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Doucette, William J; Shunthirasingham, Chubashini; Dettenmaier, Erik M; Zaleski, Rosemary T; Fantke, Peter; Arnot, Jon A

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WILLIAM J. DOUCETTE, CHUBASHINI SHUNTHIRASINGHAM, ERIK M. DETTENMAIER, ROSEMARY T. ZALESKI, PETER FANTKE, and JON A. ARNOT

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A REVIEW OF MEASURED BIOACCUMULATION DATA IN TERRESTRIAL PLANTS FOR ORGANIC CHEMICALS: METRICS, VARIABILITY AND THE NEED FOR STANDARDIZED MEASUREMENT PROTOCOLS

WILLIAM J. DOUCETTE,[a] CHUBASHINI SHUNTHIRASINGHAM,[b] ERIK M. DETTENMAIER,[c] ROSEMARY T. ZALESKI,[d] PETER FANTKE,[e] and JON A. ARNOT[f,g,h]

[a]Utah Water Research Laboratory, Utah State University, Logan, Utah, USA
[b]Air Quality Processes Research Section, Environment and Climate Change Canada, Toronto, Ontario, Canada
[c]Restoration Installation Support Team, Hill Air Force Base, Utah, USA
[d]ExxonMobil Biomedical Sciences, Occupational and Public Health, Annandale, New Jersey, USA
[e]Quantitative Sustainability Assessment Division, Department of Management Engineering, Technical University of Denmark, Lyngby, Denmark
[f]ARC Arnot Research and Consulting, Toronto, Ontario, Canada
[g]Department of Physical and Environmental Sciences, University of Toronto at Scarborough, Toronto, Ontario, Canada
[h]Department of Pharmacology and Toxicology, University of Toronto, Toronto, Ontario, Canada

* Address correspondence to william.doucette@usu.edu

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Abstract: Quantifying the transfer of organic chemicals from the environment into terrestrial plants is essential for assessing human and ecological risks, using plants as environmental contamination biomonitors, and predicting phytoremediation effectiveness. Experimental data describing chemical uptake by plants are often expressed as ratios of chemical concentrations in the plant compartments of interest (e.g., leaves, shoots, roots, xylem sap) to that in the exposure medium (e.g., soil, soil pore water, hydroponic solution, air). These ratios are generally referred to as bioconcentration factors (BCFs) but have also been named for the specific plant compartment sampled, such as root concentration factors (RCFs), leaf concentration factors (LCFs), or transpiration stream (xylem sap) concentrations factors (TSCFs). We reviewed over 350 papers to develop a database with 7,049 entries of measured bioaccumulation data for 310 organic chemicals and 112 terrestrial plant species. Various experimental approaches have been used; therefore, inter-study comparisons and data quality evaluations are difficult. Key exposure and plant growth conditions were often missing, and units were often unclear or not reported. The lack of comparable high confidence data also limits model evaluation and development. Standard test protocols, or at a minimum, standard reporting guidelines, for the measurement of plant uptake data are recommended to generate comparable, high-quality data that will improve mechanistic understanding of organic chemical uptake by plants.

Keywords: Bioconcentration, Plants, Organic contaminants

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INTRODUCTION

Plants are the largest component of the earth's biomass and are the base of all food webs. Organic chemical contaminants can directly contact and accumulate in above-ground plant tissues (shoots) through vapor and particle deposition or in below-ground tissues via the roots. The movement and distribution of the contaminants within the plant are determined by the properties of contaminants and plants. Plants and associated microorganisms (e.g., endophytes, rhizosphere organisms) can also transform organic chemicals, impacting their environmental fate and transfer to higher trophic levels. Quantifying and predicting the transfer of chemicals from the physical environment into terrestrial plants is important for assessing human and ecological risks, evaluating the use of plants as biomonitors of environmental contamination, and predicting the effectiveness of phytoremediation.

The contact of organic contaminants with above-ground vegetation (shoot) occurs through gas exchange and deposition at leaf surfaces, with the dominant pathway and kinetics dependent on the properties of the contaminant and leaf cuticle and the environmental conditions [e.g., 1, 2, 3]. The cuticle consists of several lipid or lipid-like components including cutin, cutan, and extractable waxes that exhibit varying affinities for organic contaminants [1, 4, 5]. It is also possible, but less likely to be significant for neutral hydrophobic chemicals ($1 < \log_{10}$ octanol-water (K_{ow}) partition coefficients < 8), that organic contaminants can sorb to the non-lipid organic matter fractions of leaves. Stomatal uptake might also be important for some chemicals [1]. Contaminants accumulating in shoot tissues during periods of high atmospheric concentration can also be released when exposure concentrations decrease [3, 6, 7].

The root uptake of most organic contaminants is passive. In passive transport, the more water transpired, the greater the amount of organic contaminants that moves into the plant. Once

a chemical passes through the root membrane, it can be transported to other parts of the plant, depending on its properties. For neutral compounds, hydrophobicity is one of the key transport factors [8-10], while for ionizable organics, the movement and distribution also depends on the dissociation constant (pKa), charge of the chemical, and pH of the various plant compartments [11]. Xylem channels conduct the flow of water, nutrients, and contaminants from roots to the photosynthetic sections of the plant, while phloem distributes sugars and other photosynthetic products throughout the plant. Xylem transport rates are directly related to transpiration rates, while phloem transport rates are governed by differences in solute concentrations between sites of synthesis and consumption [12]. Daytime xylem transport rates are generally 10 times greater than phloem transport rates [13], but their relative contributions to specific compartments can vary. For example, while xylem and phloem contribute roughly equally to apple fruit growth early in the growing season, from mid-to-late-growing season, the phloem dominates [13, 14]. Within the xylem, lateral movement to adjacent cells may provide a pathway for contaminants to move into the phloem [12, 15].

During transport within the plant, organic chemicals can be metabolized, sequestered within various plant tissues, and volatilized from the plant surfaces. Plants contain enzymatic systems such as cytochromes P-450, and evidence regarding the biotransformation capabilities of plants comes from cell culture and intact plant studies [16]. Plants can degrade a wide range of organic contaminants, from highly polar herbicides like glyphosate to very hydrophobic chemicals such as dichlorodiphenyltrichloroethane (DDT) and hexachlorobenzene (HCB) [e.g., 17, 18, 19]. Plant biotransformation capacity may also be chemical- and plant species-specific. For example, Liu et al. [20] showed that PCB77 was hydroxylated by poplar plants but not by switchgrass during the experiment period. Endophytic organisms can also contribute to the

metabolism of organic chemicals within plants [21]. Plant biotransformation rates are available for a few pesticides [e.g., 17, 22, 23], pharmaceutical chemicals [e.g., 24], and plasticizers [e.g., 25, 26]. Furthermore, plant dissipation rates (degradation and transport loss mechanisms) can vary considerably between different plant compartments and environmental conditions [27, 28]. For chemicals with high Henry's Law constants (K_{AW}) that have been translocated to shoots, volatilization from leaves and stems, often referred to as phytovolatilization, can be a measurable loss mechanism [e.g., 29, 30].

Differences between plant species can also be important in the root uptake of organic chemicals. For example, partitioning into the roots is a function of root lipid content in addition to the hydrophobicity of the chemical [31]. Another example of species differences is the unique ability of "gold rush" zucchini (*Cucurbita pepo,* subspecies *pepo*) to transfer hydrophobic organics from roots to above ground tissues, relative to other plants [32-35]. This enhanced root to shoot transfer is thought to be partly due to interactions with various proteins that increase the solubility of these compounds in the xylem sap [36, 37].

Empirical data describing the extent of chemical uptake by plants can be expressed as ratios of chemical concentrations in the plant compartment of interest (e.g. leaves, shoots, roots, xylem sap) to that in the exposure medium (air, soil, soil pore water, hydroponic solution) measured at the time the samples are collected [38]. These ratios are generally referred to as bioconcentration factors (BCFs) that implicitly assume steady state is approximated. The most commonly reported plant BCFs are for roots, stems or wood, leaves, shoots (above ground tissues), and xylem sap. The chemical concentration ratio between xylem sap and the external exposure solution (usually a hydroponic solution) is specifically referred to as a transpiration stream concentration factor (TSCF). When plant biomass increases faster than contaminant

uptake, growth dilution can influence BCF values. The importance of growth dilution in predicting foliar and root uptake of organic contaminants has been well documented [e.g., 28, 39, 40, 41].

Reliable, high-quality plant bioaccumulation data is critical in developing and evaluating plant bioaccumulation models, assessing human and ecological risks, using plants as environmental contamination biomonitors, and predicting phytoremediation effectiveness. Earlier reviews specifically focusing on modeling plant bioaccumulation [e.g., 42, 43-45], and more generally on terrestrial bioaccumulation [46, 47], have highlighted substantial experimental data gaps and limitations.

The objectives of the present study are to (1) summarize the common metrics for quantifying organic chemical bioaccumulation in terrestrial plants; (2) review and compile measured plant bioaccumulation data, including uptake and biotransformation rates published in the peer-reviewed literature; (3) assess the general consistency of information reported for plant bioaccumulation studies; (4) evaluate the applicability of some previously reported relationships between plant bioaccumulation metrics and physical-chemical properties (e.g., K_{OW} and octanol-air (K_{OA}) partition coefficients) to the newly compiled dataset; (5) illustrate possible data contradictions; (6) use simple theoretical partitioning models to provide a frame of reference for examining and comparing the different types of measured bioaccumulation data; and (7) provide preliminary direction for future plant bioaccumulation studies.

METHODS

Plant bioaccumulation concepts and assessment metrics

Figure 1 provides a conceptual overview of the key processes associated with organic chemical bioaccumulation in a plant and the typical metrics or test endpoints used to describe

these processes. Bioaccumulation metrics are reported using a variety of units depending how the chemical concentrations are expressed. Chemical concentrations in the plant tissues are commonly specified on either a fresh (fw) or dry weight (dw) basis. Occasionally, measured lipid contents of the plant tissues (mainly root and leaves) are reported (i.e., kg-lw/kg-dw) and the chemical concentrations are expressed on a lipid weight basis (lw). Contaminant concentrations in the environment surrounding the plant (exposure media) can also be reported in various ways. Chemical concentrations in air can be reported as total, including gaseous and particulate phases, or separately. Concentrations of chemicals in soils are typically reported on a dw basis; however, if the organic carbon content (OC) of the soil is measured (i.e., kg-OC/kg-dw), the results can also be expressed on an organic carbon normalized basis. When the concentrations for neutral organic chemicals are lipid and organic carbon normalized, chemical equilibrium partitioning approaches have been proposed to better understand chemical fate and plant bioaccumulation [48].

Table 1 lists definitions and summary calculations for the three general plant bioaccumulation metrics (endpoints) included in this review. Table S-1 in the Supporting Information (SI) provides a more detailed summary for all of the different specific metrics (n=21) included in the database. The first general plant bioaccumulation metric is defined as chemical concentration ratios between **below ground vegetation** (i.e., roots, tubers) and appropriate environmental compartments (i.e., soil or other solid phase medium, soil pore water solution or hydroponic solution). Tuber concentration factors (TCFs) and root concentration factors (RCFs) are specific examples of below ground vegetation concentration factors. TCFs and RCFs can be further sub-classified for cores and peels or total below ground tissues and whether or not the source phase is solid (e.g., soil) or liquid (e.g., hydroponic). The second

general metric characterizes chemical concentration ratios between **above ground vegetation** (i.e., foliage, shoot) or specific above ground plant compartment (i.e., stems, leaf, fruit) and appropriate environmental compartments (i.e., air, water, soil or soil solution). Leaf concentration factors (LCFs), shoot concentration factors (STCFs), stem concentration factors (SCFs), seed concentration factors (SdCFs) and fruit concentration factors (FCFs) are specific examples of above ground vegetation BCFs in the database. The third general bioaccumulation metric is the **transpiration stream concentration factor** (TSCF) defined as the ratio of chemical concentration in the xylem sap to the chemical concentration in water (hydroponic or soil solution) taken up by the plant. Ideally, bioaccumulation endpoints should be determined under steady state conditions (i.e., concentration ratios between plant compartments and exposure media are constant over time) or kinetically using uptake and elimination rates for consistency and comparability.

Plant bioaccumulation database development

The peer-reviewed literature was searched using the list of plant bioaccumulation metrics outlined in the introduction section (BCFs, RCFs, TSCFs, etc.) and biotransformation rates or corresponding half-lives in whole plants or individual plant compartments as key words. Only plant bioaccumulation metrics based on measured data were included in the database. Reported bioaccumulation metrics have various units depending on the exposure medium. If the units were documented in the study, this was noted in the database. However, in some cases, the units were not explicitly reported but could be inferred from the data provided. This was also noted in the database. In other cases, however, the units could not be readily inferred. Data from these studies were included but noted to show that the units were not available. When available, other key parameters reported from the experiments were also included in the database, such as exposure

concentration, (air) temperature, lipid and water content of sampled plant material, sampled plant mass, duration of light exposure, soil organic carbon and soil water content. The primary reference was also stated for each bioaccumulation value entered into the database.

Physical-chemical properties

The following physical-chemical properties were obtained for all chemicals in the database: molar mass (M; $g.mol^{-1}$), K_{OW}, K_{OA}, K_{AW} (dimensionless), and OC normalized sorption coefficients (K_{OC}; L-water/kg-OC). For consistency, most physical-chemical property data were obtained from the U.S. Environmental Protection Agency's EPI Suite™ [49] program. Measured chemical property data were preferentially selected over predicted values. The database also includes SMILES notations [50] and chemical abstract service (CAS) registration numbers. Chemicals that contain recognized ionizable functional groups were identified and flagged in the database as ionizable organic chemicals (IOCs). Future database additions should include dissociation constants for IOCs and more explicit evaluation of the data with respect to this chemical property.

Relationships between plant bioaccumulation metrics and organic chemical properties

Many correlations between physical-chemical properties and various plant BCFs have been reported and used in various models to predict plant bioaccumulation [8, 51, 52]. For example, root concentration factors [8, 53], stem or wood concentration factors [30, 54-57]; and above ground or shoot concentration factors [33, 43, 58] have been related to log K_{OW}. Similarly, based on the assumption that the lipophilic cuticle is the major plant component governing air-plant interactions, simple regression models have been developed that relate air-shoot BCFs to K_{OA} [59-62] or to a combination of K_{AW} (dimensionless) and K_{OW} [63].

Two different types of general relationships between log K_{OW} and TSCF have also been reported. Bell-shaped curves relating TSCF to log K_{OW} [8, 64, 65] suggest that compounds that are either highly water soluble or are highly hydrophobic will not be significantly taken up by plants. More recently, Dettenmaier et al. [9] presented an empirical relationship between TSCF and log K_{OW} that indicates that non-ionizable, polar, highly water soluble organic compounds are most likely to be taken up by plant roots and translocated to shoot tissue. Highly water soluble compounds were also predicted to be the most likely type of organic chemicals transferred from soil to above ground plant compartments [45, 66].

Despite being developed from relatively small datasets over 25 years ago, both the Travis and Arms BCF-K_{OW} regression [58] and Briggs et al. TSCF-K_{OW} [8] relationship are still used by the regulatory agencies in North America. The U.S. EPA lists the Travis and Arms relationship in its 2005 Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities [67], and the Briggs relationship is used in the 2014 Guidance for Assessing Pesticide Risks to Bees [68] developed by the U.S. EPA, Health Canada Pest Management Regulatory Agency, and State of California Department of Pesticide Regulation.

Plant bioaccumulation database evaluation

A general requirement for assessing data quality is that the reported test procedures and designs comply with, or are comparable to, published testing guidelines or are conducted with accepted methods that are described in sufficient detail (e.g., REACH). Klimisch et al. [69] and others [70, 71], have developed data quality assessment methods for ecotoxicology and fish bioaccumulation testing data, respectively, based on nationally or internationally recognized testing guidance. While plant-testing guidance exists for toxicity (e.g., OCSPP 850.4230: Early Seedling Growth Toxicity Test. United States - Environmental Protection Agency [72]), few

standard methods (e.g., OCSPP 850.4800: Plant Uptake and Translocation Test [73]) exist for plant bioaccumulation testing, making data quality assessment difficult [74] .

Using the guiding principles from “Klimisch-type” data quality assessment methods [69], we developed some preliminary criteria (Table 2) and tentatively assigned each database entry into one of three screening-level data confidence categories: high, medium, or low. Because of the wide variety of experimental methods used to develop the data and the inconsistent reporting of supporting information, data quality assessment was challenging. All of the criteria listed for the particular category had to be met for the entry to be assigned to that confidence category. Unless there was a clear indication from the publication that the criteria were not met, we assumed that they were. Thus, data screened as “high confidence” may still have significant error. Additionally, because this is a relatively simple screening exercise, data screened as “medium” or “low” confidence may still be reliable, particularly in specific contexts. For example, bioaccumulation metrics reported for homologs are considered to be of low confidence because chemical-specific identification and metrics are lacking. However, if the reported homologs (or mixtures) have similar partitioning and degradation properties, the data may still be valuable for certain contexts such as model development and testing. We encourage interested users of the database to consider our proposed criteria for assigning screening-level data confidence categorizations (Table 2) but to critically examine data entries of interest according to their context-specific objectives.

RESULTS

Database summary

More than 350 papers (published ca. 1955–2014) were initially collected and reviewed. Suitable values and parameters reported or inferred from the reviewed studies were added into a

database. The final database includes 7,049 unique database entries for plant bioaccumulation metrics or rate constants for 310 organic chemicals measured in 112 plant species from 156 peer-reviewed publications. In some cases, the papers did not report specific bioaccumulation metrics but provided sufficient measured data necessary to calculate them. In other papers, bioaccumulation metrics calculated from the measured data were displayed in figures but specific values were not reported. The bioaccumulation metrics derived from figures are noted in the database. When values of the same experimental study were reported by different literature sources, only the original source data were included in the database. The database and summary information compiled from the experiments and the selected physical-chemical properties for each entry are included in the supporting information in the form of a Microsoft Excel® spreadsheet. The spreadsheet database is also available in Digital Commons at Utah State University (digitalcommens@usu.edu) and www.arnotresearch.com.

The database includes 2,728 below ground concentration factors for 237 chemicals and 3,947 above ground concentration factors for 208 chemicals and 309 TSCFs for 104 chemicals. The database includes plant bioaccumulation metrics for polycyclic aromatic hydrocarbons (PAHs), pesticides, pharmaceutical and veterinary chemicals, polybrominated diphenyl ethers (PBDEs), polychlorinated biphenyls (PCBs), per- and polyfluoroalkyl substances (PFASs), polychlorinated dibenzo-p-dioxins (PCDDs) and polychlorinated dibenzofurans (PCDFs). Pesticides and PCBs represent the majority of the compounds, and the majority of data entries are for PAHs and pesticides. PAHs, pesticides, pharmaceutical and veterinary compounds, and PFASs make up approximately 27%, 26%, 8% and 4% of the total data entries, respectively. The number of data entries for PBDEs, PCBs, and PCDDs/PCDFs represent approximately 4%, 15%, and 10%, respectively. Chemicals not associated with the aforementioned chemical classes

represent the remainder of the total entries. Table S-2 provides a summary of values for some of the physical-chemical properties for the chemicals in the database. Approximately 30% of the 310 chemicals were identified as IOCs.

Several test parameters could be considered essential to fully interpret the data and evaluate the quality of the measured values, (e.g., Table S-3); however, these parameters were not always reported. For example, some studies did not clearly state whether the data were reported on a fresh weight or dry weight basis; some did not mention what specific tissue types (roots, shoots, stems, leaves, fruits or tubers) were sampled; and several did not report the soil concentrations or key soil properties. Clear reporting of the units for the bioaccumulation metrics was missing in about 20% of the data entries. While it may be possible to infer or assume the units for the concentration ratios, this may lead to significant uncertainties in data interpretation. For example, RCFs are expressed as both root to soil (dry-weight basis) and root to soil solution or hydroponic solution (e.g., L/kg or mL/g) ratios. When sufficient details were reported to differentiate these types of RCFs, we reported them as RCF_{solid} and RCF_{aq}, respectively.

Attainment of steady state conditions, dependent on chemical-, plant-, and exposure-specific variables, is generally not verified experimentally and/or reported for plant uptake studies. This can limit data interpretation and inter-study comparisons. Reported exposure durations were included in the database but were not used to assign screening-level data confidence scores. Finally, none of the reviewed articles reported plant growth rates, and measurements for chemical concentrations in the exposure medium at the end of the exposure period were uncommon. Approximately 16% of the database entries were assessed to be of high confidence, 12% of low confidence, and the vast majority (~72%) of medium confidence.

In the next sections, the relationships between several plant bioaccumulation metrics and physical-chemical properties such as log K_{OW} and log K_{OA} are examined using the new database. The database can test refined model hypotheses that make more explicit assumptions for chemical partitioning (e.g., distribution ratios for IOCs). We selected K_{OW} and K_{OA} over other potential descriptors such as K_{OC}, calculated distribution coefficients, membrane water coefficients and other coefficients because they are widely available and are the most frequently used chemical descriptors in organic chemical plant uptake models. We then qualitatively compare these data to previously reported empirical relationships and simple theoretical partitioning models. If the water content of the plant tissue was not reported, we assumed a factor of 0.2 (dw/ww) for converting dry weight plant values to wet weight (or vice versa) for plotting bioaccumulation metrics in the figures that follow. This assumed conversion factor is the median for database entries based on studies that reported the water content in plant tissues (reported water content values range from 70–95%).

Below Ground Concentration Factors (BGCFs)

There are 2,728 BGCFs in the database, with various units, spanning over 7 orders of magnitude for chemicals with log K_{OW}s ranging from -3.1 to 9.1 and MW ranging from 78.1 to 959.2 (g/mol). The BGCFs include different environmental exposure media (solid phase or aqueous) and different plant material analyzed (i.e., roots, tubers, peels, cores).

Root concentration factors (RCFs) and the relationship with log K_{OW}. The most widely cited relationships with log K_{OW}, for example Briggs et al. [8] have expressed RCF values with units of L-water/kg-wet root weight (RCF_{aq}s) based on exposures via hydroponic solution or soil pore water. Figure 2 summarizes 723 RCF_{aq}s in the database spanning approximately 7 orders of magnitude reported from 40 papers representing a range of experimental conditions and

methods. For the neutral chemicals with log K_{OW} > 1, RCF_{aq} increases with K_{OW} (excluding the low confidence data, slope = 0.73; r^2 = 0.65). For the IOCs, there is still a positive but weaker correlation for increasing RCF_{aq} as a function of K_{OW} (log K_{OW} > ~ 1, slope = 0.24; r^2 = 0.26). The extent of ionization is generally uncertain because the pH of the test systems was rarely reported.

Briggs et al. [8] proposed that two components determine the total amount of chemical in the roots, the chemical associated with the water in the roots and the chemical associated with the lipophilic root solids, leading to the correlation illustrated in Figure 2. For comparison, the results of two partitioning models [75] also used to calculate RCF_{aq}s are shown in Figure 2. The first equilibrium partitioning (EqP) RCF_{aq} model assumes the root is 80% water and the remaining organic solids have an assumed "octanol-equivalence" of 1.5% for partitioning to the roots. The second model (EqP_Kin) also includes a kinetic adjustment factor to address conditions in which the root does not reach equilibrium with the surrounding water. This can occur when growth rates exceed uptake rates (e.g., "growth dilution" effect) or the exposure duration is too short to approximate equilibrium [75]. The Briggs regression model and the partition-based models show similar RCF_{aq} predictions for chemicals in a log K_{OW} range of ~-2 to 3, but model divergence is greater with higher log K_{OW} chemicals. There is a large scatter over the entire range of hydrophobicity, and separating the neutrals (left) from the IOCs (right) improves the fit of all three models for the neutral chemicals. For some of the IOCs the RCF_{aq}s are higher than EqP at lower K_{OW}, perhaps due to electrostatic interactions. The K_{OW} based models were not specifically developed to include IOCs.

Database values of RCF_{aq}s for chemicals having similar log K_{OW} can span several orders of magnitude. For example, the nine poplar RCF_{aq}s for trichloroethylene (log K_{OW} = 2.4) that

were scored as low confidence values range from 5.1 to 570, while a single medium confidence RCF value was 2.5. The nine lower confidence RCFs were determined using a non-chemical-specific ^{14}C analysis. A single, high confidence RCF_{aq} for phenanthrene (log K_{OW} = 4.5) is 6.5. Thirty-five medium confidence RCF_{aq}s for phenanthrene measured in various plants from various experimental designs range from 5.0 to 1730. Variability is also notable for IOCs where uncertainties in exposure water pH may be particularly significant. Only 154 of the 481 RCF_{aq} entries for IOCs reported pH. For example, for triclosan (log K_{OW} = 4.8 (neutral form); pKa = 7.8), nine RCF_{aq}s considered medium confidence range from 0.08 to 100, and four RCF_{aq}s considered low confidence range from 1.4 to 90. For diclofenac (log K_{OW} = 4.5 (neutral form); pKa = 4.2), seven RCF_{aq}s considered to be medium confidence range from 0.08 to 0.84 using chemical-specific analysis, while two RCF_{aq}s derived using total radioactivity and hence considered to be low confidence range from 28 to 105.

Figure 3 illustrates the relationship between log K_{OW} and 1,199 RCF_{solid} values in the database expressed with units of kg-dry weight soil/kg-dry root weight. The RCFs are calculated and presented using dry weight soil concentrations rather than OC-normalized soil concentrations because OC content in soil was not regularly reported (0.02 kg-OC/kg-DW is the median value in the database, when reported in the studies). The RCF_{solid} values span about 5 orders of magnitude and show a large scatter over the entire range of hydrophobicity. The illustrative EqP model calculations shown in the figure suggest that the large majority of RCF_{solid} values have not reached equilibrium and the large variance in RCF_{solid} is not driven by variability in soil OC content.

An additional 175 BGCFs in the database (not shown in Fig. 3) classified as tuber concentration factors (TCFs) and expressed as total tuber biomass (dw) are displayed in Figure 4

(left). The TCFs span about 3.5 orders of magnitude, and there is no significant relationship with K_{OW}. The TCFs are lower than would be expected based on estimated EqP. An additional 292 peel concentration factors and 220 core concentrations factors for below ground edible vegetable concentration factors (a mixture of tubers and roots: carrots, radishes and potatoes) for neutral organic chemicals for data entries that were not included in any of the previous figures are displayed in Figure 4 (right). Most of the "total," peel, and core data are from the same study [76]. On average, partitioning to the peel is about 7 times greater than partitioning to the core of the edible vegetable. The average peel concentrations approximate the average "total" concentrations because the peel concentrations are highest. No significant relationships exist between the below ground edible vegetable concentration factors and log K_{OW} from ~ 2 to ~ 9. The edible vegetable concentrations are well below the EqP calculations and the assumption for a kinetic correction that suggests a decrease in concentration at higher K_{OW} does not capture the general trend observed in the measured data. In general, the EqP model with the assumed 1.5% lipid equivalence assumption for the vegetable and the 2% organic carbon content for the soil overpredicts the median of "total" measured edible vegetable concentrations (variable lipid contents and organic carbon contents) by a factor of about 60. However, most of these data (> 95%) are from a single field-based study [76] involving long-term "aged" chemical contamination rather than the shorter-term exposures commonly found in laboratory-based studies or in a sewage sludge-amended soil situation.

The EqP model calculations in Figures 2, 3, and 4 provide a frame of reference for examining and comparing the different types of measured bioaccumulation data. Differences between EqP model calculations and experimental data indicate that laboratory hydroponic exposures often approximate equilibrium (medium and high confidence data in Fig 2-left) for

below ground plant concentration ratios, but most field data for neutral organic chemicals with log K_{OW} > 2 do not (Figs 3 and 4). These differences may reflect reduced plant bioavailability from solid phases under typical field conditions (not sewage sludge-amended soil). Further examination of pore water and solid phase concentrations (and chemical activities) and plant uptake from field studies seems warranted to better ascertain possible differences between laboratory ("dissolved exposure conditions") and field BCFs. Passive sampling may provide insights into these issues of "bioavailability." Higher field growth rates and differences in loss kinetics (e.g., metabolism, volatilization) between laboratory and field could also play a role. Figure S-1 shows that there is no apparent decrease in root vegetable bioconcentration with increasing MW. However, the database contained only one value for a chemical with MW > 500 g/mol, indicating additional data are needed to better understand the uptake of larger molecules.

Above Ground Concentration Factors

The 3,947 above ground concentration factors (AGCFs) in the database have various units and exposure routes (air, soil, and water) for chemicals with log K_{OW}s ranging from -3.1 to 8.9 and MW ranging from 78.1 to 959.2 (g/mol). The AGCFs include a variety of environmental exposure media (solid phase or aqueous) and plant material analyzed (e.g., stem, fruit, leaves, whole plant). Plant-air concentration factors were predominantly leaf concentration factors (LCFs), and chemical concentrations in the air were expressed as gaseous ("dissolved") or total (gaseous and particulate phases).

Bioconcentration factors (BCFs) for total above ground plant compartments (Root to shoot pathways)

The 2,956 entries for BCFs describe the root uptake of chemicals into above ground vegetation reported from 95 different papers. The database includes a combination of field and

laboratory determined BCFs. Of these BCFs, 981 are based on exposures from an aqueous phase (i.e., hydroponic or soil solution) and 1,975 are based on exposures from a solid phase (i.e., soil). An additional 75 values in the database were derived from both soil and air exposure.

Figure 5 shows the relationship between log K_{OW} and 1,888 BCF_{solid}s (i.e., plant/soil concentration ratio) for a variety of plant tissues (e.g., stems, fruit, seeds, leaves). The BCF_{solid}s span about 8 orders of magnitude and show a substantial variability throughout the range of log K_{OW} values. The widely used relationship of Travis and Arms [58], developed mainly from literature field data (29 neutral organics), is also displayed as a reference.

The Travis and Arms model underestimates some of the BCFs categorized as being higher data confidence by about 4 orders of magnitude. Furthermore, Figure S-2 (sub-set of data from Figure 5) emphasizes that the Travis and Arms model [58] underestimates concentrations in above ground edible vegetation, highlighting the potential for significant error in applications of the model for risk assessments. Figure S-3 indicates that there is no apparent decline in BCF_{solid} for high molecular weight chemicals (i.e., MW > 500 g/mol).

Figure 6 shows 927 BCF_{aq}s (i.e., plant/solution) for a range of plant tissues (e.g., shoots, stems, fruit, seeds) as related to log K_{OW}. The BCF_{aq}s span almost 8 orders of magnitude, with substantial variability at any particular K_{OW} and no clear relationship between BCF_{aq} and K_{OW} over a wide range of chemical hydrophobicity. As observed for RCFs, BCFs for chemicals having the same or similar log K_{OW} can span several orders of magnitude. For example, BCF_{aq}s (L/kg-ww) in four species determined in the same study [77] and categorized in the medium confidence range for N,N-Diethyl-meta-toluamide (DEET) (log K_{OW} = 2.18) range from about 0.04 to 25 (n=7). Another study [78] reports that BCF_{aq}s for 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (log K_{OW} = 6.80) in two species considered here to be medium confidence ranged from about

0.03 to 1.7 (n=16)). Large variability is also observed for IOCs where exposure water pH is a critical variable, yet it was reported in only 7 of the 675 BCF_{aq} entries. For perfluorobutanesulfonic acid (estimated log K_{OW} of 1.82 for the neutral form, estimated pKa ~ -3) BCF_{aq}s range from about 0.15 to 70 (n=37). Similarly for perfluoro-*n*-undecanoic acid (estimated log K_{OW} of about 6.82 for the neutral form and a pKa ~ 0.5), BCF_{aq}s range from 0.0056 to 17 (n=33). Both examples are from the same study [79] and were tentatively assigned medium confidence scores. The differences in BCF values could be the result of species variability but could also be due to differences in the above ground tissues of the plant selected in the calculation, plant growth rates, and the amount of water transpired.

Plant-air concentration factors and relationships with octanol/air partition coefficients

Figure 7 summarizes 916 plant-air concentrations factors, predominantly LCFs, included in the database as a function of K_{OA}. The reported LCFs were determined from either total or dissolved (gaseous) air concentrations. The observed scatter is generally less than the other plant endpoints that have been previously discussed. This is likely due to the smaller chemical domain of compounds tested and/or the use of similar measurement methods since most of the data were generated by a small number of investigators (data are from 10 publications). However, the variability is still notable and the difference between gas and total air based concentration ratios becomes quite large at high K_{OA}. As mentioned in the introduction, it has also been suggested that some of the interspecies variability can be attributed to differences in the sorptive leaf phase (i.e., cutin, cutan, and waxes) [80, 81].

The solid line in Figure 7 represents equilibrium partitioning between the gas phase and the leaf, assuming the leaf has an octanol equivalence of 1.5% (kg/kg; assumed). The dashed line (EqP_kin1) includes a disequilibrium factor due to growth rates exceeding chemical uptake rates,

and the dotted line (EqP_kin2) additionally considers particle deposition to the plant (leaf) surface for very high K_{OA} chemicals [75]. The simplified models shown here (details in the SI) approximate mechanistic processes for chemical uptake in plants detailed by McLachlan [81]. The database contains no plant-air concentration factors for IOCs.

Transpiration stream concentration factors (TSCF)

Of the 299 TSCFs shown in Figure 8, 238 were generated using hydroponic exposure systems. Hydroponics are used more often than soil systems because the exposure concentrations are more easily measured and controlled. Assuming the passive uptake, TSCF values should have a theoretical maximum of 1 [82]. Thus, reported values of TSCF greater than 1 were categorized as low confidence in this screening exercise. The empirical relationships previously developed by Briggs [8] and Dettenmaier [9] for neutrals or chemicals in their non-ionized form under the conditions of the experiment are also shown in Figure 8.

Briggs et al. [8] determined TSCF values by indirectly calculating xylem sap concentrations from the total mass of the compound analyzed in the shoots divided by the volume of water transpired. The plants were grown hydroponically in a solution containing a known concentration of the chemical. Out of the 299 total reported values of TSCF, 100 were measured using this type of approach. Dettenmaier et al. [9] directly collected xylem sap from a de-topped plant (i.e., the above ground tissues are removed) sealed in a pressurized chamber containing a solution of a known concentration of the chemical. As the chamber is pressurized, xylem sap is collected as it exits the stem and is analyzed. The TSCF is calculated from the steady state ratio of the measured xylem sap and root exposure concentrations. The database contains 54 values measured using the pressure chamber approach.

TSCF values for chemicals having the same or similar log K_{OW} varied widely. For example, TSCF values for trichloroethylene (log K_{OW} = 2.4) range from 0.02 to 0.59 for 14 high confidence data entries and 0.02 to 0.22 for 9 low confidence data entries (radiolabelled, not corrected for parent chemical), with a single medium confidence entry of 0.81. Variability is also notable for IOCs where uncertainties in exposure water pH may be particularly significant because only 96 of the 183 TSCF entries for IOCs reported exposure water pH.

Kinetic data

One hundred sixty-four of the database entries include some information on uptake rate, chemical half-life or biotransformation rate of the organic chemicals in different plant species. Maddalena et al. [83] reported release rates and plant-air partition coefficients for phenanthrene, anthracene, fluoranthene and pyrene. From studies such as these, the uptake rates can be estimated. Uptake rates from air for PCBs, pesticides (including HCB, hexachlorocyclohexanes, DDT-related compounds, alachlor, dieldrin, trifluralin, mirex, thionazin, sulfotep, and bromacil), phenols, and nitrobenzene were reported in a few studies. A few papers indicated that plants were able to metabolize organic chemicals; however, these studies did not report biotransformation rates. For the others, measured biotransformation rates ranged from about 0.0003/h to about 0.02/h, corresponding to biotransformation half-lives of about 3,000 h to 30 h. A review of 4,513 measurement-based dissipation half-lives (possible biotransformation and transport loss processes) for 346 pesticides applied to 183 plant species has shown that, typically, only overall dissipation from plants is reported, while metabolism rates contributing to dissipation are reported in only less than 2% of all included studies [17]. However, dissipation half-lives can often be used as first proxy for biotransformation in plants under field conditions

[84], since biotransformation is generally the dominating process contributing to overall dissipation [41].

DISCUSSION

Substantial variability exists in plant bioaccumulation data. For chemicals having more than one literature BCF, the values often range over several orders of magnitude. In our opinion, much of the variability in BCF values is associated with the wide variety of experimental approaches used to conduct the plant uptake studies. Often, the experimental objective of the study was to determine relative plant uptake and/or distribution within the plant, not specifically to determine a BCF or TSCF value. Thus, a BCF or TSCF was reported as the outcome of the study, but since it was not the main objective, key supporting data describing environmental conditions (e.g., light, temperature and humidity) and plant growth and health related parameters were not reported or collected. Without this information, it is difficult to determine why chemical uptake data varies so much between studies.

The variation in testing methods and data reporting also prevented any meaningful global examination of the influence of variables related to environmental conditions (e.g., temperature, light, humidity, pH) and plant properties (e.g., growth rates, metabolism, age). Studies systematically quantifying the importance of these variables are needed.

Developing and applying data confidence assessment criteria to the values in the database was also challenging due to the lack of standard methods for plant uptake studies. In some cases, potential sources of uncertainty in the analytical methods can be identified, such as the use of radiolabelled test chemical without parent chemical-specific quantification. In other cases, the experimental approach itself was the biggest potential source of data uncertainty. For example, the TSCF is defined as the xylem/exposure solution ratio. However, in most cases, the xylem sap

concentration was determined indirectly from the total mass in the shoot/volume of water transpired. To assign a high quality assessment to a TSCF value that was measured indirectly is probably not appropriate even though the study might have been carefully done. Similarly, BCFs can be calculated from ratios of tissue and exposure concentrations; however, without knowing the volume of water transpired and plant growth rate, the relevance of the data is still uncertain, even if the overall quality of the study as determined from other criteria and considerations was high.

For these reasons it is suggested that plant bioaccumulation and in vivo biotransformation rate estimation testing and data reporting guidance be developed and recommended for future experimental testing. Without providing such a perspective and technical guidance to the scientific community it is unlikely that data and models used in exposure assessments will improve to any significant extent in the foreseeable future.

Despite the experimental data variability regarding the uptake of organic chemicals by plants, some generalizations can be made. Current empirical and equilibrium models using K_{OW} generally overestimate bioaccumulation in below ground edible vegetables (based on soil exposures) and underestimate bioaccumulation in above ground edible vegetables (based on soil exposures). This is not surprising since it is unlikely that equilibrium or even steady state conditions are attained during the relatively short-term exposure experiments typically conducted. Mechanistic models incorporating multiple exposure pathways (i.e., air to above ground plant tissues) and kinetic factors associated with plant growth and metabolism are more likely to explain the available data if study specific information is available to parameterize the models to the test conditions. Despite most existing plant uptake models predicting a decrease in

contaminant uptake by plants as a function of size and hydrophobicity, this was not observed in the available data.

In summary, we have developed a database of values quantifying the uptake of organic chemicals into terrestrial plants and developed and applied data quality criteria to preliminarily evaluate confidence in the database entries. We emphasize that the current screening-level criteria cannot explicitly identify all possible data quality issues (good or bad). Database users are encouraged to consider how these guiding principles were developed and review the original source before using the data for their particular application. A detailed strategy for developing standardized test methods for plant bioaccumulation testing has recently been proposed [74]. Some of the more commonly applied regression models and basic theoretical partitioning models were used to compare with database values; however, these analyses are not intended to be comprehensive model evaluations. We hope the database will provide opportunities for more comprehensive model evaluations. By including a broader spectrum of models and a more thorough comparison, chemicals and plants that are not well-predicted or lacking measurements could be identified and used to guide future research efforts. Differences in metabolism between plant species and variability between tissues could be confounding factors contributing to the overall variability but are impossible to reconcile from global analysis of the database due to uncertainty in data and variability in test methods.

Supplemental Data—The Supplemental Data are available on the Wiley Online Library at DOI: 10.1002/etc.xxxx.

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Data availability—Data, associated metadata, and calculation tools are available from the corresponding author (william.doucette@usu.edu).

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Figure 1. A conceptual overview of key plant bioaccumulation processes and assessment metrics (LCF = Leaf concentration factor, FCF = Fruit concentration factor, SCF = Stem concentration factor, TSCF = transpiration stream concentration factor, RCF = Root concentration factor (RCF), K_H = Henry's law constant and K_{OC} = Organic carbon normalized sorption coefficients); further summary of calculated endpoints are summarized in Table 1.

Figure 2. Measured root concentration factors derived from pore water or solution exposure media (RCF_{aq}) as a function of chemical octanol-water partition coefficient (K_{OW}). No tubers were included in this analysis. The figure on the left is for neutral compounds, on the right for ionizable organic chemicals (IOCs). Low, medium, and high refer to the data confidence screening assessment for the measured data. For IOCs the K_{OW} for the neutral form of the chemical is used. The Briggs et al. [8] RCF model is presented along with a simple equilibrium partitioning (EqP) model ($RCF_{aq} = 0.8 + 0.015K_{OW}$). A kinetic adjustment factor is also included in a version of the EqP model [75]. Equilibrium partitioning (EqP) models with (EqP_Kin) and without a kinetic adjustment factor are presented for reference.

Figure 3. Measured root concentration factors derived from solid exposure media (RCF_{solid}) as a function of chemical octanol-water partition coefficient (K_{OW}). The figure on the left is for neutral compounds, on the right for ionizable organic chemicals (IOCs). Low, medium, and high refer to the data confidence screening assessment for the measured data. For IOCs the K_{OW} for the neutral form of the chemical is used. Equilibrium partitioning (EqP) models with (EqP_Kin) and without a kinetic adjustment factor are presented for reference. Variability in predicted RCF_{solid} for a range of soil organic carbon (OC) contents is demonstrated.

Figure 4. Measured tuber concentration factors (TCFs; left) for potatoes and below ground edible vegetable concentration factors (BGEVCFs; right) for carrots, potatoes, and radishes as a

function of chemical octanol-water partition coefficient (KOW). Low and medium refer to the data confidence screening assessment for the measured data. The BGEVCFs are separated into data analyzed for peels, cores, and "total" below ground vegetable. Equilibrium partitioning (EqP) models with (EqP_Kin) and without a kinetic adjustment factor are presented for reference.

Figure 5. Measured bioconcentration factors derived from solid phase exposure media (BCF_{solid}) as a function of chemical octanol-water partition coefficient (K_{OW}). The figure on the left is for neutral compounds, on the right for ionizable organic chemicals (IOCs). Low, medium, and high refer to the data confidence screening assessment for the measured data. For IOCs the K_{OW} for the neutral form of the chemical is used. The Travis and Arms [58] relationship for above ground edible plant parts and soil as a function of K_{OW} derived in 1982 is also displayed ($BCF = 1.58 – 0.58 \times \log K_{OW}$, n=29).

Figure 6. Measured bioconcentration factors derived from aqueous media (BCF_{aq}) as a function of chemical octanol-water partition coefficient (K_{OW}). The figure on the left is for neutral compounds, on the right for ionizable organic chemicals (IOCs). Low, medium, and high refer to the data confidence screening assessment for the measured data. For IOCs the K_{OW} for the neutral form of the chemical is used.

Figure 7. A summary of 916 plant-air measurements included in the database as a function of the chemical octanol-air partition coefficient. The measurements are based on either bulk air or gas phase (no particles) estimates. Low, medium, and high refer to the data confidence screening assessment assignments for the measured data. An Equilibrium Partitioning (EqP) model is included that assumes that sampled plant material has 1.5% (kg/kg) octanol equivalence [75]. A kinetic adjustment factor is also included in the EqP_kin1 model to account for competing rates

of chemical uptake and growth. A second adjustment factor is additionally included in the EqP_kin2 model that accounts for particle deposition to the plant surface to illustrate the potential role of these processes on measured data.

Figure 8. Measured transpiration stream concentration factor (TSCF) values as a function of K_{OW} with the relationships developed by Briggs et al. 1982 and Dettenmaier et al. 2009. The figure on the left is for neutral compounds, on the right for ionizable organic chemicals (IOCs). Low, medium, and high refer to the data confidence screening assessment for the measured data. For IOCs the K_{OW} for the neutral form of the chemical is used. IOCs may or may not be ionized under the conditions of the experiment.

Table 1 General plant bioaccumulation factors.

General bioaccumulation endpoint	Summary calculations
Below ground vegetation concentration factor (BGCF)	Conc. in below ground tissues (mg/kg)[a] / Conc.in soil (mg/kg)[a] OR in exposure solution (mg/L)[b]
Above ground vegetation concentration factor (AGCF)	Conc. in above ground tissues (mg/kg.) [a] / Conc. in air[c] (mg/L), OR in soil (mg/kg) [a] OR in exposure solution (mg/L) [b]
Transpiration stream concentration factor (TSCF)	Conc. in xylem sap (mg/L) / Conc. in exposure solution (mg/L)[b]

[a]Concentration in soils or tissues expressed on wet (fresh) or dry basis

[b]Exposure solution = hydroponic solution (measured) or soil solution (calculated or estimated)

[c]Total or dissolved

Table 2. Screening-level criteria for assigning tentative data confidence categories (high, medium, and low) to the database entries. A database entry screened as "high confidence" satisfies (or is assumed to satisfy) all of the criteria outlined for "high confidence". A database entry that does not meet all of the high confidence criteria but meets all of the medium confidence criteria is considered to be of "medium confidence". Data that satisfy at least one of the criteria outlined for low confidence are considered to be of "low confidence".

Category	Criteria
High	Chemical (CAS RN or name) and plant species (botanical and common name) identified; units for reported bioaccumulation metric(s) are explicitly defined; chemical-specific analysis for exposure medium and plant; chemical concentration in exposure media measured at the beginning, during, and at the end of the exposure period; or rate constants (or associated half-lives) are used to calculate kinetic bioaccumulation metrics from measured concentrations; no apparent toxicity to the exposed plant; reasonable growth conditions typical for the selected plant species (i.e. hours of light and provision of nutrients); a negative control included; measures of key parameters influencing chemical partitioning between the exposure medium and the plant or plant compartment such as organic carbon content in the soil, dissolved organic carbon in hydroponic systems, pH for ionogenic organics, dissolved concentrations; composition of the plant compartments (i.e. lipid and water contents), plant mass, growth rate, and amount of water transpired.
Medium	Chemical (CAS RN or name) and plant species (botanical or common name) identified; bioaccumulation metric units can be readily inferred from reported concentrations; bioaccumulation values are estimated from a graph or figure; concentrations in exposure media are measured at some point in time concentration in plant measured at end of exposure period; chemical-specific analysis; no apparent toxicity to the exposed plant.
Low	Chemical (CAS RN or name) and plant species (botanical or common name)

	identified; bioaccumulation metric units are not clearly defined nor readily interpretable; unclear nature of test substance or use of homologs or mixtures; only assumed nominal concentrations in exposure medium and plant reported; aqueous exposure concentrations exceeding solubility in hydroponic test systems; documented toxicity to plant.

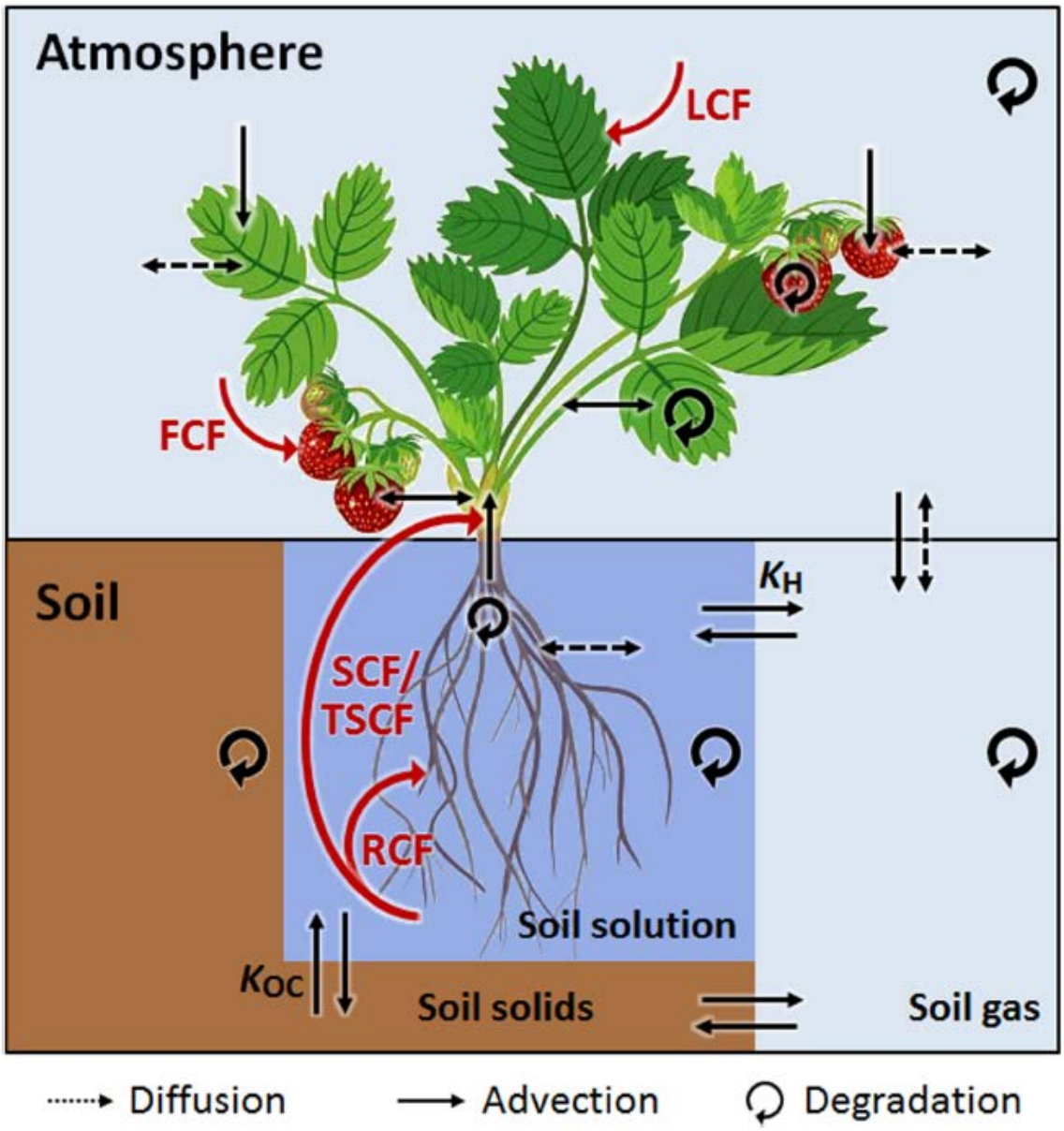

Figure 1

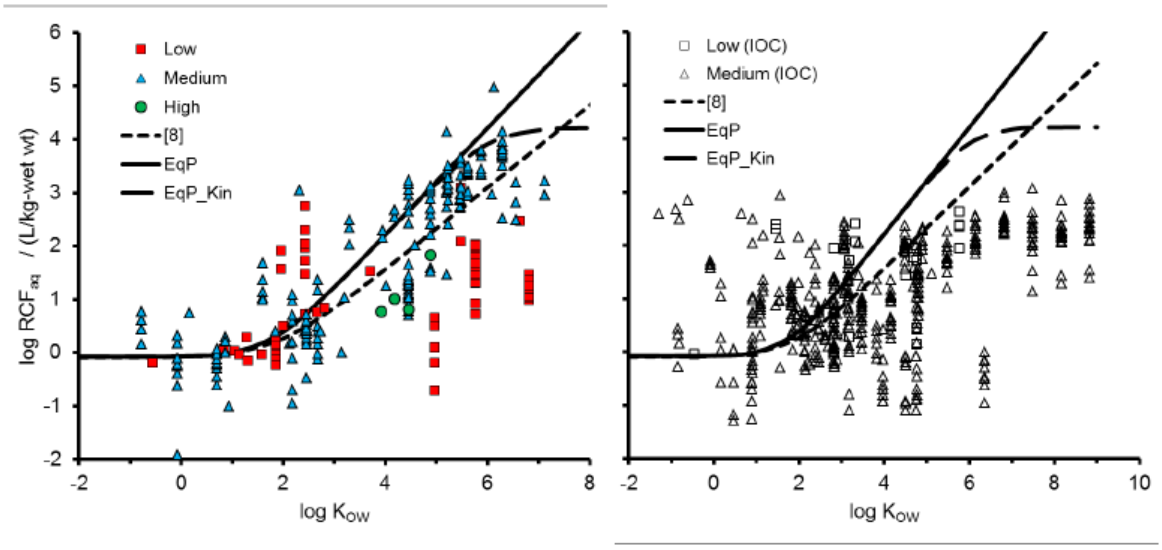

Figure 2

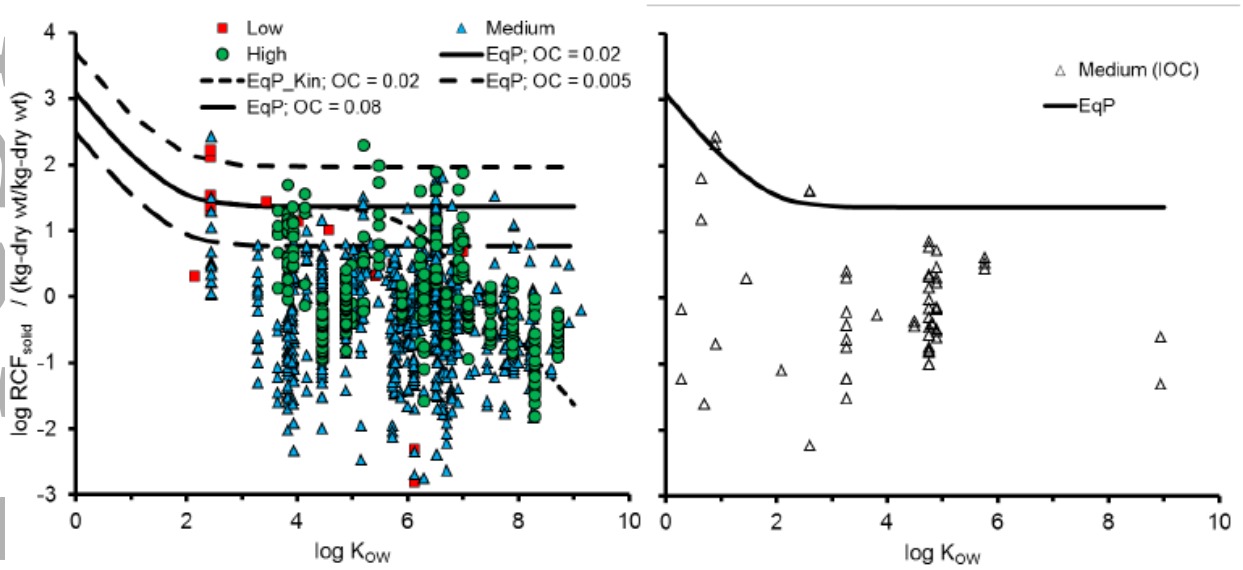

Figure 3

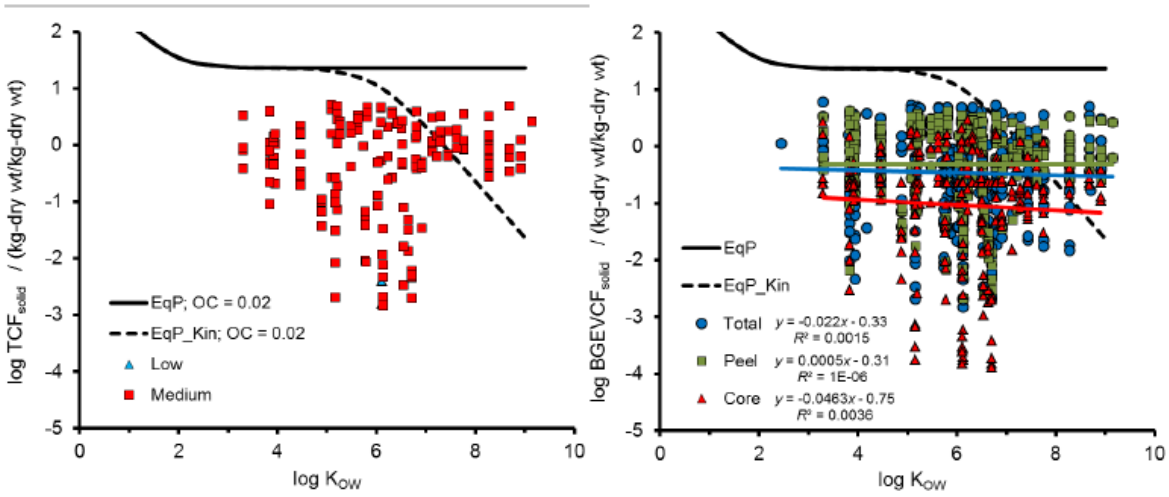

Figure 4

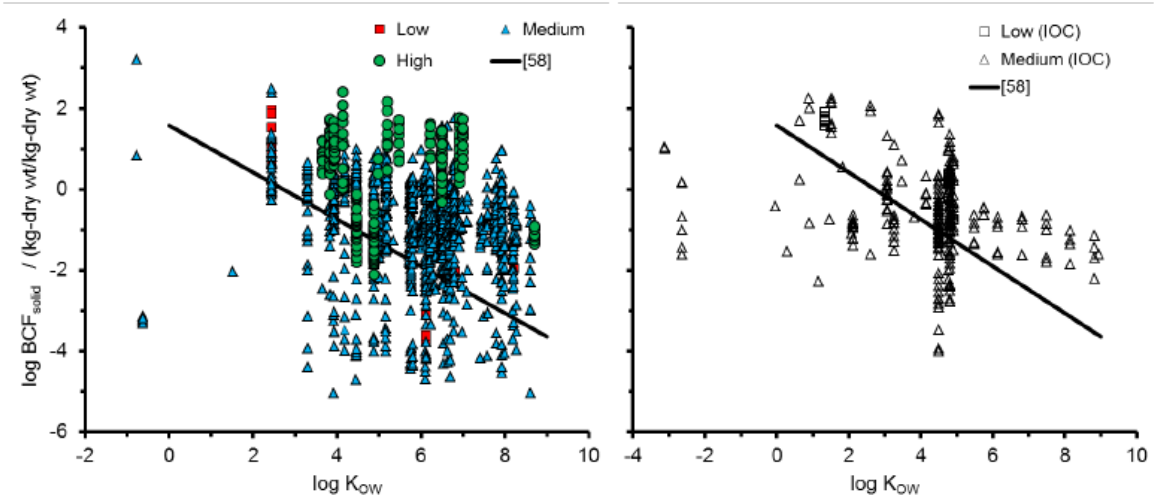

Figure 5

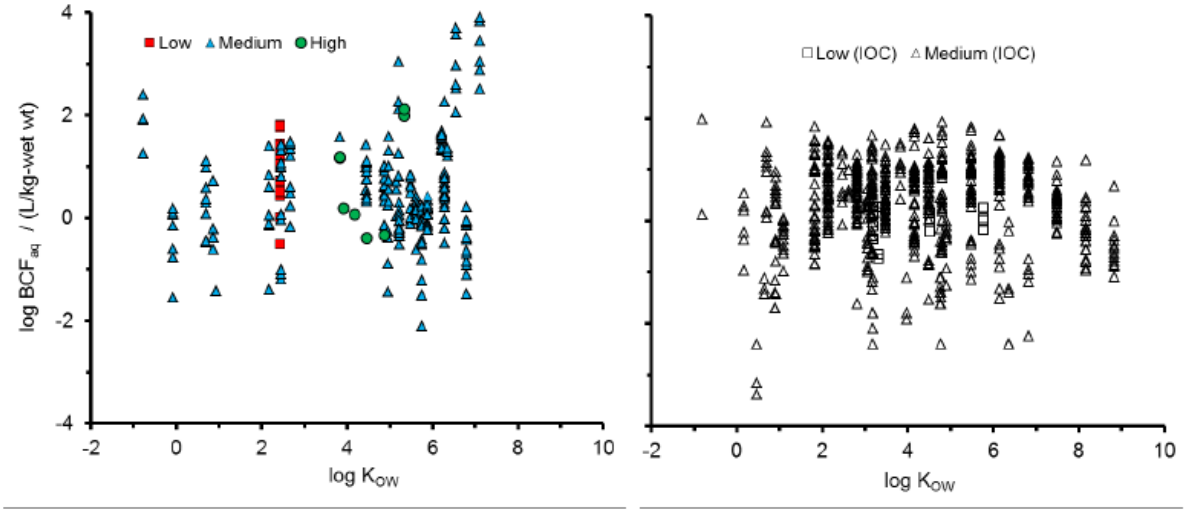

Figure 6

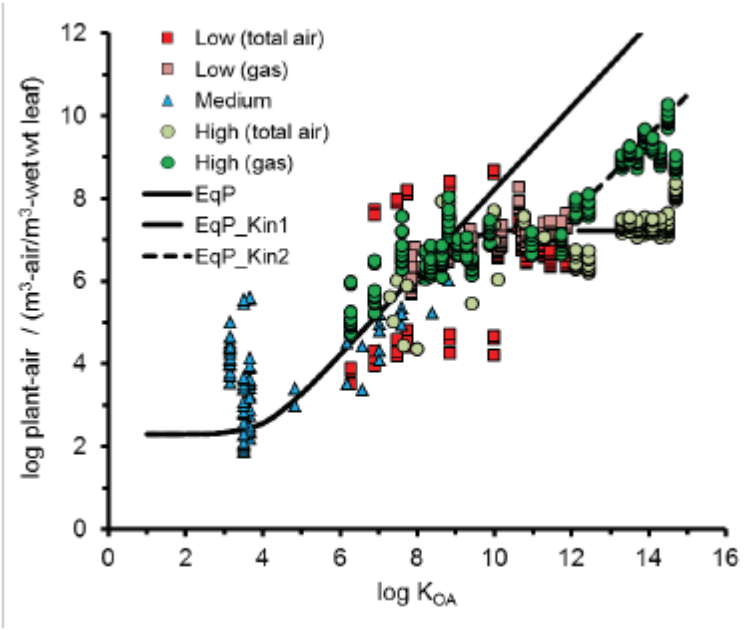

Figure 7

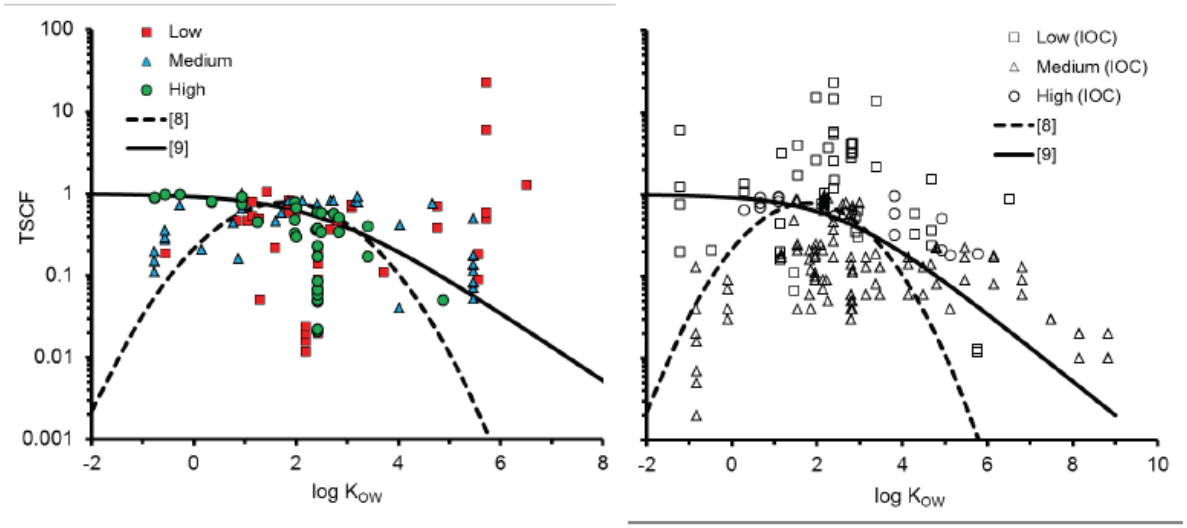

Figure 8