.03	$0.94 \pm .03^{\dagger}$	
CH <sub>3</sub> Cl	15	5	1.06±07	0.98±.06	$1.05 \pm 06$	
C <sub>2</sub> H <sub>6</sub>	15	5	0.87±.21	0 85±.41	$1.05 \pm 72$	

Table H-1. MkIV and ER-2 Measurement Accuracies and Calculated Biases (from Toon et al. 1999).

Despite high sensitivity, solar occultation has not been extensively applied to the remote sensing of  $CO_2$  or other GHGs. Early applications of solar occultation assumed that atmospheric  $CO_2$  was well mixed and constant (e.g., Rodgers 2000, p. 7) and used the information content in the  $CO_2$  absorption features to retrieve pressure, temperature, and/or tangent height. The inability of solar occultation to provide measurements for lower altitudes has also hindered its application to GHG remote sensing. However, Pak and Prather suggested that vertical profiles of  $CO_2$  from the stratosphere down to 5 km altitude, with a monthly mean uncertainty of 1% (3-4 ppm) contain key longitudinal information and can improve the derivation of  $CO_2$  fluxes from continent-scale regions, equal to or better than what can be achieved with column measurements (Pak and Prather 2001). Observational system simulation experiments (OSSEs) showed that measurements of free-tropospheric  $CO_2$  abundances at coarse spatial resolution improve a posteriori flux estimates as well as more highly resolved  $CO_2$  column abundances. Improvements are greatest over tropical landmasses, where observational uncertainties of even 3 ppm would reduce flux errors by half (Pak and Prather 2001).



Figure H-3. A comparison of gas VMR profiles measured by MkIV (black squares) and by instruments on board the ER-2 aircraft (colored symbols). In the upper panels, the comparison is illustrated as a function of altitude, while in the lower panel they are plotted as a function of  $N_2O$  (Toon et al. 1999).

Satellite data are less useful over high latitudes in either hemisphere where uncertainties less than 1 ppm would be needed to show notable improvements. Vertical profiles of  $CO_2$  abundance in the free troposphere from solar occultation with a full spectrum FTIR have the added advantage of potentially retrieving the abundance of more than 30 other trace gases and aerosols in the same air mass as the  $CO_2$ . Such observations, combined with a multi-species inversion, could further reduce uncertainty in  $CO_2$  fluxes (Pak and Prather 2001).

The most detailed study of  $CO_2$  vertical profiling from solar occultation measurements to date is the work of Foucher et al. (2009) using data from the Atmospheric Chemistry Experiment (ACE) satellite (Figure H-4). A major innovation of the Foucher et al. method is to determine tangent heights and pressure-temperature profiles in the 5 to 25 km altitude range independently of  $CO_2$ using the N<sub>2</sub> absorption continuum (Lafferty et al. 1996). Foucher et al. overcome the potential impact of uncertainties in the temperature knowledge on the retrieved  $CO_2$  profile through careful selection of the  $CO_2$  microwindows used in the retrieval (Table H-2). The results show a vertical resolution close to 2.5 km and accuracy of ~2 ppm after averaging over 25 profiles. Table H-2. Microwindows used for ACE-FTS  $CO_2$  profile determination and error budget for  $CO_2$  profile retrievals from ACE-FTS spectra (from Foucher et al. 2009).

number of m	w $CO_2$ spectral domain (cm <sup>-1</sup> )	altitude range <sup>a</sup> (km)	$E'' (cm^{-1})^{b}$	$E'' (cm^{-1})^{c}$	
12	1920–1955/ <sup>12</sup> C <sup>16</sup> O <sub>2</sub>	9–25	150.2	512.2	
13	2010-2030/ <sup>13</sup> C <sup>16</sup> O <sub>2</sub>	7-20	162.8		
32	2600-2635/ <sup>18</sup> OC <sup>16</sup> O	5-15	61.6		
9	3150-3205/ <sup>12</sup> C <sup>16</sup> O <sub>2</sub>	5-25	182.6		
16	3315-3355/ <sup>12</sup> C <sup>16</sup> O <sub>2</sub>	5-25	154.6	777.4	

 $^{\rm a}$  not all microwindows of each family are used for the same altitude range  $^{\rm b}$  mw used for CO\_2 retrieval

<sup>c</sup> mw used for T retrieval

Table 3. CO2 error budget evolution as a function of the number of micro-windows selected.

Number of mw	Noise error <sup>a</sup>		Temperature error a			Total error <sup>b</sup>			
	5-10 km	10–15 km	15–20 km	5–10 km	10–15 km	15–20 km	5-10 km	10–15 km	15-20 km
10	0.759	0.746	0.742	0.694	0.789	0.397	0.738	0.805	0.723
15	0.499	0.573	0.578	0.277	1.18	0.663	0.440	0.702	0.585
20	0.409	0.479	0.480	0.363	1.03	0.437	0.394	0.601	0.477
25	0.378	0.451	0.436	0.177	0.892	0.757	0.324	0.547	0.464
30	0.365	0.421	0.423	0.365	0.959	0.857	0.388	0.582	0.467

<sup>a</sup> ratio between retrieval error and retrieval error from the initial set containing 5 micro-windows

<sup>b</sup> in ratio as <sup>a</sup>, total error includes random noise, temperature and non target species uncertainty errors



Figure H-4.  $CO_2$  profile retrievals from ACE-FTS spectra for a region in the Northern Hemisphere covering 50-70N and 0-90W in July 2005 (grey lines) and July 2006 (red lines) (Foucher et al. 2009). Retrievals in the 10 to 22 km region used  ${}^{16}O^{12}C^{16}O$  microwindows. Retrievals in the 7 to 12 km range used  ${}^{16}O^{12}C^{18}O$  microwindows.

## H.4 Active Remote Sensing

Laser-based active remote sensing could potentially revolutionize the detection of atmospheric GHG concentrations. It would enable continuous 24-hr sampling of the total column as well as vertical profiles, can potentially operate over all latitudes and seasons, and should perform equally well over land and ocean, since the observation geometry for nadir detection is always viewing the "glint." However, technical challenges in developing lasers with the required wavelength coverage, power, and lifetime have limited the advancement of active GHG remote sensing instruments, at least to date.

Menzies and Tratt (2003) analyzed the system requirements for CO<sub>2</sub> differential absorption LIDAR (DIAL), examining both the 2.0  $\mu$ m and 1.5  $\mu$ m absorption bands. In this technique, the relative absorption is compared for excitation near the absorption line center and at one, or more, frequencies along the wings of the absorption feature where the absorbance is less intense. The CO<sub>2</sub> detection sensitivity at a given altitude is a function of the total round-trip absorption for each of the frequencies employed (Figure H-5).



Figure H-5. Left panel: Weighting functions for frequency offsets of 0.07, 0.14 and 0.21 cm<sup>-1</sup> from the 4875.749 cm<sup>-1</sup> line center of the R(30) 20013  $\leftarrow$  00001 transition. Right panel: Weighting functions for frequency offsets of 0.020, 0.030, 0.040 and 0.070 cm<sup>-1</sup> from the 6327.061 cm<sup>-1</sup> line center of the P(24) 30012  $\leftarrow$  00001 transition (Menzies and Tratt 2003).

Menzies and Tratt (2003) concluded that the susceptibility of the optical depth to uncertainties in knowledge of the atmospheric temperature profile is a sensitive function of the lower energy level of the transition and also dependent on the sounding frequency offset from line center. Only a small number of absorption lines in the  $30012 \leftarrow 00001$ ,  $30013 \leftarrow 00001$ , and  $20013 \leftarrow 00001$  bands of  ${}^{16}O^{12}C^{16}O$  exhibit the optimum combination of acceptable temperature susceptibility, target altitude of emphasis for the weighting functions, and adequate round-trip optical depth. The 6246 – 6365 cm<sup>-1</sup>(1.57 – 1.60 µm) sounding frequencies appear to be better suited to CO<sub>2</sub> mixing-ratio retrieval in the mid-troposphere to upper troposphere, whereas those in the 4828 – 4876 cm<sup>-1</sup> (2.05 – 2.07 µm) region are most appropriate for measurements in the lower troposphere where the signals relevant to CO<sub>2</sub> source and sink fluxes are most evident.

Ehret et al. (2008) reported a similar sensitivity analysis for detection of  $CO_2$ ,  $CH_4$ , and  $N_2O$  (see Figure H-6). Soundings in the vibration-rotational bands around 1.6 and 2.1 µm were found adequate for monitoring  $CO_2$ , the spectral regions at 1.6 and 2.3 µm are suited for  $CH_4$ , and

wavelengths around 3.9  $\mu$ m can be used for N<sub>2</sub>O measurements. For CO<sub>2</sub> and CH<sub>4</sub>, the following target observational requirements for the relative random error can be met: 0.2% for CO<sub>2</sub> and 0.4% for CH<sub>4</sub> for soundings at 1.6  $\mu$ m, as well as 0.4% for CO<sub>2</sub> at 2.1  $\mu$ m and 0.6% for CH<sub>4</sub> at 2.3  $\mu$ m. The IPDA instruments considered in the simulation are expected to be of moderate size in terms of required telescope aperture (0.5 – 1.5m) and laser average power (0.4 – 4W).



Figure H-6. Absorption line shape of the  $CO_2$  transition centered at  $v_0 = 6361.2509 \text{ cm}^{-1}$  with the absorption cross section marked for detuning one  $(v_L = v_0 + \gamma)$  and two  $(v_L = v_0 + 2\gamma)$  line widths from line center (Ehret et al. 2008).



Figure H-7. LIDAR estimated CO2 column number density to surface with 1 $\sigma$  deviation error bars (in black) made at the indicated altitudes versus calculated CO2 column density to surface (in orange) from the in situ sensor as a function of flight altitude (Abshire et al. 2010).

Several groups have developed CO<sub>2</sub> DIAL demonstrator instruments for the upcoming ASCOPE and ASCENDS satellite missions. Amediek et al. (2009) reported airborne reflectance measurements from a 1.57  $\mu$ m CO<sub>2</sub> DIAL system, but did not retrieve column CO<sub>2</sub> from these data. There are three airborne demonstration instruments under development in support of the ASCENDS Decadal Survey mission, but only Abshire et al. (2010) have reported retrieving CO<sub>2</sub> estimates from their measurements (Figure H-7) to date.

Finally, ground-based LIDAR profiling systems are also under development (Gibert et al. 2008, Koch et al. 2008, Sakaizawa et al. 2009). These systems provide high sensitivity and detailed vertical-profile data on boundary-layer  $CO_2$ , as well as valuable test beds for  $CO_2$  LIDAR technology development.

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"σώφρονος δ' ἀπιστίας οὐκ ἔστιν οὐδὲν χρησιμώτερον βροτοῖς." <sup>1</sup> "Nothing's more useful to mortals than judicious disbelief." <sup>2</sup>

"Trust, but verify and validate."<sup>3</sup>

<sup>&</sup>lt;sup>1</sup> This also, partly, motivated the present study and is typically quoted as, "Man's most valuable trait is a judicious sense of what not to believe." It is the opening quote in the book *Cleopatra* (2010, p. 1) by Stacy Schiff, who attributes it to Euripides, as also attributed in many sites on the Web, but with no citation. The passage was located by G.W. Pigman III, Professor of English at Caltech, who was asked for help. It is in the play *Helen* (1617f) by Euripides (e.g., <a href="http://www.perseus.tufts.edu/hopper/text;jsessionid=BD3AA7E7C51EEC10F8616508F5DB91FA?doc=Perseus%3Atext%3A1999.01.0099%3Acard%3D1577">http://www.perseus.tufts.edu/hopper/text;jsessionid=BD3AA7E7C51EEC10F8616508F5DB91FA?doc=Perseus%3Atext%3A1999.01.0099%3Acard%3D1577</a>).

<sup>&</sup>lt;sup>2</sup> Translation by Paul Dimotakis.

 $<sup>^3</sup>$  The GHGIS team's proposed update to Ronald Reagan's quote on the inside of the front cover.

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