Feng Sha (Orcid ID: 0000-0002-2376-0868)
Lauvaux Thomas (Orcid ID: 0000-0002-7697-742X)
Keller Klaus (Orcid ID: 0000-0002-5451-8687)
Davis Kenneth, J. (Orcid ID: 0000-0002-1992-8381)
Rayner Peter (Orcid ID: 0000-0001-7707-6298)
Oda Tomohiro (Orcid ID: 0000-0002-8328-3020)
Gurney Kevin R. (Orcid ID: 0000-0001-9218-7164)

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A road map for improving the treatment of uncertainties in high-resolution regional carbon flux inverse estimates

Sha Feng[1, *], Thomas Lauvaux[1, †], Klaus Keller[2, 3], Kenneth J. Davis[1, 3], Peter Rayner[4], Tomohiro Oda[5, 6], Kevin R. Gurney[7]

[1]Department of Meteorology and Atmospheric Science, The Pennsylvania State University, State College, Pennsylvania 16803, USA.

[2]Department of Geoscience, The Pennsylvania State University, State College, Pennsylvania 16803, USA.

[3]Earth and Environmental Systems Institute, The Pennsylvania State University, State College, Pennsylvania 16803, USA.

[4]School of Earth Sciences, University of Melbourne, 3010, Vic, Australia.

[5]Global Modeling and Assimilation Office, NASA Goddard Space Flight Center, Greenbelt, Maryland 20771, USA.

[6]Goddard Earth Sciences, Technology and Research, Universities Space Research Association, Columbia, Maryland 20771, USA.

[7]School of Informatics, Computing and Cyber Systems, Northern Arizona University, Flagstaff, Arizona 86011, USA.

[*]Corresponding author: Sha Feng (sfeng@psu.edu)

[†]Now at Laboratoire des Sciences du Climat et de l'Environnement, CEA, CNRS, UVSQ/IPSL, Université Paris-Saclay, Orme des Merisiers, 91191 Gif-sur-Yvette cedex, France

Key Points:

- We quantify biospheric flux, fossil fuel emission, atmospheric transport, and boundary inflow uncertainties in modeled atmospheric CO_2.
- Biospheric fluxes and fossil fuel emissions are the largest contributors to atmospheric CO_2 uncertainty over North America.

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- Transport uncertainties can be approximated by random errors, while boundary inflow uncertainties are persistent and can be sizeable.

Abstract

Atmospheric inversions allow us to estimate the terrestrial carbon sink by combining atmospheric observations with atmospheric transport models. However, these inverse estimates remain highly uncertain. Here we quantify uncertainties in simulations of North American atmospheric CO_2 concentrations using a probabilistic approach. We demonstrate that uncertainty in fossil fuel emissions is a key factor in the uncertainty surrounding biospheric flux estimates. We show that atmospheric transport uncertainties in state-of-the-art numerical weather models diminish when averaged over time, while uncertainties in large-scale CO_2 boundary inflow considerably impair our ability to quantify regional fluxes. Current estimates of the North America land sink which neglect the uncertainties in CO_2 boundary inflow and fossil fuel emissions are likely overconfident. Our findings suggest that targeted use of new atmospheric observations and improved quantification of uncertainty components are a promising avenue to improve atmospheric inversions with the goal to refine estimates of biospheric CO_2 fluxes on regional and continental scales.

Plain Language Summary

The uncertainty in biospheric carbon dioxide (CO_2) flux estimates drives divergent projections of future climate and uncertainty in prescriptions for climate mitigation. The terrestrial carbon sink can be inferred from atmospheric CO_2 observations with transport models via inversion methods. Regional CO_2 flux estimates remain uncertain due to the mixture of uncertainties caused by transport models, prior estimates of biospheric fluxes, large-scale CO_2 boundary inflow, the assumptions in the inversion process, and the limited density of atmospheric CO_2 observations. Understanding the characteristics of these uncertainties in space and time is essential for accurate biospheric CO_2 flux estimates. Here we identify the terms that most confound biospheric flux estimates. Our results show that, over North America, (i) biospheric fluxes dominate the model uncertainty over all timescales. (ii) Contrary to expectation, fossil fuel emissions are the second largest source of uncertainty at all timescales. (iii) Transport uncertainties are large at short timescales, but act like random errors decreasing with time averaging. (ix) Continental boundary inflow uncertainties are large near the boundaries and become significant at seasonal to annual timescales. We propose sampling and analysis strategies that can better quantify and reduce uncertainties in both fossil fuel emission and biospheric flux estimates.

1 Introduction

The terrestrial biosphere is a vast sink for anthropogenic carbon dioxide (CO_2) emissions. On average it removes roughly 2.6 ± 1.2 Pg C per year [*Ballantyne et al.*, 2012; *Ciais et al.*, 2013; *IPCC*, 2014; *Keenan et al.*, 2016]. Understanding how this sink responds to climate change is crucial to inform climate projections and the design of climate risk management strategies [*Friedlingstein et al.*, 2014; *Reichstein et al.*, 2013; *Stocker et al.*, 2013]. Terrestrial ecosystem models that simulate terrestrial CO_2 fluxes (sources and sinks) generally exhibit large regional differences in land CO_2 uptake (Fig. S6). Atmospheric inversions, on the other hand, quantify biospheric CO_2 fluxes by combining terrestrial ecosystem models, fossil fuel emission inventories and atmospheric transport models with atmospheric CO_2 concentration measurements [e.g., *Bousquet et al.*, 2000; *Ciais et al.*, 2005]. Both approaches offer invaluable insights into the global extent and latitudinal distribution of terrestrial carbon sinks [*IPCC*, 2014]. However, considerable uncertainties remain with regard to (i) the magnitude of biospheric carbon fluxes on continental and regional scales [*Peylin et al.*, 2013; *Sarmiento et al.*, 2010], and (ii) the distribution of fluxes across continents [*Stephens et al.*, 2007]. Furthermore, the mechanisms driving long-term trends and climate change remain unclear, causing considerable uncertainty in climate projections [*Bonan and Doney*, 2018]. The uncertainties in our ability to estimate regional-scale CO_2 fluxes by atmospheric inversions stem from the multiple components of inversion systems, including atmospheric transport models, prior estimates of biospheric fluxes, large-scale CO_2 boundary inflow, and the assumptions in the inversion process along with the atmospheric CO_2 observations [*Schuh et al.*, 2013]. While the CO_2 observation network over North America has been rapidly expanded in the last decade [*Andrews et al.*, 2014], researchers still commonly prescribe uncertainties arising from these components in a statistically-consistent way but prone to under- or over-estimation as only the total uncertainty is verifiable. Most inverse studies assume that atmospheric transport uncertainty has the greatest impact on the inversion models' accuracy [*Baker et al.*, 2006; *Gurney et al.*, 2002; *Stephens et al.*, 2007]. Inverse studies typically prescribe terrestrial biospheric CO_2 flux uncertainty and are thus silent on the effects of the complex spatiotemporal error structures (Fig. S6). Most importantly, inversion studies generally assume perfect knowledge of fossil fuel emissions [e.g., *Gurney et al.*, 2002; *Liu et al.*, 2017]. However, the uncertainty in inventories of national, annual bottom-up fossil fuel emissions ranges from 4% to 20% across countries, depending on data collection and management [*Andres et al.*, 2014]. While annual estimates agree within 4% over the whole of North America [*Oda et al.*, 2018], the uncertainties in spatially explicit fossil fuel emissions at the city scale can increase to 30- 200% [*Andres et al.*, 2014; *Asefi-Najafabady et al.*, 2014]. Finally, few studies have assigned and documented boundary inflow uncertainty in ways that represent errors in large-scale CO_2 inflow advected over the simulation domain [e.g., *Alden et al.*, 2016; *Göckede et al.*, 2010; *He et al.*, 2018]. Overconfident treatment of fossil fuel emissions, under-confident treatment of transport, and hesitation to proceed with a regional high-resolution model because of the difficulty of including boundary inflow uncertainties result in incomplete uncertainty assessments. Poor uncertainty estimates can bias inverse estimates. The

often-prohibitive computational demands of uncertainty assessment are frequently addressed by prescribing uncertainties from expert judgment. And while expert judgment can provide useful insights, the complexity of those uncertainties poses considerable challenges [*O'Hagan and Oakley*, 2004; *Werner et al.*, 2017]. Here, we present comprehensive assessments of the different sources of model uncertainty at the continental scale in order to better inform the development of regional inversion models. We address this problem by creating the first ensemble-based modeling system able to explicitly quantify uncertainties from a variety of sources in atmospheric CO_2 simulations. Uncertainties in atmospheric CO_2 mole fractions are directly related to the potential of an inversion to inform about surface fluxes and boundary inflow. The forward modeling approach used here allows us to circumvent the use of a deterministic system, which is inherently influenced by subjective choices of *a priori* information, by using a well-calibrated, high-resolution, ensemble-based, forward modeling system to quantify the various uncertainty terms (Fig. S1; see SI for full description of the model evaluation and calibration). Note that the uncertainties in atmospheric boundary layer CO_2 mole fractions that are calculated here may be directly related to the uncertainties in surface CO_2 fluxes that inversions calculate through the spread of the ensemble: the spread in surface flux across the ensemble is transformed, through use of the transport model, into a spread in atmospheric boundary layer CO_2 mole fractions across the domain; the spread of the whole ensemble, and the uncertainties calculated from it, may be scaled up or down to match what the best estimate of uncertainty actually should be. This is assured by the calibration process of the ensemble spread based upon the observations. Thus, while this study does not directly calculate surface flux uncertainties, it provides a means for estimating those through examination of atmospheric boundary layer CO_2 mole fraction uncertainties.

2 Data and Methods

We quantify the uncertainty in the simulated atmospheric CO_2 concentrations using the root-mean-square difference (RMSD) between the ensemble members and the observations or the ensemble mean (see SI for a full description). In this work, we focus on the midday atmospheric boundary layer CO_2 concentrations over North America, similar to the data assimilated in current regional inversions. The domain of interest includes the majority of North America land and the surrounding ocean (see color-shaded area in Figure 2). For simplicity, the modeled CO_2 concentrations at Level 5 in our transport model WRF-Chem, ~550 m above ground level, and at 20 UTC are used to represent the well-mixed midday atmospheric boundary layer atmospheric boundary layer conditions. Our modeling system samples four sources of uncertainty in an atmospheric inversion: (i) atmospheric transport, (ii) biospheric fluxes, (iii) fossil fuel emissions, and (iv) large-scale CO_2 boundary inflow. We construct an ensemble suite for each component and calculate the associated uncertainty in the simulation accordingly. A summary of the members of ensemble suites and the associated uncertainty quantifications can be found in Table S1.

For the transport ensemble suite, we generate the ensemble by perturbing the model physics and initial and boundary conditions using the multiple physics and Stochastic Kinetic Energy Backscattering scheme (SKEBS) [e.g., *Rayner et al.*, 2010], ten members in total. For the boundary inflow suite, we use the global modeled posterior CO_2 concentrations from CT2016 [*Peters et al.*, 2007], NASA Carbon Monitoring System [*Liu et al.*, 2014], TM5 [*Basu et al.*, 2016], and GEOS-Chem [*Schuh et al.*, 2015] taking into full consideration the conservation of mass along the boundaries of our regional model domain, four in total; for the biospheric flux suite, we include the simulated net ecosystem exchanges (NEE) from 15 terrestrial vegetation models and their mean [*Fisher et al.*, 2016; *Huntzinger et al.*, 2013], SiB3 [*Baker et al.*, 2010; *Baker et al.*, 2008], and the posterior biospheric fluxes from CarbonTracker CT2016 [*Peters et al.*, 2007], 18 in total. All of the CO_2 boundary inflow and biospheric fluxes members are coupled with every WRF-Chem transport simulation at 27 km × 27 km with 51 vertical levels for the time period of 2010. Details about transport model setup can be found in Section 2.3 of SI.

For fossil fuel emissions, we use two methods to estimate the associated uncertainty for the simulations: an ensemble approach and an error propagation from national to tower-footprint resolutions. Our final estimate simply corresponds to the mean of the results from these two estimates to avoid over- or under-estimation of fossil fuel uncertainties. A full description of the fossil fuel CO_2 uncertainty estimates can be found in SI. Briefly, the ensemble approach is based on 25 perturbations of annual fossil fuel emission realizations from the Fossil Fuel Data Assimilation System (FFDAS) [*Asefi-Najafabady et al.*, 2014; *Rayner et al.*, 2010] with various parameters and input fields. Because the FFDAS perturbation artificially generates a few negative emission values (<10%) from small sources, we zero out the negative values in the ensemble suite. As a result, we use standard statistics for non-Gaussian distributions, i.e., half of the interquartile range of the fossil fuel CO_2 concentrations are used to represent the annual fossil fuel uncertainty. We introduce constant emissions (without any diurnal and seasonal variations) into the transport simulations, which allows us to propagate annual uncertainties of fossil fuel emissions into atmospheric CO_2 concentrations.

The second method relies on an error propagation approach. Since the errors propagate linearly from surface emissions/fluxes to atmospheric CO_2 concentrations, the ratio of the uncertainty to the mean in emissions remains the same in concentration space. Annual uncertainty estimates from four different gridded fossil fuel emission products at $3^\circ \times 3^\circ$ resolution is about 30%, defined as the upper bound [*Andres et al.*, 1996; *Andres et al.*, 2011]. We account for potential spatial error correlations and decrease the errors by half (from 30% down to 14%) due to emission factors, disaggregation biases, etc., to define the lower bound of fossil fuel uncertainties. Based on the linear relationship between the flux and concentration spaces, we translate the range of flux-based uncertainty estimates into the atmospheric CO_2 concentration (in ppm) using these ratios.

Because none of the fossil emission uncertainty estimates are available at the daily timescale, we use existing studies of whole-city aircraft mass balance, bottom-up emissions comparisons, and inversion approaches to define the range of daily uncertainties at 100% and 50% for the upper and lower bounds, respectively [*Gurney et al.*, 2019; *Oda et al.*, 2019; *Turnbull et al.*, 2011]. This range takes the consideration of daily and seasonal variations of the fossil fuel CO_2 uncertainty. In the error propagation approach, we determine the upper and lower bounds of the fossil fuel CO_2 uncertainty estimates at the daily timescale by scaling the mean of simulated CO_2 mole fractions 100% and 50%, respectively. In the ensemble-based (FFDAS) approach, we scale the median 100% to determine at the daily fossil fuel CO_2 uncertainty. Considering that differences among different emission products were estimated at 20% annually over large cities [*Gurney et al.*, 2019], our daily estimates are higher due to additional errors in prescribed day-to-day variations (e.g. weekly climatology, absence of weather-related variability).

We interpolate uncertainty estimates between daily and annual timescales with an exponentially decaying function of time to produce consistent uncertainty estimates, with the following justification. There are no robust estimates of temporal error correlations available at sub-annual scales for fossil fuel emissions. At short timescales within a week, fossil fuel emission uncertainties decrease rapidly by removing day-to-day variations caused by weather events and economic activities. Between weekly to monthly time scales, the errors remain similar with no additional information used by bottom-up products. We only expect a faster decrease once aggregating the uncertainties at seasonal to annual time scales. We acknowledge that this function is a simple interpolation for two estimates because there is not any better information. We justify the shape by considering the level of information available in bottom-up products.

The ensemble modeling system consists of 18,720 members (10-transport×4-boundary condition×18-biospheric fluxes×26-fossil fuel emissions). We apply a series of evaluation and calibration procedures, i.e. Taylor diagrams and rank histograms, to ensure the reliability of the ensemble system. We begin by examining the simulated transport with NOAA rawinsonde data (http://www.esrl.noaa.gov/raobs/fsl-format-new.cgi) to ensure that we have accurately calibrated uncertainty bounds in boundary layer wind fields and heights. We next evaluate the CO_2 boundary inflow from global models with high-altitude NOAA aircraft data (>3km above sea level) [*Sweeney et al.*, 2015]. We calibrate the ensemble system using NOAA tall tower CO_2 data [*Andrews et al.*, 2014]. The full description of our evaluation and calibration of the ensemble system is provided in the supplementary information.

3 Results

3.1 Timescale dependence of modeled CO_2 uncertainties

Atmospheric CO_2 concentrations are driven by an intricate interplay of atmospheric, biospheric, and anthropogenic processes. As a result, simulated concentrations have complex temporal and spatial structures on daily to yearly and local to continental scales (Fig. 1a/2/3). Note that, to reflect the estimates from the current inversions, we display the CO_2 uncertainty estimates at the locations of the NOAA in-situ tower measurement. While independent random errors would lead to a simple decrease in errors as the time window grows, our results (Fig. 1a) reveal more complex processes. The biospheric flux uncertainty dominates from daily to seasonal averaging windows, representing, as is commonly assumed in atmospheric inversions [*Peters et al.*, 2007], 50% or more of the model variance (fig. 1c). The contribution of biospheric flux uncertainty decreases from seasonal to annual time frames (44% of variance annually). Summertime ecosystem net productivity and wintertime net respiration are nearly balanced over a year (-0.75 $\pm$0.25 Pg C/year over North America [*Crowell et al.*, 2019]), hence reducing the absolute uncertainty of the net ecosystem exchange over a full year. The fossil fuel emission uncertainty, which is ranked second in importance on short timescales, becomes nearly equal to the biospheric flux uncertainty on the annual timescale. Meanwhile, the downscaling of national estimates increases fossil fuel emission uncertainties considerably (cf. SI). Boundary inflow uncertainty, representing large-scale CO_2 conditions in regional simulations, comprises 10% to 15% of the model variance in daily to half-year timescales but declines to 5% annually because, in global inversions, the annual atmospheric growth rate is constrained by observations rather than simulations. The transport uncertainty closely resembles a series of random errors when aggregated over time; the associated model variance decreases rapidly from 20% to 5% beyond the synoptic scale (i.e. a few days to a week). As a result, in our high-resolution, regional modeling system, it appears to be the least important factor on seasonal to annual timescales, less influential than is typically assumed in global inversions [*Baker et al.*, 2006; *Basu et al.*, 2016; *Gurney et al.*, 2002]. Atmospheric transport models perform quite well over North America, perhaps in part because of the relatively dense network of operational weather observations which are fed into state-of-the-art reanalysis products. Others such as higher spatial resolutions likely having a better representation of the transport and a domain-limited setup largely avoiding error growth could also lead smaller transport uncertainty in the regional modeling than the global modeling.

3.2 Implications for the interpretation and design of atmospheric inversion studies

The accuracy of atmospheric inversion results relies on accurately estimating uncertainty for each component of the system [*Tarantola*, 2005] (see also description in SI). Atmospheric inversion studies have typically relied on simplifying assumptions to produce these uncertainty estimates. As mentioned above, continental and global fossil fuel emissions are often assumed to be perfectly known [e.g., *Gurney et al.*, 2002; *Liu et al.*, 2017]. We re-examine this assumption

by quantifying the ratio of the biospheric CO_2 flux uncertainty to the sum of the remaining uncertainty components both with and without the fossil fuel emission uncertainty (Fig. 1b). Consider the common – though unrealistic – assumption of perfectly known fossil fuel emissions. In this case, the ratio of biospheric flux uncertainty to the sum of the remaining uncertainty source components reveals a complex pattern. It increases as the averaging time window grows up to monthly-to-seasonal timescales, drops abruptly at the half-year point, and increases again to reach its maximum at the annual timescale (Fig. 1b). On monthly-to-seasonal timescales, the biospheric uncertainty is more than twice the sum of other uncertainty terms. This unrealistic assumption would suggest that the monthly-to-seasonal periods are an optimal temporal window for improving biospheric CO_2 flux estimates and confronting divergent terrestrial biospheric CO_2 flux models with atmospheric inverse flux estimates.

Adopting a more realistic approach to the uncertainty of fossil fuel emissions changes the results drastically (Fig. 1b). The contribution of biospheric flux uncertainty is significantly decreased. Furthermore, the monthly-to-seasonal maximum in the biospheric flux share disappears almost entirely. Fossil fuel emissions now account for 20% or more of the total variance across all timescales (Fig. 1c). Fossil fuel emission uncertainty therefore plays a key role in biospheric CO_2 flux estimation and must certainly be included in continental-scale inversion studies. Without it, regional uncertainties in fossil fuel emission inventories may render accurate determination of biospheric CO_2 fluxes impossible.

3.3 Improving sampling strategies to reduce inversion uncertainties

Quantifying the individual components of the uncertainty in CO_2 fluxes and emissions is critical for regional inversion studies. We next analyze the relative contribution of each component of CO_2 flux variance to the total uncertainty across space and time to inform the design of optimal atmospheric CO_2 sampling strategies (Fig. 2). Spatially, the biospheric uncertainty dominates the total annual uncertainty across North America, excepting only the very edges of our domain. A few regions, namely the Canadian and Mexican West Coast, the Pacific Northwest, the Corn Belt, Florida, and the Canadian East Coast, show the variance of a biospheric flux uncertainty that is higher than 70% (Fig.2a). Biospheric flux uncertainties, integrated across North America, peak around the middle of the summer (Fig. 3) and are the largest contributor to monthly atmospheric CO_2 uncertainty for the entire year.

As expected in domain-limited inverse estimates, the CO_2 boundary inflow uncertainty is most important at the lateral boundaries of the domain. The northern and western boundaries are most visible, highlighting the large-scale CO_2 inflow from higher latitudes, (40-60°N) driven over North America by the North Pacific Jet (Fig. 2b). The colocation of the CO_2 boundary inflow uncertainty with the jet stream suggests the importance of synoptic-scale variations to annual biospheric flux estimates. The boundary inflow uncertainty shows seasonal variation similar to that of the biospheric uncertainty (Fig. 3). We hypothesize that this is due to large and uncertain biospheric fluxes in the northern hemisphere but outside of our study domain. Our

ability to constrain this inflow is limited by the sparsity of atmospheric CO_2 observations near the western boundary of the domain (Fig. S7).

Fossil fuel emissions uncertainty contributes the highest percentage to the annually-averaged total in the regions offshore of the East and Gulf Coast, the northwestern coastal region and most of California (Fig. 2c). The climatological mean flow, composed of mid-latitudinal westerly winds, drives fossil fuel CO_2 signals off the east coast. Monthly variations remain nearly level, with just a slight increase in winter and summer. While fossil emission uncertainty is never dominant over North America, when combined with uncertainty in the boundary inflow these components contribute a substantial fraction to the total uncertainty (Fig. 3). Note that the sum of fossil fuel and boundary inflow uncertainties has monthly variations nearly identical to those of biospheric flux uncertainty. This makes them practically indistinguishable in an inverse problem, unless our observations take advantage of the spatial structures in their uncertainties (Fig. 2) or measurements of additional trace gases, such as radiocarbons, are used [*Basu et al.*, 2016; *Rayner et al.*, 2010].

At the annual timescale, our results suggest that the transport uncertainty plays the least important role in regional biospheric CO_2 flux estimation, while uncertainties in CO_2 boundary inflow and fossil fuel emissions have greater potential to confound efforts to estimate North American biospheric fluxes. Observing the flow of air upstream, over the north-eastern Pacific Ocean and the northern boundary of the model domain, is a promising first step toward reduce the uncertainty introduced by large-scale CO_2 boundary inflow [*Alden et al.*, 2016; *He et al.*, 2018]. Accounting for fossil fuel uncertainty can further improve the accuracy of North American biospheric flux estimates. Additional targeted atmospheric CO_2 data, therefore, could substantially reduce the uncertainties in current regional and continental carbon flux estimates.

4 Discussion and Conclusions

Our study based on a calibrated ensemble modeling system suggests that, at seasonal to annual timescales, uncertainties in CO_2 boundary inflow and fossil fuel emissions have greater potential to confound efforts to estimate North American biospheric fluxes, and that atmospheric transport uncertainty plays the least important role in regional biospheric CO_2 flux estimation. These findings may be specific to moderately high-resolution, numerical weather models; atmospheric transport may be a larger source of uncertainty for coarser resolution transport models at the global scale. We suggest increasing the number of observations of atmospheric CO_2 concentrations taken at the northern and western boundaries of North America as a first step to reduce the uncertainty introduced by continental CO_2 boundary inflow. Accounting for uncertainty in fossil fuel emissions and including them in the inversion framework, with observations targeted to reduce uncertainty in fossil fuel emissions, can further improve the accuracy of North American biospheric CO_2 flux estimates. While the uncertainties presented here are in terms of atmospheric concentrations, the conclusions obtained are directly transferable to the surface fluxes, since the spread of flux and concentration is fixed for each

ensemble. Unrealistic assumptions about either of these two sources of uncertainty is likely to lead to erroneous conclusions about the other component of the North American CO_2 budget. Most challenging to inversions, transport model uncertainties at sub-monthly timescales remain critical, suggesting potential improvement in flux estimation from the joint assimilation of meteorological and CO_2 data, or more sophisticated meteorological transport schemes. Evaluation of inverse fluxes will also benefit from independent data over regions where independent components to the atmospheric CO_2 budget dominate, allowing improvements of the components to be evaluated.

We acknowledge that this work is based on the midday atmospheric boundary layer CO_2 simulations, and the implications can be limited to the regional carbon flux inverse estimates with surface in-situ atmospheric CO_2 data. The sensitivity of the model uncertainties is very likely different to the airborne in-situ and column-averaged measurements. *Chen et al.* [2019] studied the modeled CO_2 uncertainties in full-column CO_2 concentrations due to biospheric fluxes, transport and CO_2 boundary inflow using an ensemble system. They found that the model uncertainty from CO_2 boundary inflow stays consistent throughout the entire column of atmosphere, while both of the transport and biospheric CO_2 uncertainty decrease rapidly with the increase of the height; therefore, CO_2 boundary inflow plays the most important role for column-averaged CO_2 among the uncertainty components studied. A comprehensive study on the seasonal characteristics of these uncertainty components in the column-integrated CO_2 is underway. However, none of similar studies have been done with airborne in-situ measurements so far. Urgent investigations on the sensitivity of the model uncertainty to various measurement platforms, such as the airborne in-situ and column-averaged measurements is needed due to the fact that the availability of aircraft and remote sensing data has grown rapidly in the past few years.

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None of the authors are aware of conflicts of interests.

Data and Materials Availability

The three-hourly output from Multi-scale Synthesis and Terrestrial Model Intercomparison Project (MsTMIP; http://nacp.ornl.gov/MsTMIP.shtml) can be found the Modeling and Synthesis Thematic Data Center at Oak Ridge National Laboratory (ORNL; http://nacp.ornl.gov). CarbonTracker CT2016 results are provided by NOAA ESRL, Boulder, Colorado, USA from the website at http://carbontracker.noaa.gov. A set of GEOS-Chem simulated CO_2 mole fractions are provided by NASA Carbon Monitoring System (https://carbon.nasa.gov/). ODIAC can be downloaded from http://db.cger.nies.go.jp/dataset/ODIAC/collaborators.html. The CO_2 mole fraction data used in this work are prepared by the in-situ tall tower and aircraft programs at Network at National Oceanic and Atmospheric Administration (NOAA) Global Greenhouse Gas Reference. The dataset is archived in Observation Package (ObsPack) Global View Plus version 3.1 data products. The meteorological data used are from the NOAA rawindsonde stations (http://www.esrl.noaa.gov/raobs/fsl-format-new.cgi).

Author contributions

S. Feng and T. Lauvaux took lead roles in writing this paper and the design of the model framework. S. Feng carried out the forward model simulations and data analysis. K. Keller and K. J. Davis contributed to the design of the model framework. P. Rayner and K. R. Gurney provided the Fossil Fuel Data Assimilation System (FFDAS) realizations. T. Oda produced the $1° \times 1°$ uncertainty estimates of fossil fuel emissions. S. Feng, T. Lauvaux, P. Rayner, K. R. Gurney, and T. Oda conducted the analysis and interpretation of uncertainty in fossil fuel signals. S. Feng wrote the initial draft. All authors edited and approved the final manuscript.

References

Alden, C. B., et al. (2016), Regional atmospheric CO_2 inversion reveals seasonal and geographic differences in Amazon net biome exchange, *Global Change Biology*, *22*(10), 3427-3443.

Andres, R. J., T. A. Boden, and D. Higdon (2014), A new evaluation of the uncertainty associated with CDIAC estimates of fossil fuel carbon dioxide emission, *Tellus B: Chemical and Physical Meteorology*, *66*(1), 23616.

Andres, R. J., G. Marland, I. Fung, and E. Matthews (1996), A 1° × 1° distribution of carbon dioxide emissions from fossil fuel consumption and cement manufacture, 1950–1990, *Global Biogeochemical Cycles*, *10*(3), 419-429.

Andres, R. J., J. S. Gregg, L. Losey, G. Marland, and T. A. Boden (2011), Monthly, global emissions of carbon dioxide from fossil fuel consumption, *Tellus B*, *63*(3), 309-327.

Andrews, A. E., et al. (2014), CO_2, CO, and CH_4 measurements from tall towers in the NOAA Earth System Research Laboratory's Global Greenhouse Gas Reference Network: instrumentation, uncertainty analysis, and recommendations for future high-accuracy greenhouse gas monitoring efforts, *Atmos. Meas. Tech.*, *7*(2), 647-687.

Asefi-Najafabady, S., P. J. Rayner, K. R. Gurney, A. McRobert, Y. Song, K. Coltin, J. Huang, C. Elvidge, and K. Baugh (2014), A multiyear, global gridded fossil fuel CO_2 emission data product: Evaluation and analysis of results, *Journal of Geophysical Research: Atmospheres*, *119*(17), 10,213-210,231.

Baker, D. F., et al. (2006), TransCom 3 inversion intercomparison: Impact of transport model errors on the interannual variability of regional CO_2 fluxes, 1988–2003, *Global Biogeochemical Cycles*, *20*(1).

Baker, I. T., A. S. Denning, and R. Stockli (2010), North American gross primary productivity: regional characterization and interannual variability, *Tellus B*, *62*(5), 533-549.

Baker, I. T., L. Prihodko, A. S. Denning, M. Goulden, S. Miller, and H. R. da Rocha (2008), Seasonal drought stress in the Amazon: Reconciling models and observations, *Journal of Geophysical Research: Biogeosciences*, *113*(G1).

Ballantyne, A. P., C. B. Alden, J. B. Miller, P. P. Tans, and J. W. C. White (2012), Increase in observed net carbon dioxide uptake by land and oceans during the past 50 years, *Nature*, *488*, 70.

Basu, S., J. B. Miller, and S. Lehman (2016), Separation of biospheric and fossil fuel fluxes of CO_2 by atmospheric inversion of CO_2 and $^{14}CO_2$ measurements: Observation System Simulations, *Atmos. Chem. Phys.*, *16*(9), 5665-5683.

Bonan, G. B., and S. C. Doney (2018), Climate, ecosystems, and planetary futures: The challenge to predict life in Earth system models, *Science*, *359*(6375).

Bousquet, P., P. Peylin, P. Ciais, C. Le Quéré, P. Friedlingstein, and P. P. Tans (2000), Regional Changes in Carbon Dioxide Fluxes of Land and Oceans Since 1980, *Science*, *290*(5495), 1342.

Chen, H. W., F. Zhang, T. Lauvaux, K. J. Davis, S. Feng, M. P. Butler, and R. B. Alley (2019), Characterization of Regional-Scale CO_2 Transport Uncertainties in an Ensemble with Flow-Dependent Transport Errors, *Geophysical Research Letters*, *0*(0)., 46, 4049–4058. https://doi.org/10.1029/2018GL081341

Ciais, P., T. Gasser, J. D. Paris, K. Caldeira, M. R. Raupach, J. G. Canadell, A. Patwardhan, P. Friedlingstein, S. L. Piao, and V. Gitz (2013), Attributing the increase in atmospheric CO_2 to emitters and absorbers, *Nature Climate Change*, *3*, 926.

Ciais, P., et al. (2005), Europe-wide reduction in primary productivity caused by the heat and drought in 2003, *Nature*, *437*, 529.

Crowell, S., et al. (2019), The 2015–2016 carbon cycle as seen from OCO-2 and the global in situ network, *Atmos. Chem. Phys.*, *19*(15), 9797-9831.

Fisher, J. B., M. Sikka, D. N. Huntzinger, C. Schwalm, and J. Liu (2016), Technical note: 3-hourly temporal downscaling of monthly global terrestrial biosphere model net ecosystem exchange, *Biogeosciences*, *13*(14), 4271-4277.

Friedlingstein, P., M. Meinshausen, V. K. Arora, C. D. Jones, A. Anav, S. K. Liddicoat, and R. Knutti (2014), Uncertainties in CMIP5 Climate Projections due to Carbon Cycle Feedbacks, *Journal of Climate*, *27*(2), 511-526.

Göckede, M., D. P. Turner, A. M. Michalak, D. Vickers, and B. E. Law (2010), Sensitivity of a subregional scale atmospheric inverse CO_2 modeling framework to boundary conditions, *Journal of Geophysical Research: Atmospheres*, *115*(D24).

Gurney, K. R., J. Liang, D. O'Keeffe, R. Patarasuk, M. Hutchins, J. Huang, P. Rao, and Y. Song (2019), Comparison of Global Downscaled Versus Bottom-Up Fossil Fuel CO_2 Emissions at the Urban Scale in Four U.S. Urban Areas, *Journal of Geophysical Research: Atmospheres*, *124*(5), 2823-2840.

Gurney, K. R., et al. (2002), Towards robust regional estimates of CO_2 sources and sinks using atmospheric transport models, *Nature*, *415*, 626.

He, W., et al. (2018), CTDAS-Lagrange v1.0: a high-resolution data assimilation system for regional carbon dioxide observations, *Geosci. Model Dev.*, *11*(8), 3515-3536.

Huntzinger, D. N., et al. (2013), The North American Carbon Program Multi-Scale Synthesis and Terrestrial Model Intercomparison Project – Part 1: Overview and experimental design, *Geosci. Model Dev.*, *6*(6), 2121-2133.

IPCC (2014), The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change [Core Writing Team,

R.K. Pachauri and L.A. Meyer (eds.)]. 151 pp, IPCC, Geneva, Switzerland.

Keenan, T. F., I. C. Prentice, J. G. Canadell, C. A. Williams, H. Wang, M. Raupach, and G. J. Collatz (2016), Recent pause in the growth rate of atmospheric CO_2 due to enhanced terrestrial carbon uptake, *Nature Communications*, *7*, 13428.

Liu, J., et al. (2014), Carbon monitoring system flux estimation and attribution: impact of ACOS-GOSAT XCO_2 sampling on the inference of terrestrial biospheric sources and sinks AU - Liu, Junjie, *Tellus B: Chemical and Physical Meteorology*, *66*(1), 22486.

Liu, J., et al. (2017), Contrasting carbon cycle responses of the tropical continents to the 2015–2016 El Niño, *Science*, *358*(6360).

O'Hagan, A., and J. E. Oakley (2004), Probability is perfect, but we can't elicit it perfectly, *Reliability Engineering & System Safety*, *85*(1), 239-248.

Oda, T., S. Maksyutov, and R. J. Andres (2018), The Open-source Data Inventory for Anthropogenic CO_2, version 2016 (ODIAC2016): a global monthly fossil fuel CO_2 gridded emissions data product for tracer transport simulations and surface flux inversions, *Earth Syst. Sci. Data*, *10*(1), 87-107.

Oda, T., et al. (2019), Errors and uncertainties in a gridded carbon dioxide emissions inventory, *Mitigation and Adaptation Strategies for Global Change*. 24: 1007. https://doi.org/10.1007/s11027-019-09877-2

Peters, W., et al. (2007), An atmospheric perspective on North American carbon dioxide exchange: CarbonTracker, *Proceedings of the National Academy of Sciences*, *104*(48), 18925-18930.

Peylin, P., et al. (2013), Global atmospheric carbon budget: results from an ensemble of atmospheric CO_2 inversions, *Biogeosciences*, *10*(10), 6699-6720.

Rayner, P. J., M. R. Raupach, M. Paget, P. Peylin, and E. Koffi (2010), A new global gridded data set of CO_2 emissions from fossil fuel combustion: Methodology and evaluation, *Journal of Geophysical Research: Atmospheres*, *115*(D19).

Reichstein, M., et al. (2013), Climate extremes and the carbon cycle, *Nature*, *500*, 287.

Sarmiento, J. L., M. Gloor, N. Gruber, C. Beaulieu, A. R. Jacobson, S. E. Mikaloff Fletcher, S. Pacala, and K. Rodgers (2010), Trends and regional distributions of land and ocean carbon sinks, *Biogeosciences*, *7*(8), 2351-2367.

Schuh, A. E., D. F. Baker, and A. Jacobson (2015), GEOS-Chem-CarbonTracker, in *ESRL/Global Monitoring Annual Conference*, edited, Boulder, CO.

Schuh, A. E., et al. (2013), Evaluating atmospheric CO_2 inversions at multiple scales over a highly inventoried agricultural landscape, *Global Change Biology*, *19*(5), 1424-1439.

Stephens, B. B., et al. (2007), Weak Northern and Strong Tropical Land Carbon Uptake from Vertical Profiles of Atmospheric CO<sub>2</sub&gt, *Science*, *316*(5832), 1732.

Stocker, B. D., R. Roth, F. Joos, R. Spahni, M. Steinacher, S. Zaehle, L. Bouwman, R. Xu, and I. C. Prentice (2013), Multiple greenhouse-gas feedbacks from the land biosphere under future climate change scenarios, *Nature Climate Change*, *3*, 666.

Sweeney, C., et al. (2015), Seasonal climatology of CO_2 across North America from aircraft measurements in the NOAA/ESRL Global Greenhouse Gas Reference Network, *Journal of Geophysical Research: Atmospheres*, *120*(10), 5155-5190.

Tarantola, A. (2005), *Inverse Problem Theory and Methods for Model Parameter Estimation*, 348 pp., Society for Industrial and Applied Mathematics.

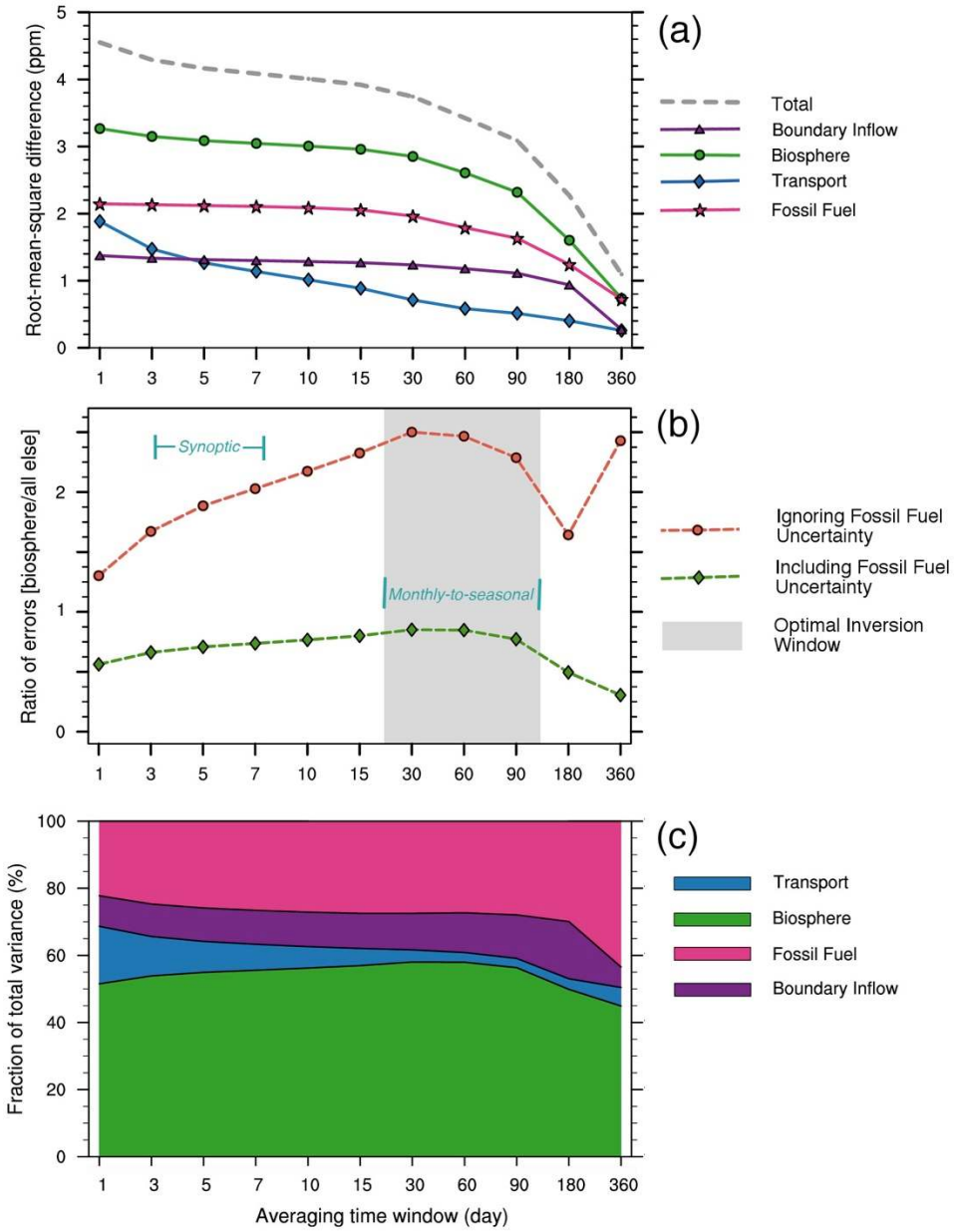
Turnbull, J. C., et al. (2011), Assessment of fossil fuel carbon dioxide and other anthropogenic trace gas emissions from airborne measurements over Sacramento, California in spring 2009, *Atmos. Chem. Phys.*, *11*(2), 705-721.

Werner, C., T. Bedford, R. M. Cooke, A. M. Hanea, and O. Morales-Nápoles (2017), Expert judgement for dependence in probabilistic modelling: A systematic literature review and future research directions, *European Journal of Operational Research*, *258*(3), 801-819.

Figure 1. Uncertainty metrics of the modeled midday atmospheric boundary layer CO_2 concentrations as a function of timescale presented for four model components (transport models, biospheric fluxes, fossil fuel emissions, and the boundary inflow) over North America for 2010. The domain of interest includes the majority of North America land and the surrounding ocean (color-shaded area in Figure 2). (a) Root-mean-square difference (RMSD) of simulated CO_2 from the observations, as contributed to by each of the inversion components and the total); (b) Ratio of the uncertainty (in the same RMSD) due to biospheric fluxes over that due to the rest of the error terms with and without consideration of the fossil fuel uncertainty; (c) Fraction of each variance-term to the total variance in the simulated CO_2. The uncertainties plotted are those from the ensemble sampled at the location of six NOAA CO_2 tall tower measurements, indicated by red triangles in Figure S2. The locations of these towers can be found in Figure 2 and Figure S2.

Figure 2. Spatial distribution of the fractions of variance in atmospheric boundary layer CO_2 concentrations due to (a) biosphere, (b) boundary inflow, and (c) fossil fuel emission uncertainties to the sum of these three terms at the annual timescale. These three components are coupled with atmospheric transport when we run the simulations. As a result, transport uncertainty scales with one of the components and cannot be independently presented. Given that annual transport uncertainty weights the least and act as random noise in Figure 1, we only show the fraction maps for the variance of the biospheric flux, boundary inflow, and fossil fuel emission uncertainties. Similar to Figure 1, the modeled midday atmospheric boundary layer CO_2 concentrations are used. The circled crosses denote the location of the NOAA tower measurements used for calculating RMSD in Figure 1.

Figure 3. Monthly mean variations of the modeled midday atmospheric boundary layer CO_2 uncertainties from biospheric fluxes, fossil fuel emissions, and boundary inflow over North America for 2010. The uncertainty of a given component is calculated by RMSD of simulated CO_2 across the associated ensemble members from the ensemble mean. The domain considered in computing the statistics includes the majority of North America land and the surrounding ocean (color-shaded area in Figure 2). The dashed line denotes the sum of the model uncertainty attributed to fossil fuel emissions and boundary inflow.



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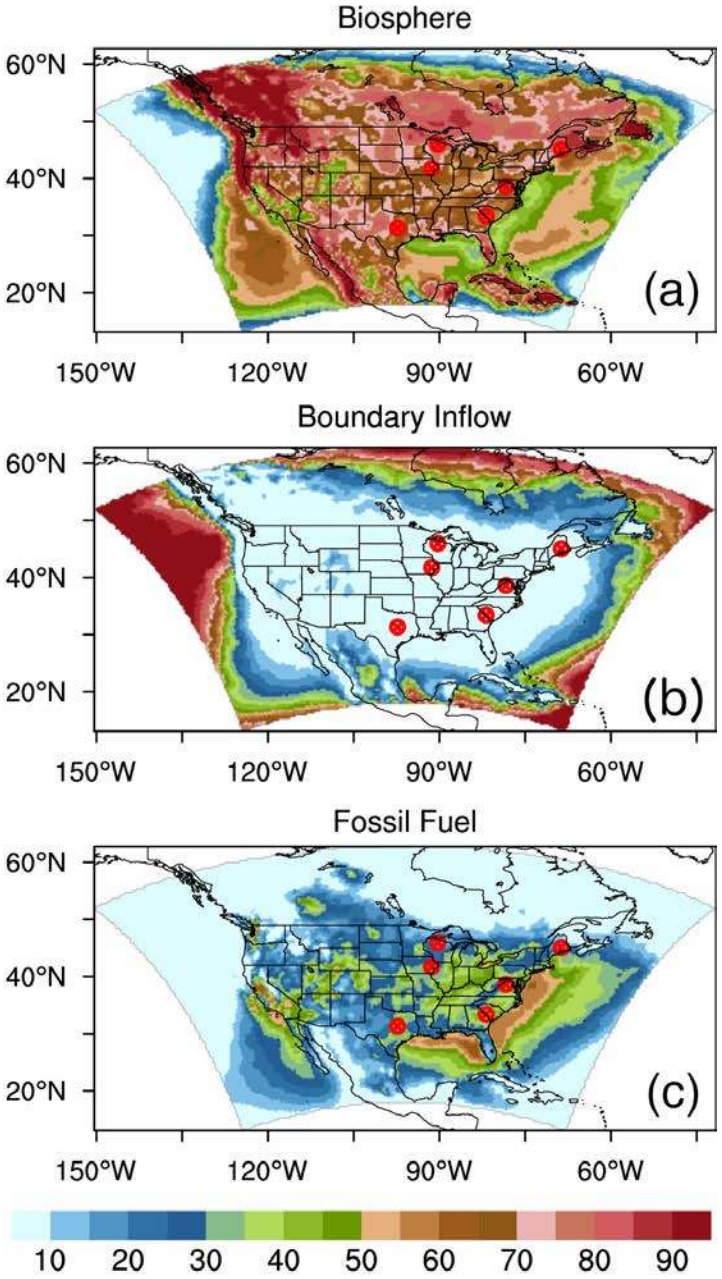

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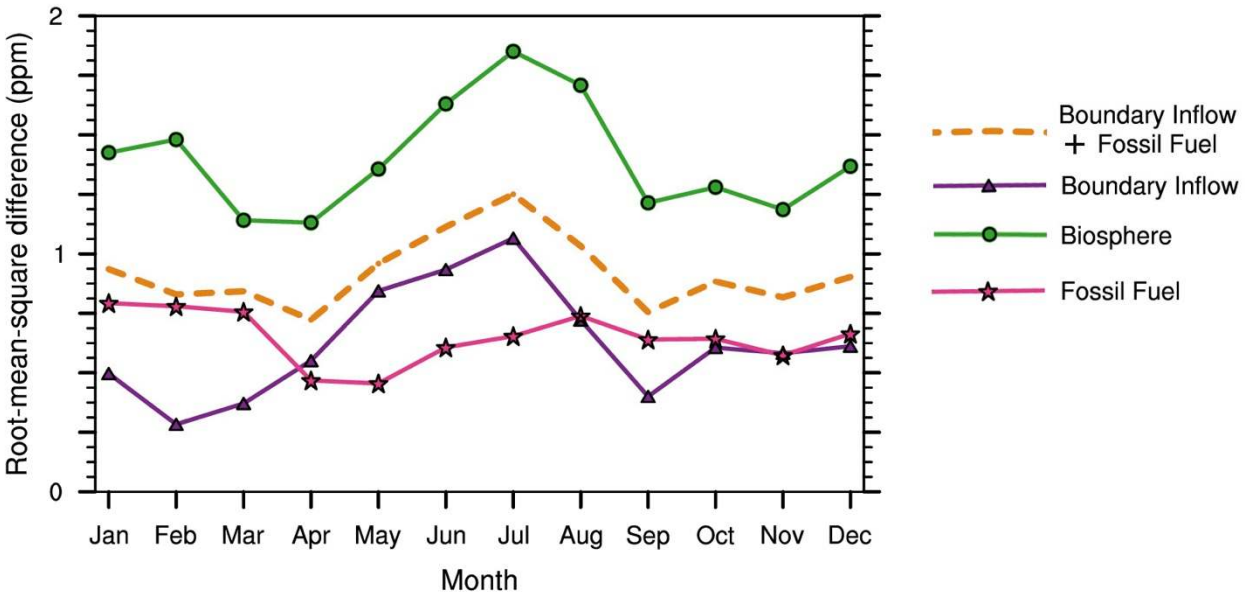

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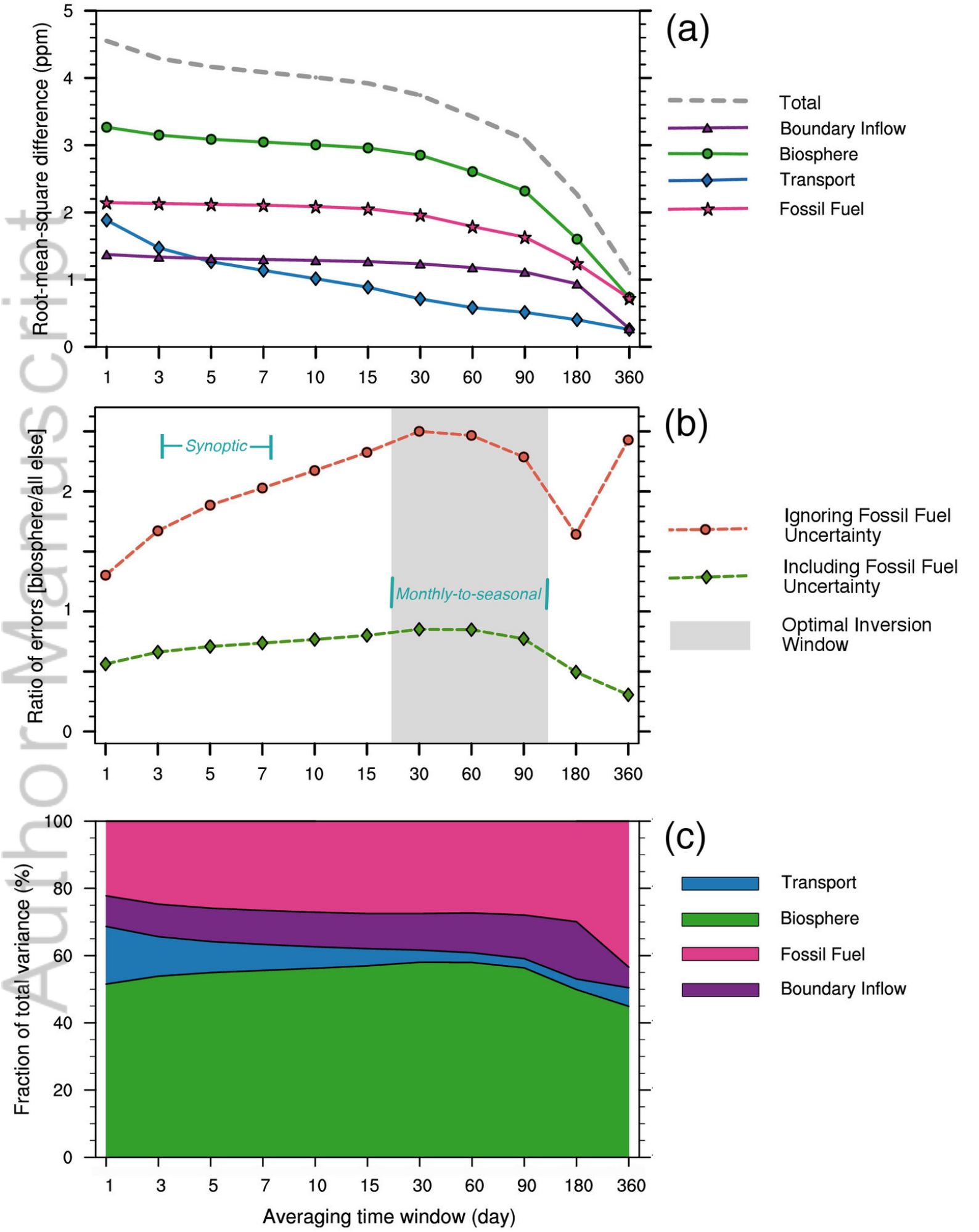

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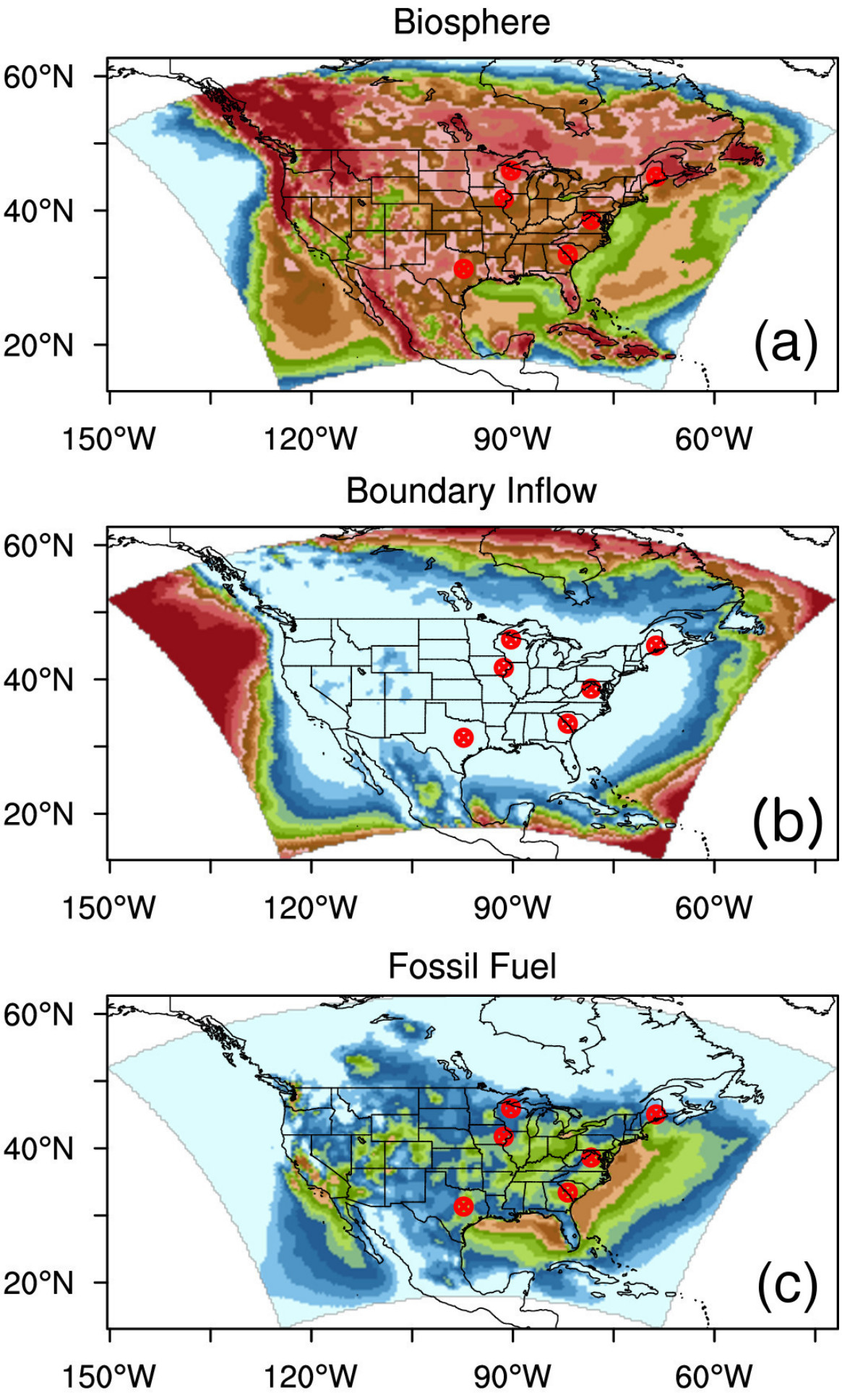

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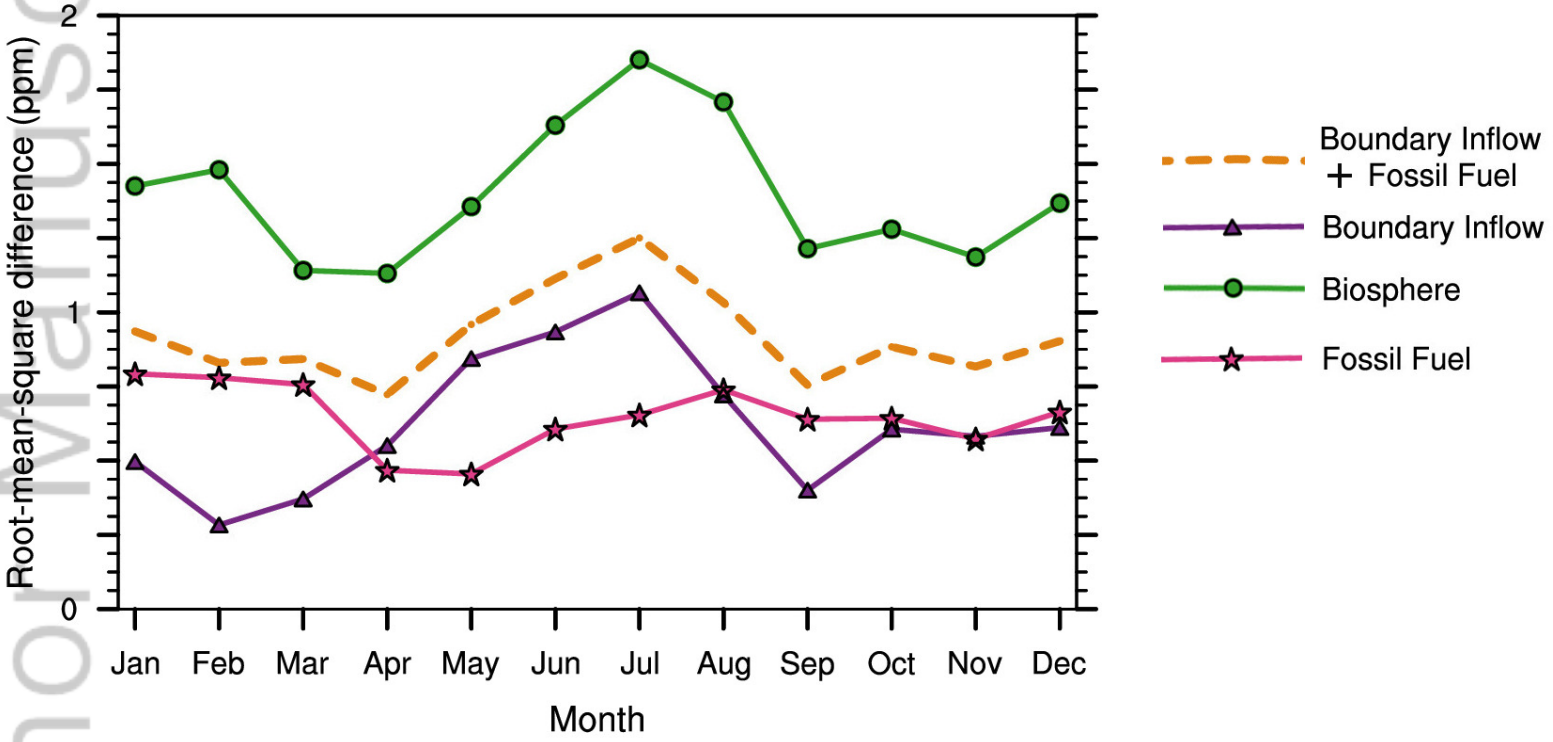

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Author/s:
Feng, S;Lauvaux, T;Keller, K;Davis, KJ;Rayner, P;Oda, T;Gurney, KR

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