Improved prediction of the bioconcentration factors of organic contaminants from soils into plant/crop roots by related physicochemical parameters

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Abstract

There has been an on-going pursuit for relations between the levels of chemicals in plants/crops and the source levels in soil or water in order to address impacts of toxic substances on human health and ecological quality. In this research, we applied the quasi-equilibrium partition model to analyze the relations for nonionic organic contaminants between plant/crop roots and external soil/water media. The model relates the in-situ root concentration factors of chemicals from external water into plant/crop roots (RCF\textsubscript{(water)}) with the system physicochemical parameters and the chemical quasi-equilibrium states with plant/crop roots ($\alpha_{pt}$). With known RCF\textsubscript{(water)} values, root lipid contents ($f_{lip}$), and octanol-water $K_{ow}$'s, the chemical-plant $\alpha_{pt}$ values and their ranges of variation at given $f_{lip}K_{ow}$ could be calculated. Because of the inherent relation between $\alpha_{pt}$ and $f_{lip}K_{ow}$, a highly distinct correlation emerges between log RCF\textsubscript{(water)} and log $f_{lip}K_{ow}$ ($R^2 = 0.825$; $n = 368$), with the supporting data drawn from 19 disparate soil-plant studies covering some 6 orders of magnitude in $f_{lip}K_{ow}$ and 4 orders of magnitude in RCF\textsubscript{(water)}. This correlation performs far better than any relationship previously developed for predicting the contamination levels of pesticides and toxic organic chemicals in plant/crop roots for assessing risks on food safety.

Keywords

Organic contaminants; Pesticides; Food contamination; Root concentration factor; Root lipid content; Soil pore water

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Appendix A. Supplementary data

Table S1, the root concentration factors (RCFs) from water and related data; Table S2, RCFs from soils, log $K_{ow}$, and related data; Table S3, the sources of log $K_{ow}$ and log $K_{om}$ data listed in Table S2; Table S4, the shoot concentration factors (SCFs) and related data; Table S5, a glossary of terms used; Fig. S1, relations between log RCF\textsubscript{(som)} and log $K_{ow}$ for organic chemicals with plant/crop roots; Fig. S2, relations between log SCF\textsubscript{(water)} and log $[f_{lip}K_{ow}]$ for PAHs with plant/crop shoots; Fig. S3, relations between $\alpha_{pt}$ and log $[f_{lip}K_{ow}]$ for PAHs with plant/crop shoots. Supplementary data to this article can be found online at https://doi.org/10.1016/j.envint.2019.02.020.
1. Introduction

Since the advent of pesticides in 1950s for the control of insects and weeds, there has been a strong demand for a basic understanding of the transfer of pesticides and toxic chemicals from soils to food crops (Harris and Sans, 1967; Iwata et al., 1974; King et al., 1965; Fuhremann and Lichtenstein, 1980). Such knowledge is needed for estimating the levels of harmful substances in food chains and the associated human health impacts. To meet this demand, extensive greenhouse and field-plot studies were performed by scientists (Beestman et al., 1969; Harris and Sans, 1967; Lichtenstein, 1959) to explore relations between the levels of pesticides in soils ($C_s$) and the levels absorbed by crops ($C_{pt}$). The crop samples examined included whole plants and their roots and shoots. These studies revealed that: when a pesticide in a soil was absorbed by a crop species or its segment (e.g., root) at a fixed system setting, a relatively good linear relation existed between $C_{pt}$ and $C_s$; however, the $C_{pt}/C_s$ ratio of a chemical with a crop varied widely between soils. In spite of these findings, the soil-to-plant bioconcentration factors, i.e., BCF$^{(soil)} = C_{pt}/C_s$, are routinely measured as reference indices.

Investigation on relations between levels of organic chemicals in plants/crops and in external sources (soil or water) receives increasing attention since 1970s as more varieties and higher quantities of chemicals are being emitted into natural systems that arouses concerns for food safety. In the 1990s, theoretical models were being developed by Riederer (1990), Trapp et al. (1990), Paterson et al. (1994), Trapp and Matthies (1995), and Burken and Schnoor (1998) for plant uptakes of chemicals in terms of their interfacial transfer rates and partition constants between plants and associated media: soil, water, and air. The models were executed with estimated transfer rates and coefficients along with estimated plant transpiration and chemical-breakdown rates. Later, Chiou et al. (2001) formulated a quasi-equilibrium partition model by relating the levels of chemicals in a plant to their quasi-equilibrium partitions to the associated plant components, with the quasi-equilibrium values ($\alpha_{pt} \leq 1$) depending on chemical properties and system settings. The latter model was substantiated by the disparate quasi-equilibrium states of different chemicals in a plant (or its segment) following an exposure. The model has since been further tested and verified by many water-plant and soil-plant contamination data (Barbour et al., 2005; Card et al., 2012; Chiou, 2002; Gao et al., 2005; Huang et al., 2011; Li et al., 2005; Li et al., 2002; Su and Zhu, 2006; Su et al., 2009; Yang et al., 2017; Zhang et al., 2005).

A critical parameter to be dealt in the quasi-equilibrium partition model is the quasi-equilibrium $\alpha_{pt}$ value, which is a function of the chemical’s property ($K_{ow}$) and the plant-uptake setting. Since the ranges of variation in $\alpha_{pt}$ for chemicals under diverse system settings have not been established (Chiou et al., 2001), we here extended the basic model to analyze the ranges of $\alpha_{pt}$ values for various chemicals with plant/crop roots based on the observed root concentration factors (RCFs) from extensive laboratory/greenhouse/field studies. Incorporating the observed $\alpha_{pt}$ ranges into the model enables one to construct helpful correlations of RCFs with relevant parameters to aid in estimation of the crop-contamination level that is timely needed. This objective is further motivated by findings that when the driving force of a chemical from soil to plant roots is based on the level in
soil pore water \((C_{pw})\), instead of the level in bulk soil \((C_s)\), the chemical RCFs with roots from extensive sources converge sharply. A brief overview of the quasi-equilibrium partition model is given next to facilitate the subsequent account of extensive literature data toward the formation of improved predictive correlations.

### 2. Theoretical considerations

The fact that no general relation exists between the levels of chemicals in plants \((C_{pt})\) and sustaining soils \((C_i)\) suggests that \(C_s\) is not a rigorous intensity index (Hung et al., 2009). It is known that the sorption of relatively water-insoluble nonionic organic chemicals by a water-saturated soil occurs predominantly by partition into the soil organic matter (SOM) (Chiou et al., 1979); adsorption by soil minerals is relatively insignificant except for soils having very low SOM contents because of the adsorptive competition by water (Chiou et al., 1981, 1983). Therefore, the level of a chemical in soil pore water (i.e., \(C_{pw}\)), which serves as the driving force for plant uptake, depends primarily on the level in SOM (i.e., \(C_{om}\)), not the level in bulk soil (\(C_i\)), i.e.,

\[
C_{pw} = C_{om}/K_{om} = (C_s/f_{om})/K_{om}
\]  
(1)

where \(K_{om} (= C_{om}/C_{pw})\) is the chemical’s equilibrium partition coefficient between SOM and water and \(f_{om}\) is the SOM fraction in soil. Here \(K_{om}\) is related to the soil-water distribution coefficient \((K_d)\) by

\[
K_{om} = K_d/f_{om}
\]  
(2)

The term \(C_{om}\) in Eq. (1) expresses the contamination intensity in a water-saturated soil as sensed by the equilibrium \(C_{pw}\) in soil pore water. Since \(C_s (= f_{om}C_{om})\) varies not only with \(C_{pw}\) but also with \(f_{om}\), the term RCF_{(soil)} based on \(C_s\) is elusive. The finding (Kile et al., 1995) that the \(K_{om}\) of a chemical is practically constant between soils from wide sources enables the \(C_{pw}\) with various soils to be rapidly estimated via Eq. (1).

To analyze the soil-plant contamination data, the needed \(C_{pw}\) values could thus be derived from \(C_s, f_{om},\) and estimated \(K_{om}\) using the above procedure, if the soil-specific experimental \(K_d\) values are not available. Using the \(C_{pw}\) as the driving force in soils, the levels of chemicals absorbed by a plant segment after an exposure could be set as:

\[
C_{pt} = \alpha_{pt}C_{pw}[f_{pw} + f_{pom}K_{pom}]
\]  
(3)

where \(C_{pt}\) is the level in a plant segment on the fresh-weight basis; \(f_{pw}\) is the weight fraction of water in the plant segment; \(f_{pom}\) is the weight fraction of all organic constituents in the plant segment (with \(f_{pw} + f_{pom} = 1\)); \(K_{pom}\) is the partition coefficient of a chemical between the (dry) plant organic matter and water; and \(\alpha_{pt}\) is the quasi-equilibrium factor expressing the deviation from equilibrium of a chemical in a plant segment relative to its level in external water when the plant is sampled. The \(\alpha_{pt}\) value \((\leq 1)\) has a logical upper limit of 1 when the chemical in a plant segment of interest reaches equilibrium with its external water phase.
For simplicity, the most important plant constituents are assumed to be water, carbohydrates, and lipids, such that Eq. (3) may be expressed as

\[
C_{pt} = \alpha_{pt}C_{pw}\left[f_{pw} + f_{ch}K_{ch} + f_{lip}K_{lip}\right]
\]

where subscripts “ch” and “lip” refer respectively to carbohydrates and lipids, with \( f_{pw} + f_{ch} + f_{lip} = 1 \). Since experimental \( C_{pw} \) data are usually unavailable, they are estimated from \( C_{om}/K_{om} \) via Eq. (1) to give

\[
C_{pt} = \alpha_{pt}\left(C_{om}/K_{om}\right)\left[f_{pw} + f_{ch}K_{ch} + f_{lip}K_{lip}\right]
\]

Thus, the in-situ root concentration factor of a chemical relative to its level in external soil water (\( C_{pw} \)), \( \text{RCF}_{(water)} \), may thus be defined as:

\[
\text{RCF}_{(water)} = C_{pt}/\left(C_{om}/K_{om}\right) = \alpha_{pt}\left[f_{pw} + f_{pom}K_{pom}\right]
\]

or alternatively as

\[
\text{RCF}_{(water)} = C_{pt}/\left(C_{om}/K_{om}\right) = \alpha_{pt}\left[f_{pw} + f_{ch}K_{ch} + f_{lip}K_{lip}\right]
\]

The \( \text{RCF}_{(water)} \) as defined is a quasi-equilibrium distribution coefficient. Unlike many equilibrium BCFs, the \( \text{RCF}_{(water)} \) depends not only on the chemical-plant properties but also on the \( \alpha_{pt} \) (≤1) when soils and plants are collected.

Under a system setting, the \( \alpha_{pt} \) may be calculated via either Eq. (6) based on the measured \( f_{pw} \), \( f_{pom} \), and \( K_{pom} \) or via Eq. (7) using available \( f_{pw} \), \( f_{ch}K_{ch} \), and \( f_{lip}K_{lip} \). Generally, if \( f_{pom}K_{pom} \) or \( f_{lip}K_{lip} \) is only a small multiple of \( f_{pw} \) (~0.9), as for chemicals with \( K_{ow} < 500 \) and roots with \( f_{lip} < 0.01 \), the \( \alpha_{pt} \) should be close to 1 after short plant exposures (Briggs et al., 1982; Chiou et al., 2001). Here the \( f_{ch}K_{ch} \) term is usually small relative to \( f_{lip}K_{lip} \) (Hung et al., 2010) such that \( f_{ch}K_{ch} \) could be neglected in most cases. If \( f_{lip}K_{lip}/f_{pw} \) is large (say, > 50–100), the \( \alpha_{pt} \) value will be small and highly system-dependent, as described later. In the latter case, it is practical to determine the ranges of \( \alpha_{pt} \) for common pesticides and contaminants on food crops under assumed system settings. Such information serves to estimate the BCF_{(water)} ranges and contamination levels of the chemicals in crops.

### 3. Data processing and manipulation

To analyze the \( \text{RCF}_{(water)} \) of chemicals in Eq. (7), the needed \( K_{om} \) data consist of either the experimental values or those estimated from \( K_{ow} \) using the empirical equations described below. For relatively nonpolar substituted aromatic compounds other than polycyclic aromatic hydrocarbons (PAHs), the log \( K_{om} \)-log \( K_{ow} \) correlation of Chiou et al. (1983) is used to estimate the soil \( K_{om} \):

\[
\log K_{om} = 0.904 \log K_{ow} - 0.779
\]
For PAHs and their derivatives, the original log $K_{oc}$-log $K_{ow}$ correlation established by Karickhoff et al. (1979) with sediments is converted to that for soils using the relation of $K_{oc}$ (sediment) $\cong 2K_{oc}$ (soil) (Kile et al., 1995) along with $K_{oc} = 1.85K_{om}$ (Chiou, 2002) to give:

$$\log K_{om} = 1.00 \log K_{ow} - 0.778$$

(9)

For polar chemicals, the empirical correlation of Briggs (1981) could be used for estimation if no experimental $K_{om}$ are available:

$$\log K_{om} = 0.52 \log K_{ow} + 0.64$$

(10)

When the reported RCF$_{soil}$ or RCF$_{water}$ data of chemicals are based on the dry plant weight, they are converted to the fresh-weight values for consistency of the treatment. This conversion is made by assuming the water content to be 90% by weight for all fresh roots. This water content is the average for the edible portions of 172 crops/plants given in the USDA Nutrient Database (https://ndb.nal.usda.gov/ndb/search/list).

As indicated, the $f_{ch}K_{ch}$ term in Eqs. (5) and (7) is generally small relative to $f_{lip}K_{lip}$. The value of $K_{ch}$ may be estimated from the respective $K_{ow}$ via the correlation (Hung et al., 2010):

$$\log K_{ch} = 0.741 \log K_{ow} - 1.86$$

(11)

Finally, the $K_{lip}$ term in Eqs. (5) and (7) is assumed to be equal to $K_{ow}$ for the model execution because of the lack of $K_{lip}$ data for most chemicals. This assumption is justified by the similarity of $K_{lip}$ and $K_{ow}$ for a diversity of chemicals according to Hung et al. (2014):

$$\log K_{lip} = 1.03 \log K_{ow} + 0.105$$

(12)

As seen, the difference between $\log K_{lip}$ and $\log K_{ow}$ is not a serious concern to the predicted log RCF$_{water}$ for all chemicals.

4. Sources of literature data

The RCF$_{water}$ data of 37 chemicals with a number of plants/crops from 11 hydroponic studies (Briggs et al., 1982; De Carvalho et al., 2007; Gao et al., 2008; García-Valcárcel et al., 2016; Hinman and Klaine, 1992; Namiki et al., 2015; Romeh, 2014; San Miguel et al., 2013; Su and Zhu, 2006; Su et al., 2009; Xia and Ma, 2006) are listed in Table S1 (Supporting Information). Total data points are 48. Plant roots studied include rice seedlings, lettuce, parrot feather, red clover, Hydrilla verticillata, Phragmites australis, Hordeum vulgare, Brassica aleracea, barley, and many others. Chemicals studied include industrial wastes (e.g., benzaldehyde, chlorophenols, and chlorobenzenes), various pesticides (e.g., atrazine, oxamyl, aldicarb, phenylureas, carbamates, chlordane, ethion, lindane, dieldrin,
etc.), and pharmaceuticals (e.g., fluconazole and clotrimazole), with the log $K_{\text{ow}} = -0.57$ to 5.41.

A similar compilation of the RCF_{water} data for 66 chemicals from various soils to various plants/crops is listed in Table S2. Total data points are 376. The compiled values are from 4 field experiments (Harris and Sans, 1967; Kipopoulou et al., 1999; Mikes et al., 2009; Zhang et al., 2005) and 15 laboratory/greenhouse studies (Beestman et al., 1969; Boxall et al., 2006; Cai et al., 2008; Carter et al., 2014; Gao et al., 2005; Huang et al., 2011; Jiang et al., 2016; Macherius et al., 2012; Pannu et al., 2012; Prosser et al., 2014; Scheunert et al., 1994; Tao et al., 2009; Trapp et al., 1990; Wu et al., 2012; Zhu et al., 2016). The source data comprise a wide range of log $K_{\text{ow}}$ (0.91–8.70), plants/crops, and soil $f_{\text{om}}$ values. Major studied chemicals include organochlorine pesticides (Beestman et al., 1969; Harris and Sans, 1967; Mikes et al., 2009), chlorinated benzenes (Scheunert et al., 1994; Trapp et al., 1990; Zhang et al., 2005), PAHs (Cai et al., 2008; Gao et al., 2005; Kipopoulou et al., 1999; Tao et al., 2009), and poly-brominated diphenyl ethers (PBDEs) (Huang et al., 2011), which make for > 90% of the total data points. Minor chemical classes include polychlorinated biphenyls (PCBs) (Mikes et al., 2009) and personal-care products (Macherius et al., 2012; Pannu et al., 2012; Prosser et al., 2014; Wu et al., 2012). Studied plant roots and their lipid contents ($f_{\text{lip}} \times 100$) are wheat (1.14), barley (1.00), carrot (0.24), radish (0.10), celery (0.17), maize (0.53), pumpkin (0.70), turnip (0.10), onion (0.10), spinach (0.34), Chinese cabbage (0.68), ryegrass (0.32), and amaranth (0.32). If the $f_{\text{lip}}$ data are not reported in original sources, available values from the USDA Food Composition Database (https://ndb.nal.usda.gov/ndb/search/list) are selected. Also listed in Table S2 are the log $K_{\text{ow}}$, soil organic-matter contents ($f_{\text{om}}$), plant species, root lipid contents ($f_{\text{lip}}$), and plant exposure times. The sources of log $K_{\text{ow}}$ values and experimental or model-estimated log $K_{\text{om}}$ values of chemicals in Table S2 are indicated in Table S3.

The hydroponic RCF_{water} data selected for analysis are restricted to the plant samples with > 1-day exposure. For the soil-plant RCF_{water} data from laboratory or field studies, only the data for samples with > 7 days (up to 93 days) of exposure were selected, with most data (~85%) having exposure times of 39–70 days. In either case, no RCF_{water} data of ionic and ionizable chemicals were selected since their uptakes by plants may involve more than a partition process (Tanoue et al., 2012; Wu et al., 2013; Li et al., 2019). When adopting the soil-plant data from literature, only the studies with reported soil $f_{\text{om}}$ and accessible plant $f_{\text{lip}}$ values were selected. For given chemicals with different soils or plants, or with same soils and plants but at very different dosed levels in soil or very different exposure times, the associated RCF_{water} values were treated as independent data in the correlation analysis.

5. Results and discussion

5.1. Root concentration factors from water solutions

We evaluate first the RCF_{water} values of chemicals, i.e., the levels in fresh roots ($C_{\text{pt}}$) relative to those in water ($C_{w}$), from 11 hydroponic studies listed in Table S1. As shown in Fig. 1, a plot of log RCF_{water} versus log $K_{\text{ow}}$ of the chemicals creates two distinctive groups. Over the range of log $K_{\text{ow}} \geq 1.5$, a good linear relation is observed between log RCF_{water} and log $K_{\text{ow}}$, i.e.,

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\[
\log \text{RCF}_{(\text{water})} = 0.720 \log K_{\text{ow}} - 1.14 \quad (n = 38)
\]  

with a correlation coefficient \( R^2 = 0.908 \). The 95% confidence interval and prediction interval for the \( \log \text{RCF}_{(\text{water})} \) data are drawn in Fig. 1. Conversely, in the range of \( \log K_{\text{ow}} \leq 1.1 \), the data fall close to the horizontal line of \( \log \text{RCF}_{(\text{water})} \approx 0.9 \), as first noted by Briggs et al. (1982). The latter results are much anticipated because when the \( K_{\text{ow}} \) of a chemical is small the \( f_{\text{lip}}K_{\text{lip}} \) will be small compared to \( f_{\text{pw}} \) (which is \( \sim 0.9 \)) if \( f_{\text{lip}} \) is small. In this case, \( \log \text{RCF}_{(\text{water})} \) approaches \( \log f_{\text{pw}} \), or essentially zero, as the lower limit. As shown in Table S2, the \( f_{\text{lip}} \) values for most fresh roots are < 0.01 (i.e., 1%) such that for all chemicals with \( K_{\text{ow}} \leq 10 \) the \( \log \text{RCF}_{(\text{water})} \) is practically zero.

The \( \log \text{RCF}_{(\text{water})} \) at a \( \log K_{\text{ow}} \geq 1.5 \) displays a moderate scatter due to the different root \( f_{\text{lip}} \) and \( \alpha_{\text{pt}} \) values as impacted by the chemical \( K_{\text{lip}} \), plant type, plant growth/size, exposure time, and system setting. Whereas calculations of the \( \alpha_{\text{pt}} \) values for individual chemicals with roots in Table S1 require the \( f_{\text{lip}} \) data that are inaccessible, except the \( f_{\text{lip}} (\sim 0.01) \) for barley roots (Briggs et al., 1982), one expects the \( \alpha_{\text{pt}} \) value to decrease largely with increasing \( K_{\text{ow}} \), as found with limited data earlier (Chiou et al., 2001). In principle, with \( K_{\text{ow}} < 500 \) or \( f_{\text{lip}}K_{\text{lip}} < 5 \), the \( \alpha_{\text{pt}} \) should be generally close to 1. If the \( f_{\text{lip}} \) is very small (e.g., \( \sim 0.1\% \) for radishes), even the uptakes of chemicals with \( K_{\text{ow}} = 1000-2000 \) could approach their equilibrium limits (i.e., \( \alpha_{\text{pt}} = 1 \)) in short times. In contrast, the \( \text{RCF}_{(\text{water})} \) values of high-\( K_{\text{ow}} \) chemicals tend to be much more system-dependent. In later analyses of diverse soil-plant data with known \( f_{\text{lip}} \) values, the observed pattern between \( \alpha_{\text{pt}} \) and \( f_{\text{lip}}K_{\text{ow}} \) reflects the impacts of various system parameters on \( \text{RCF}_{(\text{water})} \).

### 5.2. RCFs based on chemical levels in soils and SOM

Consider next the \( \text{RCF}_{(\text{soil})} \) values based on the levels of chemicals in plant roots on a fresh-weight basis \( (C_{\text{pt}}) \) and the corresponding levels in whole soils on a dry-weight basis \( (C_{\text{so}}) \). The relevant data are listed in Table S2, the SI. As noticed, when \( \log \text{RCF}_{(\text{soil})} \) is plotted against \( \log K_{\text{ow}} \) in Fig. 2(A), no distinct patterns emerge \( (R^2 < 0.16) \), as recognized in various reports (Cai et al., 2008; Doucette et al., 2018; Macherius et al., 2012; Mikes et al., 2009; Scheunert et al., 1994; Takaki et al., 2014; Tao et al., 2009; Trapp et al., 1990; Wu et al., 2012). Here the \( \text{RCF}_{(\text{soil})} \) at a given \( K_{\text{ow}} \) varies by as high as 1400-fold. In addition, many observed \( \text{RCF}_{(\text{soil})} \) values are < 1, which is in contrast with the trend for organic chemicals concentrating from water into an organic phase. In analyzing a large set of chemical soil-plant data, Doucette et al. (2018) and Takaki et al. (2014) found a similar wide scatter in plots of \( \log \text{RCF}_{(\text{soil})} \) versus \( \log K_{\text{ow}} \). The lack of a specific relation between \( \log \text{RCF}_{(\text{soil})} \) and \( K_{\text{ow}} \) comes with no surprise in view of \( C_{\text{so}} = f_{\text{om}}C_{\text{om}} \) for relatively water-insoluble (high-\( K_{\text{ow}} \)) chemicals with a water-saturated soil, where the soil contamination intensity \( C_{\text{om}} \) is independent of the value of \( f_{\text{om}} \) (see more discussion in Hung et al., 2009). Since the \( f_{\text{om}} \) varies between soils, the influence of \( f_{\text{om}} \) alone on \( \text{RCF}_{(\text{soil})} \) could well exceed two orders of magnitude in extreme cases. Thus, the observed \( \text{RCF}_{(\text{soil})} \) of a high-\( K_{\text{ow}} \) chemical with a plant tends to be inversely related to soil \( f_{\text{om}} \) as manifested by the dieldrin \( \text{RCF}_{(\text{soil})} \) data (Beestman et al., 1969; Harris and Sans, 1967). Moreover, the
RCF\text{\textsubscript{(soil)}} of a chemical with a given soil tends to increase with increasing plant \textit{f}\text{\textsubscript{lip}}, although not in a strictly proportional manner.

With above considerations, it is expected that if the distribution of chemicals between soil and plant is expressed in terms of the levels in SOM (i.e., \textit{C\textsubscript{om}}), the resulting log RCF\text{\textsubscript{(som)}} values should correlate better with the respective log \textit{K\textsubscript{ow}}. The needed RCF\text{\textsubscript{(som)}} data are obtained by multiplying the RCF\text{\textsubscript{(soil)}} data by associated \textit{f\textsubscript{om}} values (see Eqs. (1) and (7)). The plot of log RCF\text{\textsubscript{(som)}} versus log \textit{K\textsubscript{ow}} is shown in Fig. S1, the SI. As seen, although this adjustment does significantly enhance the correlation (\textit{R\textsuperscript{2}} = 0.421) with a reduced RCF\text{\textsubscript{(som)}} spread, the correlation coefficient is not high enough to be practically useful. In essence, the log RCF\text{\textsubscript{(som)}}-log \textit{K\textsubscript{ow}} plot exhibits a relatively small negative slope (-0.282), implicating that other factors and system parameters also contribute significantly to in-situ RCF values.

5.3. RCFs based on chemical levels in soil water

Recognizing that the RCF\text{\textsubscript{(soil)}} is not a rigorous index and the SOM-based RCF\text{\textsubscript{(som)}} offers only a moderate improvement, we now examine the ability of the soil-water-based RCF\text{\textsubscript{(water)}} in Eq. (7) to reconcile the same set of data in Table S2. The desired RCF\text{\textsubscript{(water)}} data can be obtained by multiplying the RCF\text{\textsubscript{(soil)}} by respective \textit{f\textsubscript{om}}\textit{K\textsubscript{om}}. As shown in Fig. 2(B), a plot of log RCF\text{\textsubscript{(water)}} versus log \textit{K\textsubscript{ow}} for the soil-plant data generates a reasonably distinct and positive correlation, i.e.,

\[
\text{log RCF}_{\text{water}} = 0.565 \text{log } \textit{K}_{\text{ow}} - 1.05 \text{ (n = 374)}
\]  

(14)

with a correlation coefficient \textit{R\textsuperscript{2}} = 0.700, which reduces enormously the RCF\text{\textsubscript{(soil)}} scatter in Fig. 2(A). This improvement signifies the merit of RCF\text{\textsubscript{(water)}} values based on chemical levels in soil water, which serves to link the RCF\text{\textsubscript{(water)}} data derived from soils and water solutions. The observed spread in RCF\text{\textsubscript{(water)}} at a given \textit{K\textsubscript{ow}} reflects the combined impacts of the root \textit{f\textsubscript{lip}} and chemical-root \textit{a\textsubscript{pt}}, which are a function of plant species, plant growth, plant health, exposure time, and system variables, when the soil-plant samples are collected.

Based on the model, the plant \textit{f\textsubscript{lip}} is a prime factor to the RCF\text{\textsubscript{(water)}} of a chemical whenever the \textit{f\textsubscript{lip}}\textit{K\textsubscript{ow}} far exceeds \textit{f\textsubscript{pw}} (~0.9). This expectation is substantiated by a further vastly improved correlation of log RCF\text{\textsubscript{(water)}} with associated log \textit{f\textsubscript{lip}}\textit{K\textsubscript{ow}}, as shown in Fig. 3, where the data split into two groups. For the group with log \textit{f\textsubscript{lip}}\textit{K\textsubscript{ow}} < 0, the observed log RCF\text{\textsubscript{(water)}} approaching 0 at the lower end is well in line with Eq. (7) for many low-\textit{K\textsubscript{ow}} chemicals, as shown in Fig. 1. Conversely, for the group at log \textit{f\textsubscript{lip}}\textit{K\textsubscript{ow}} > 0, the log RCF\text{\textsubscript{(water)}} data, except those of hexachlorocyclohexanes (HCHs) discussed later, are eminently linearly related to the log \textit{f\textsubscript{lip}}\textit{K\textsubscript{ow}} to give

\[
\text{log RCF}_{\text{water}} = 0.587 \text{log } \textit{f\textsubscript{lip}}\textit{K}_{\text{ow}} + 0.172 \text{ (n = 368)}
\]  

(15)

with a correlation coefficient \textit{R\textsuperscript{2}} = 0.825, which covers about 6 orders of magnitude in \textit{f\textsubscript{lip}}\textit{K\textsubscript{ow}} and 4 orders of magnitude in RCF\text{\textsubscript{(water)}}. The associated 95\% confidence interval and prediction interval are also shown. The success of Eq. (15) is due to a large extent to the inverse relation between \textit{a\textsubscript{pt}} and \textit{f\textsubscript{lip}}\textit{K\textsubscript{ow}} to be illustrated later. As is expected, the log
5.4. Dependence of $\alpha_{pt}$ on chemical lipophilicity and system setting

In Fig. 4, the mean $\alpha_{pt}$ value at a $f_{lip}K_{ow}$ shows an expected inverse relation with $f_{lip}K_{ow}$, decreasing from about 1 for many chemicals at log $f_{lip}K_{ow} \leq 0$, or $f_{lip}K_{ow} \leq 1$, to about 0.001–0.002 at log $f_{lip}K_{ow} = 6.5$ or $f_{lip}K_{ow} = 3 \times 10^6$ for highly brominated PBDEs. The observed positive slope between log RCF$_{(water)}$ and log $f_{lip}K_{ow}$ at log $f_{lip}K_{ow} > 0$ in Fig. 3 implies that the decrease in mean $\alpha_{pt}$ with increasing $f_{lip}K_{ow}$ is less than the net increase in $f_{lip}K_{ow}$ (or $f_{lip}K_{ow}$). As manifested in Fig. 4, the log $\alpha_{pt}$-log $f_{lip}K_{ow}$ relation over log $f_{lip}K_{ow}$ is clearly nonlinear, consistent with the quasi-equilibrium partition model. Only at log $f_{lip}K_{ow} \geq 1$, the log $\alpha_{pt}$-log $f_{lip}K_{ow}$ plot is approximately linear, similar to the largely linear relation of log RCF$_{(water)}$ versus log $f_{lip}K_{ow}$ at log $f_{lip}K_{ow} > 0$. Thus, a simple algorithm to find the (approximate) mean $\alpha_{pt}$ at any log $f_{lip}K_{ow} \geq 1$ is to first find the mean RCF$_{(water)}$ via Eq. (15) and then substitute it into Eq. (7) to calculate the mean $\alpha_{pt}$. Calculations of $\alpha_{pt}$ may be expedited with $f_{pw} = 0.9$ and $f_{ch}K_{ch} = 0$ without causing significant errors. Here the calculated mean $\alpha_{pt}$ values for chemicals in roots (Table S2) at log $f_{lip}K_{ow} = 1, 2, 3$, and 4, for example, are 0.53, 0.22, 0.085, and 0.033, respectively, under the assumed exposure conditions.

In theory, the width or spread in $\alpha_{pt}$ and RCF$_{(water)}$ at a $f_{lip}K_{ow}$ should diminish with reducing $f_{lip}K_{ow}$ because the related mean $\alpha_{pt}$ would be closer to the upper limit of 1; therefore, the log RCF$_{(water)}$-log $f_{lip}K_{ow}$ or log $\alpha_{pt}$-log $f_{lip}K_{ow}$ relation generally becomes sharper at reduced $f_{lip}K_{ow}$. On this basis, the unusually small RCF$_{(water)}$ (0.15 to 0.35) or $\alpha_{pt}$ (0.024–0.056) values of $\alpha$, $\beta$, and $\gamma$-HCH on radishes, which result from an unusually large spread in RCF$_{(water)}$ at small $f_{lip}K_{ow}$ (5.2–6.5) in a field study (Mikes et al., 2009), are considered abnormal as well as the RCF$_{(water)}$ of 1,4-dichlorobenzene on barley (Scheunert et al., 1994), which yields $\alpha_{pt} = -2$. Excluding these outliers, the $\alpha_{pt}$ or RCF$_{(water)}$ values at given $f_{lip}K_{ow}$ differ only by a factor of < 2 to 30, which is rather small considering that the RCF$_{(water)}$ values encompass a wide variety of chemicals under a wide diversity of system settings.
It is beneficial to pinpoint essential factors affecting the $\alpha_{pt}$ value. Among all potential factors, accuracies of $K_{om}$ and $K_{ow}$ data have a direct impact on $\alpha_{pt}$ especially for high-$K_{ow}$ chemicals (e.g., PAHs, PCBs, and PBDEs). In addition, calculations of $C_{pw}$ via $C_{om}/K_{om}$ tend to overestimate $C_{pw}$ for chemicals with high $f_{lip}K_{ow}/f_{pw}$ and thus underestimate the actual RCF$_{\text{(water)}}$ and $\alpha_{pt}$. This is because the model assumes $C_{pw}$ to be in instant equilibrium with $C_{om}$ during the plant uptake, which is doubtfully valid when $f_{lip}K_{ow}$ is large. There is, however, a benefit gained by using the estimated $K_{om}$ data for homologous chemicals because the data usually yield right relative orders to enhance the relative consistency of the estimated RCF$_{\text{(water)}}$. In theory, the extent of underestimation in $\alpha_{pt}$ increases with increasing $f_{lip}K_{lip}/f_{pw}$.

Based on the model, the plant $f_{lip}$ is a major factor on the RCF$_{\text{(water)}}$ of lipophilic chemicals. When assessing the $f_{lip}$ impact on RCF$_{\text{(water)}}$, the root $f_{lip}$ is assumed, as approximation, to be independent of the plant size, plant growth/health, and system settings. This assumption introduces certain uncertainties in RCF$_{\text{(water)}}$. Other factors, e.g., the magnitude and uniformity of $f_{om}$ and $C_{om}$ and the plant/crop exposure time, could also affect the observed RCF$_{\text{(water)}}$ or $\alpha_{pt}$ values. Accounts for some of these factors based on relevant available soil-plant contamination data are presented next.

### 5.5. Influences of soil chemical level and plant exposure time

The potential impacts of $C_s$ and the plant exposure time on RCF$_{\text{(water)}}$ are of immediate interest. When the studied soils are well homogenized in a laboratory study, the resulting RCF$_{\text{(water)}}$ and $\alpha_{pt}$ values of dieldrin with maize roots (Beestman et al., 1969) show only a small dependence (by a factor of $<2$) on $C_s$ (from 1 and 5 mg/kg) and on the time of exposure (39 to 90 days). Results of Harris and Sans (1967) on dieldrin uptakes by carrots from three well-mixed soils in well-maintained field plots over a period of 93 days also yield comparable RCF$_{\text{(water)}}$ and $\alpha_{pt}$ values despite that the soil $f_{om}$ varies by nearly 50-fold (0.014 to 0.665). These findings disclose that the chemical-plant $\alpha_{pt}$ values are not sensitively affected by $C_s$ and $f_{om}$ or the exposure period if the time of exposure is sufficiently long and if the soil $f_{om}$ (or chemical $C_{om}$) is kept relatively uniformly.

### 5.6. Influences of plant species and system settings

In the preceding reports of Beestman et al. (1969) and Harris and Sans (1967), the observed $\alpha_{pt}$ values of dieldrin (i.e., 0.4–0.6 and 0.2, respectively) are however notably different. It suggests that system settings and plant species significantly affect the $\alpha_{pt}$ values of chemicals with large $f_{lip}K_{lip}/f_{pw}$ in plants. This view is supported by extensive data on the root uptakes of phenanthrene (PHN) and other PAHs under different (laboratory and field) settings over exposure times of 45–64 days (Cai et al., 2008; Gao et al., 2005; Kipopoulou et al., 1999; Tao et al., 2009). Here, the $\alpha_{pt}$ or RCF$_{\text{(water)}}$ values of PHN and pyrene taken up from a soil at 7–8 different initial PHN or pyrene levels ($C_s$ or $C_{om}$) by a plant (e.g., Chinese cabbage) in a laboratory differ only by about 2-fold (Gao et al., 2005). In contrast, the RCF$_{\text{(water)}}$ values of PHN and pyrene with different plants and system settings differ by 30 to 40-fold (Gao et al., 2005; Kipopoulou et al., 1999; Tao et al., 2009), in which the $f_{lip}$ varies by about 5-fold and the $\alpha_{pt}$ by 5 to 8-fold. On the $f_{lip}$ impact, Gao et al. (2005) found that the RCF$_{\text{(water)}}$ of PHN and pyrene with Chinese cabbage ($f_{lip} = 0.0068$) and ryegrass ($f_{lip}$
are largely proportional to root f$_{lip}$ values. Similarly, the observed RCF$_{water}$ of di- and tri-chlorobenzenes with three crop roots (spinach, carrot, and radish) from farm sites conform largely to the order of root f$_{lip}$ values (Zhang et al., 2005). The results demonstrate that plant f$_{lip}$ and system settings have a major impact on RCF$_{water}$ for chemicals in roots with large f$_{lip}$K$_{ow}$/f$_{pw}$. However, as the f$_{lip}$K$_{ow}$/f$_{pw}$ ratio becomes small, the influences of both plant f$_{lip}$ and system settings should decline sharply or become unnoticeable.

5.7. Influences of field sample inhomogeneity

The field RCF$_{water}$ data are expected to be more variable due to spatially inhomogeneous f$^om$ or C$^om$. This effect could be best illustrated by the field RCF$_{water}$ data with small f$_{lip}$K$_{ow}$ (say, ≤5) because the expected variation in RCF$_{water}$ for systems having relatively uniform f$^om$ and C$^om$ in soil should be small according to the quasi-equilibrium model. In a field study of Mikes et al. (2009), the collected soil and radish samples of α-, β-, and γ-HCH, which have f$_{lip}$K$_{ow}$ = 5.2–6.5, exhibit about a 10-fold scatter in RCF$_{water}$, with many (but not all) measured RCF$_w$ values (0.15–0.35) falling far below ~0.9 to yield very small α$_{pt}$ values (0.024–0.056). These anomalous data might have resulted from multiple causes, including highly non-uniform soil f$^om$ or chemical C$^om$ values, the combined errors in sample preparation and analyses, and/or other unknown causes. In contrast, the RCF$_{water}$ data reported by Zhang et al. (2005) for several chlorobenzenes on a few crop roots from soils (with f$_{lip}$K$_{ow}$ = 2.5–35) at some farm sites display only 2 to 5-fold changes. As the field-sample homogeneity could vary widely, a potentially large variation in RCF$_{water}$ or α$_{pt}$ may occur.

5.8. Influences of chemical degradation and metabolism

Chemical degradation in soil rhizosphere and metabolism inside plants affect the plant contamination levels or RCF$_{water}$. The impact of either an abiotic breakdown or a microbial degradation in the rhizosphere on plant/crop uptake could be treated in terms of the reduced C$_{om}$ or C$_{pw}$ value in Eq. (6), which mitigates the plant uptake level (C$_{pt}$) but exerts no direct effect on the RCF$_{water}$. In this case, the degraded species is viewed as a new chemical subject to the same partition-limited plant uptake. On the other hand, a metabolic process in a plant may or may not affect the C$_{pt}$ or RCF$_{water}$ of the parent chemical depending on the situation. Although the current data is inadequate to fully settle this issue, one expects that only when the chemical metabolic rate far exceeds the rate of chemical uptake by plants will the metabolism have a strong impact on the RCF$_{water}$ or α$_{pt}$ value.

The above view is compatible with the observation of Trapp et al. (1990) on uptakes of atrazine (log K$_{ow}$ = 2.71), 1,2,4-trichlorobenzene (TCB) (log K$_{ow}$ = 3.98), and other chemicals in a soil by barley seedlings (f$_{lip}$ = ~0.01) over one week of exposure. Here the log RCF$_{water}$ of atrazine and TCB are 0.80 and 1.28 and the α$_{pt}$ 1.0 and 0.20, respectively (see Table S2). Masses of atrazine and TCB metabolites in barley are 148% and 90%, respectively, of the parent chemicals. As seen, log RCF$_{water}$ values of atrazine and TCB fall close to the regressed line in Fig. 3 and the α$_{pt}$ values (≤5), especially 1.0 for atrazine, also score well with others in Fig. 4. This indicates that metabolism in plants does not necessarily affect the partition uptake of parent chemicals. Thus, for atrazine and TCB in barley (with f$_{lip}$K$_{lip}$/f$_{pw}$ = 5.7 and 105, respectively), the metabolism seems to have
no major effects on RCF\textsubscript{(water)} and/or $\alpha_{pt}$. For other compounds (e.g., hexachlorobenzene and DDT) having large $f_{lip}\cdot K_{lip}/f_{pw}$ but insignificant metabolic breakdown in barley (Trapp et al., 1990), observed RCF\textsubscript{(water)} and $\alpha_{pt}$ values are also compatible with those of other chemicals. Thus, unless the $\alpha_{pt}$ values are exceptionally small and high levels of metabolites are detected, small $\alpha_{pt}$ values for chemicals with high $f_{lip}\cdot K_{lip}/f_{pw}$ could well be the result of slow chemical uptakes by plants alone.

5.9. Chemical uptakes by shoots and plant seedlings

With the observed efficiency of the quasi-equilibrium partition model for estimating the levels of chemicals in plant/crop roots, a brief account of the model applicability for shoot uptakes is in order. Although the current shoot-uptake studies with reported shoot $f_{lip}$ values are limited, the shoot concentration factors, SCF\textsubscript{(water)} of many PAHs (Gao et al., 2005; Tao et al., 2009) based on their levels in soils and shoots and estimated $C_{pw}$ are compatible with $\alpha_{pt} \leq 1$ imposed by the model. Related SCF\textsubscript{(water)} and $\alpha_{pt}$ data with plant/crop shoots are listed in Table S4, the SI. Observed log SCF\textsubscript{(water)} or $\alpha_{pt}$ values for PAHs with shoots scatter widely when plotted against the shoot log $f_{lip}\cdot K_{ow}$ (see Figs. S2 and S3, the SI). Overall, with a plant/crop, the SCF\textsubscript{(water)} for given PAHs are lower than the respective RCF\textsubscript{(water)} by 2–100 times such that no simple correlation stands out for estimating the SCF\textsubscript{(water)} with shoots.

On the other hand, it is encouraging to find that the quasi-equilibrium partition model (Eq. (15)) gives satisfactory estimates of the RCF\textsubscript{(water)} values with whole plant seedlings (Li et al., 2002; Su and Zhu, 2006; Su et al., 2009; Trapp et al., 1990). This outcome reflects that the total transport paths of chemicals from external water to small plants are relatively short. This observation adds values to the quasi-equilibrium partition model to estimate the levels of contamination in small food crops from soils or water solutions. However, more studies on latter systems are needed to increase the database for developing improved system-specific correlations.

5.10. Prospects on estimation of crop contamination

As exhibited in Figs. 1, 3, and 4, the partition-limited model (Eq. (7)) consolidates the water-plant and soil-plant RCF\textsubscript{(water)} data encompassing diverse system settings. The observed convergence of the RCF\textsubscript{(water)} values with soils and water stems from the use of soil $C_{pw}$ in Eq. (1) as the chemical driving force for plant uptake. The other key parameter sharpening the RCF\textsubscript{(water)} estimation is the $f_{lip}\cdot K_{ow}$ used for quantifying the lipophilic capacity of a specific chemical-plant pair. In essence, the highly improved correlation of Eq. (15) delineates the dependence of RCF\textsubscript{(water)} on the chemical hydrophilicity/lipophilicity and the system setting.

There is a special merit to estimate the RCF\textsubscript{(water)} for chemicals with log $f_{lip}\cdot K_{ow} \leq 2$. With root $f_{lip}$ being $\sim 0.001–0.01$, this log $f_{lip}\cdot K_{ow}$ corresponds to log $K_{ow} \leq 4–5$, which covers a great many pesticides. In this range, the average $\alpha_{pt}$ values with roots fall into 0.20–1.0; consequently, the variation of $\alpha_{pt}$ with system settings is much reduced. Thus, once the ranges of $\alpha_{pt}$ for chemicals with certain plant roots and system settings are determined, they could be used for estimating the RCF\textsubscript{(water)} values or chemical levels in roots at some
chemical levels in soil or water under similar settings. In this practice, the finding that $\alpha_{pt}$ is not sensitive to $f_{om}$ or $C_{om}$ for well-mixed soils (Beestman et al., 1969; Gao et al., 2005; Harris and Sans, 1967; Tao et al., 2009) facilitates the said $\text{RCF}_{\text{water}}$ estimation, with the more variable field-site samples excluded.

6. Conclusions

Analysis of the extensive soil-plant distribution data for a wide variety of nonionic organic chemicals shows clear evidence that the $\text{RCF}_{\text{soil}}$ based on $C_s$ in a soil is an uncritical distribution index because it is a function of the SOM content. By adopting the chemical levels in soil pore water ($C_{pw}$), based on the estimated levels in SOM ($C_{om}$), the resulting $\text{RCF}_{\text{water}}$ effectively overcomes the deficiency of $\text{RCF}_{\text{soil}}$. To further improve the analysis, a more quantitative lipophilic parameter ($f_{lip}K_{ow}$) is employed to account for the lipid effect on $\text{RCF}_{\text{water}}$. By these adjustments, the observed log $\text{RCF}_{\text{water}}$ from diverse soil-plant settings are eminently related to the associated log $f_{lip}K_{ow}$ ($R^2 = 0.825$, $n = 368$). This suggests that $\text{RCF}_{\text{water}}$ is an effective bioconcentration index and $f_{lip}K_{ow}$ an essential parameter for the organic-chemical uptake by roots. The quasi-equilibrium values ($\alpha_{pt}$) found for chemicals under different system settings exhibit an anticipated trend that the ranges of $\alpha_{pt}$ or $\text{RCF}_{\text{water}}$ at given $f_{lip}K_{ow}$ are reduced at small $f_{lip}K_{ow}$ values, with the field data excluded. This effect aids in estimation of the root contamination levels of chemicals (especially, pesticides) with log $K_{ow} \leq 5$. The intimate correlation of $\text{RCF}_{\text{water}}$ with $f_{lip}K_{ow}$ should enhance the transport-fate modeling of nonionic contaminants in soil-plant systems. Information from this work offers a far more accurate prediction of the organic bioaccumulation by plant/crop roots and thus a more accurate risk assessment of the human exposure.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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Fig. 1.
Plots of log RCF<sub>(w)</sub> versus log <i>K<sub>ow</sub></i> for organic chemicals on plant/crop roots from 11 hydroponic studies described in the text. The “expected line” to the lower left is based on Eq. (7) with <i>α<sub>pt</sub></i> = 1, <i>f<sub>pw</sub></i> = 0.9, <i>f<sub>ch</sub></i><i>K<sub>ch</sub></i> = 0, and <i>f<sub>lip</sub></i><i>K<sub>ow</sub></i> = 0.
Fig. 2.
Plots of log $R_{\text{CF(soil)}}$ versus log $K_{\text{ow}}$ (A) and log $R_{\text{CF(water)}}$ versus log $K_{\text{ow}}$ (B) for organic chemicals on plant/crop roots from 19 soil-plant studies described in the text.
Fig. 3.
Plots of log RCF\textsubscript{(water)} versus log [f\textsubscript{lp}K\textsubscript{ow}] for organic chemicals on plant/crop roots from 19 soil-plant studies described in the text. The solid-redcircle data points are suspected outliers excluded from the regression analysis. The “expected line” to the lower left is based on Eq. (7) with $\alpha$\textsubscript{pt} = 1, $f$\textsubscript{pw} = 0.9, and $f$\textsubscript{ch}K\textsubscript{ch} = 0. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
Fig. 4.
Plots of $\alpha_{pt}$ versus log $[f_{lip}K_{ow}]$ for organic chemicals on plant/crop roots from 19 soil-plant studies described in the text ($n = 376$).