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Revising the EPA dilution-attenuation soil screening model for PFAS

Mark L. Brusseau [a,b,*], Bo Guo [b]

[a] Environmental Science Department, The University of Arizona, Tucson, AZ 85721, USA
[b] Hydrology and Atmospheric Sciences Department, The University of Arizona, Tucson, AZ 85721, USA

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ABSTRACT

Per and polyfluoroalkyl substances (PFAS) have been shown to be ubiquitous in the environment, and one issue of critical concern is the leaching of PFAS from soil to groundwater. The risk posed by contaminants present in soil is often assessed in terms of the anticipated impact to groundwater through the determination of soil screening levels (SSLs). The U.S. Environmental Protection Agency (EPA) established a soil screening model for determining SSLs. However, the model does not consider the unique retention properties of PFAS and, consequently, the SSLs established with the model may not represent the actual levels that are protective of groundwater quality. The objective of this work is to revise the standard EPA SSL model to reflect the unique properties and associated retention behavior of PFAS. Specifically, the distribution parameter used to convert soil porewater concentrations to soil concentrations is revised to account for adsorption at the air-water interface. Example calculations conducted for PFOS and PFOA illustrate the contrasting SSLs obtained with the revised and standard models. A comparison of distribution parameters calculated for a series of PFAS of different chain length shows that the significance of air-water interfacial adsorption can vary greatly as a function of the specific PFAS. Therefore, the difference between SSLs calculated with the revised versus standard models will vary as a function of the specific PFAS, with greater differences typically observed for longer-chain PFAS. It is anticipated that this revised model will be useful for developing improved SSLs that can be used to enhance site investigations and management for PFAS-impacted sites.

Synopsis: The widely used EPA SSL model is revised for PFAS applications to account for adsorption at the air-water interface.

Introduction

Recent meta-analyses of field investigations have determined that the vadose zone is a primary reservoir of per and polyfluoroalkyl substances (PFAS) at many PFAS-impacted sites (Anderson et al., 2019; Brusseau et al., 2020). A primary concern for these sites is the leaching of PFAS through the vadose zone to groundwater, and the subsequent impairment of groundwater quality and associated potential risks to human health. The risk posed by contaminants present in the vadose zone is often assessed in terms of the anticipated impact to groundwater. An initial assessment of this risk is typically conducted by comparing measured soil concentrations to soil screening levels (SSLs) that are established to be protective of groundwater quality. It is important to note that SSLs are not cleanup standards (EPA, 1996a).

The U.S. Environmental Protection Agency (EPA) established a soil screening guidance in 1996 as a means to develop SSLs (EPA, 1996a, 1996b). The SSL is defined as the concentration of contaminant in soil that is determined to be protective of human exposure via a specified exposure pathway. For example, the methodology for calculating SSLs for the migration-to-groundwater pathway was developed to identify concentrations in soil that have the potential to contaminate groundwater. SSLs are risk-based concentrations derived from equations combining exposure information with EPA toxicity data. The exposure information refers to the exposure pathway selected for assessment (such as migration to groundwater) and to the soil concentrations present at the site. The toxicity data refers to the standard used to set the target concentration for the relevant medium, such as a maximum contaminant level used to establish the target groundwater concentration for the migration-to-groundwater pathway.

The primary purpose of the EPA SSL approach is to conserve resources by identifying and targeting the sites that pose the greatest concern and therefore warrant further investigation. It is designed for use during the early stages of site investigations, when there is typically limited information about subsurface properties and conditions. The SSL

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* Corresponding author at: Environmental Science Department, The University of Arizona, Tucson, AZ 85721, USA.
E-mail address: Brusseau@arizona.edu (M.L. Brusseau).

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guidance was developed specifically for application at Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) national priorities list (Superfund) sites. However, the EPA SSL guidance has been widely used for a diversity of sites and applications. It is the standard approach for developing SSLs for sites with soil contamination.

The magnitudes of leaching and mass discharge to groundwater are governed by the concentration of contaminant in soil porewater and the infiltration/recharge rate. The porewater concentration in turn is mediated by multiple processes that affect the retention, attenuation, and leaching of the contaminant in the vadose zone. The EPA SSL guidance employs a simple dilution-attenuation (DAF) mass-balance model. As for any screening model, the EPA DAF model is based on a suite of simplifying assumptions. These include the assumption that retention of the contaminant occurs solely by sorption to the soil solids and partitioning into the soil atmosphere, and that sorption is linear, instantaneous (under equilibrium conditions), and associated only with the organic-carbon component of the soil. The SSL guidance was established for application to standard Superfund contaminants such as metals, chlorinated-solvent compounds, and hydrocarbon-fuel constituents. Hence, the model does not consider the unique retention properties of PFAS and, consequently, the SSLs established with the method may not represent the actual levels that are protective of groundwater quality.

Field investigations, mathematical modeling, and bench-scale transport studies have demonstrated that PFAS retention and transport in unsaturated porous media is typically more complex than other types of contaminants such as chlorinated-solvent compounds and hydrocarbon-fuel constituents. Specifically, as surfactants, PFAS adsorb at air-water interfaces in soils, which can provide a source of significant retention in some cases (Brusseau, 2018, 2020; Brusseau et al., 2019a, 2021; Brusseau and Guo, 2022; Guo et al., 2020; Li et al., 2021; Lyu et al., 2018, 2022; Schaefer et al., 2022; Silva et al., 2020; Wallis et al., 2022; Yan et al., 2020; Zeng et al., 2021; Zeng and Guo, 2021). The magnitude of retention by air-water interfacial adsorption depends upon several factors, including PFAS structure and concentration, soil properties, solution chemistry, and the presence of co-solutes (Brusseau, 2018, 2019, 2021; Brusseau et al., 2019a, 2021; Brusseau and Guo, 2021; Brusseau and Van Glubt, 2019, 2021; Costanza et al., 2019; Huang et al., 2022; Li et al., 2021; Lyu et al., 2018, 2022; Schaefer et al., 2019; Silva et al., 2019; Yan et al., 2020). Sorption by the solid phase (soil particles) is another process of significance for PFAS. Due to their molecular properties, PFAS sorption is often more complex compared to other contaminants in that multiple soil constituents and associated mechanisms may be involved (Li et al., 2018; Brusseau et al., 2019b; Knight et al., 2019; Nguyen et al., 2020; Fabregat-Palau et al., 2021; Wang et al., 2021). As a result of air-water interfacial adsorption and multi-mechanism sorption, the retention of PFAS in the vadose zone can be significantly greater compared to traditional organic contaminants. Therefore, efforts to characterize the distribution or transport of PFAS in the vadose zone, including the determination of representative SSLs, should consider the unique properties of PFAS.

The objective of this work is to revise the standard EPA SSL guidance to reflect the unique properties and associated retention behavior of PFAS. The development of the standard EPA DAF model is first presented, along with the accompanying assumptions. This model is then revised by incorporating a term for air-water interfacial adsorption into the distribution parameter used to convert soil porewater concentrations to soil concentrations. Example calculations are conducted to illustrate the contrasting results obtained with the revised and standard models. The additional input parameters required for the revised model are discussed.

Methods

The standard EPA DAF SSL model

The present work is focused on SSLs developed specifically for the migration-to-groundwater pathway. The conceptual basis of this specific approach is discussed in Section 1 in the Supplemental Information (SI) file. The basic procedure to determine SSLs starts with the identification of a relevant target concentration for groundwater (i.e., saturated-zone porewater) that is determined to be protective of groundwater quality. This target concentration is then multiplied by the DAF to obtain the corresponding target leachate or soil porewater concentration in the vadose zone. This step accounts for relevant dilution and attenuation of contaminant concentrations during migration through the vadose zone to the receptor well. This soil porewater concentration is then multiplied by a distribution term to calculate the corresponding soil concentration. This latter step is conducted for two reasons. First, soil porewater concentrations are rarely directly measured at field sites, whereas soil concentrations are the standard for vadose-zone characterization and are routinely measured. Second, most contaminants of concern are present in additional phases in a soil sample beyond the aqueous phase (porewater), such as sorbed by the solids, and thus total concentrations in the soil are typically greater than porewater concentrations. It is observed that the procedure involves a set of backward-moving calculations starting with the target groundwater concentration and progressing to the SSL.

There are two key parameters of the DAF model, the DAF term and the distribution term. The DAF comprises the product of two components, the dilution factor (DF) and the attenuation factor (AF), i.e., DAF = DF × AF. The EPA soil screening guidance addresses only one of these dilution-attenuation processes, specifically contaminant dilution in groundwater. The DF is determined by a simple mixing-zone equation derived from a water-balance relationship that compares the rates of infiltration/recharge and groundwater flow. Detailed discussion of this term is presented in the original EPA documents (EPA, 1996a, 1996b). The default value set by the EPA is 20. It is critical to note that the standard EPA SSL model does not account for attenuation during transport in the vadose zone or groundwater. Hence, the AF is set by default to 1, and the default DAF is 20. It is also important to recognize that the default assumption of AF = 1 is the most conservative approach possible in terms of accounting for the impacts of attenuation processes on leaching in the vadose zone. Namely, this approach assumes that there is no attenuation and, therefore, that leaching rates of the contaminant are equivalent to those of a nonreactive (conservative) solute.

The distribution term is developed from a standard mass balance of contaminant distribution in a soil volume sample. The complete development is given in the SI file (Section 2 in SI), along with underlying assumptions (Section 3 in SI). The EPA DAF SSL model is given as (EPA, 1996a, 1996b):

$$SSL = C_{soil} = C_{gw} DAF\left[K_d + (\theta_w + \theta_a H)\frac{1}{\rho_b}\right] \tag{1}$$

where C_{gw} is the target groundwater concentration deemed to be protective of groundwater quality, C_{pw} = vadose-zone porewater concentration, C_{soil} = soil concentration, $C_{pw} = C_{gw}\ DAF$, K_d (L^3/M) is the sorption coefficient, H (-) is Henry's law constant, ρ_b is porous-medium bulk density (M/L^3), θ_a is volumetric air content (L^3/L^3), and θ_w is volumetric water content (L^3/L^3). Note that the soil concentration determined from this calculation is the SSL.

The standard EPA DAF model accounts for contaminant specificity through the magnitudes of K_d and H in the distribution term. The larger the term in brackets in Eq. (1), the larger the SSL will be for a given target groundwater concentration. AF values may also vary as a function of the contaminant, with for example larger resultant DAF values producing larger SSLs. However, with the default setting of AF = 1, the DAF is independent of the contaminant and solely a function of hydraulic (dilution) factors.

Development of the revised DAF SSL model

The standard DAF model is revised to account for adsorption of PFAS at the air-water interface. It is critical to note that this revision is directed to only the distribution term, which converts the calculated target soil porewater concentration to a corresponding soil concentration. Hence, the revision accounts for the additional mass present in a soil sample that is adsorbed at the air-water interface, the representation of which is critical to produce an accurate porewater-to-soil conversion for PFAS. The revision does not account for the potential impact of air-water interfacial adsorption on retention and associated attenuation during transport through the vadose zone. As noted above, the default assumption for the standard DAF model is that there is no attenuation in the vadose zone. Therefore, this revision does not impact the AF or DAF.

Brusseau and colleagues have developed comprehensive retention models for the distribution of PFAS in the vadose zone (Brusseau, 2018; Brusseau et al., 2019a; Brusseau and Guo, 2022). The complete nondimensional distribution term, R_d^{comp}, is given as (Brusseau and Guo, 2022):

$$R_d^{comp} = \left(1 + K_{d*}\frac{\rho_b}{\theta_w} + H\frac{\theta_a}{\theta_w} + K_n\frac{\theta_n}{\theta_w} + K_{aw*}\frac{a_{aw}}{\theta_w} + K_{nw*}\frac{a_{nw}}{\theta_w} + K_{an*}\frac{a_{an}}{\theta_w} + K_{c*}X_c\right) \tag{2}$$

where a_{an} is the specific air-NAPL interfacial area (L^2/L^3), a_{aw} is the specific air-water interfacial area (L^2/L^3), a_{nw} is the specific NAPL-water interfacial area (L^2/L^3), K_{an^*} is the nonlinear air-NAPL interfacial adsorption coefficient (L^3/L^2), K_{aw^*} is the nonlinear air-water interfacial adsorption coefficient (L^3/L^2), K_{c^*} is the nonlinear distribution coefficient for sorption by colloids (L^3/M), K_{d^*} is the nonlinear solid-phase adsorption coefficient (L^3/M), K_n is the NAPL-water partition coefficient (-), K_{nw^*} is the nonlinear NAPL-water interfacial adsorption coefficient (L^3/L^2), X_c is the concentration of colloidal material in porewater (M/L^3) and θ_n is volumetric NAPL content (L^3/L^3).

Eq. (2) accounts for the contributions of all potential relevant phases and domains within a soil sample volume, with the exception of supramolecular structures such as micelles that may exist as a separate phase. The R_d^{comp} term would be used to convert soil porewater concentrations to soil concentrations by accounting for the presence of PFAS in all relevant retention domains. Eq. (2) can be modified on a site-specific basis by employing only those terms that are relevant for that site. In the present work, it will be assumed that adsorption at the air-water interface is the only additional source of retention beyond that of solid-phase sorption and partitioning to soil atmosphere. The modified distribution term for this case is given by:

$$R_d^{Rev} = \left(1 + K_d\frac{\rho_b}{\theta_w} + H\frac{\theta_a}{\theta_w} + K_{aw}\frac{a_{aw}}{\theta_w}\right) \tag{3}$$

where the K_d and K_{aw} have been simplified by assuming linear adsorption. Methods to account for nonlinear adsorption are discussed by Brusseau and Guo (Brusseau and Guo, 2022). The revised SSL model in terms of the nondimensional distribution factor format of Brusseau and Guo (Brusseau and Guo, 2022) is given by:

$$SSL^{Rev} = C_{gw}DAF\frac{\theta_w}{\rho_b}R_d^{Rev} \tag{4}$$

The revised DAF SSL model presented in the original EPA format is given by:

$$SSL^{Rev} = C_{gw}DAF\left[K_d + (K_{aw}a_{aw} + \theta_w + \theta_a H)\frac{1}{\rho b}\right] \tag{5}$$

Comparison of Eqs. (1) and (5) reveals that the revised model differs from the original model by the presence of the $K_{aw}a_{aw}$ term in the brackets, which accounts for contaminant that is adsorbed at the air-water interface.

Results and discussion

Illustrative calculations of SSLs

An illustrative application is presented to compare the differences in SSLs determined with the revised and standard models due to the impact of air-water interfacial adsorption. A vadose zone soil collected from a site in Tucson, AZ, is used as the representative porous medium. Perfluorooctanesulfonic acid (PFOS) and perfluorooctanoic acid (PFOA) are selected as the representative PFAS. Values for the sorption coefficient, air-water interfacial adsorption coefficient, and air-water interfacial area were obtained from prior studies (see references in Table 1). The input parameters used for the calculations are presented in Table 1, along with the SSLs determined with the two models.

A SSL of 4.3 μg/kg is calculated for PFOS using the standard model. In comparison, a SSL of 75.6 μg/kg is obtained with the revised model. The revised SSL is more than an order of magnitude higher due to the impact of air-water interfacial adsorption. This difference could have a significant impact on identification of sites or areas of sites of greatest concern. It is important to recall that the revised SSL is based solely on correcting the distribution term used to convert soil porewater concentration to soil concentration to account for the additional retention accrued to air-water interfacial adsorption. Potential impacts of retention processes on PFAS leaching and attenuation are not considered.

The impact of contaminant properties on the SSL in the standard model was represented through the values used for K_d and H in the distribution term. The air-water interfacial adsorption coefficient employed in the revised model is also a function of the contaminant. Air-

Table 1
Example Parameters and Calculated SSLs for PFOS and PFOA.

	PFOS		PFOA	
Parameter	**Standard Model**	**Revised Model**	**Standard Model**	**Revised Model**
Dilution Factor (DF)	20	20	20	20
Attenuation Factor (AF)	1	1	1	1
Dilution-Attenuation Factor (DAF)	20	20	20	20
Bulk density (ρ_b, g/cm^3)	1.5	1.5	1.5	1.5
Water content (θ_w, -)	0.2	0.2	0.2	0.2
Air content (θ_a, -)	0.2	0.2	0.2	0.2
Porosity (n, -)	0.4	0.4	0.4	0.4
Sorption coefficient (K_d, cm^3/g)[a]	2	2	1	1
Henry's Law constant (H, -)	0	0	0	0
Air-water interfacial adsorption coefficient (K_{aw}, cm)[b]	NA	0.12	NA	0.008
Air-water interfacial area (a_{aw}, cm^{-1})[c]	NA	446	NA	446
Distribution term (R_d, -)	16	283.6	8.5	26.3
Target groundwater concentration (C_{gw}, μg/L)[d]	0.1	0.1	0.1	0.1
Soil Screening Level (SSL, μg/kg)	4.3	75.6	2.3	7.0

[a] Measured values from (Brusseau et al., 2021)

[b] Measured values from (Costanza et al., 2019; Silva et al., 2019; Brusseau and Van Glubt, 2021)

[c] Measured value from (Guo et al., 2020)

[d] The target groundwater concentration employed is an arbitrary value used for illustration only

water interfacial adsorption is a strong function of the molecular structure of the individual PFAS (Brusseau, 2019; Brusseau and Van Glubt, 2019; Costanza et al., 2019; Schaefer et al., 2019; Silva et al., 2019; Brusseau and Van Glubt, 2021; Brusseau, 2021). This is illustrated by comparing the SSLs determined for PFOA using all of the same parameters as used for PFOS, with the exception of the sorption and air-water interfacial adsorption coefficients (Table 1). The SSL determined for PFOA with the revised model is 7 μg/kg, compared to 75.6 μg/kg for PFOS. In addition, it is observed that the SSL calculated for PFOA with the revised model is only a factor of three larger than the SSL calculated with the standard model. Conversely, the two values differ by more than an order of magnitude for PFOS. These results are due to the differential impact of air-water interfacial adsorption, wherein PFOS has significantly greater interfacial activity compared to PFOA (as shown by their respective K_{aw} values in Table 1).

The impact of chain length on the magnitude of air-water interfacial adsorption for a series of PFAS is illustrated in Fig. 1. The K_{aw} is observed to increase log-linearly with increasing fluorinated-carbon chain length. More generally, K_{aw} is a log-linear function of the molar volume (Brusseau, 2019; Brusseau and Van Glubt, 2019, 2021). As a result, the significance of air-water interfacial adsorption can vary greatly as a function of the specific PFAS. This means that the magnitude of the distribution term in Eqs. 4 and 5 will vary as well. For example, as illustrated in Fig. 1, the distribution factors for PFCAs with < 7 fluorinated carbons are close to 1 because of their comparatively small K_{aw} values. Concomitantly, SSLs determined with the revised model for these PFAS will be similar to the values determined with the standard model due to the minimal impact of air-water interfacial adsorption. Therefore, the difference between SSLs calculated with the revised versus standard models will vary as a function of the specific PFAS, with greater differences typically observed for longer-chain PFAS.

The revised model requires two additional input parameters, namely the air-water interfacial adsorption coefficient and the air-water interfacial area. Measurement and estimation of these parameters is discussed in the SI (Section 4), along with potential impacts of nonideal processes. Also discussed in that section is the estimation of K_d.

Conclusions

There is currently great interest in determining SSLs for PFAS-impacted sites to protect groundwater quality (e.g., Anderson, 2021; Guo et al., 2022; Pepper et al., 2023). This issue is of great significance given the ubiquitous presence of PFAS in soils across the globe. The standard EPA DAF model, which is the most widely used method to establish SSLs, does not account for the unique properties of PFAS and how they may impact retention and distribution in soil. This includes representing adsorption at air-water interfaces, which can be a significant source of retention for many PFAS. The current model is revised by incorporating a term for air-water interfacial adsorption into the distribution parameter used to convert soil porewater concentrations to soil concentrations. Illustrative examples showed that the SSLs determined for PFAS with the revised model may be significantly different from those determined with the standard model. A comparison of distribution parameters calculated for a series of PFAS of different chain length showed that the significance of air-water interfacial adsorption can vary greatly as a function of the specific PFAS. Therefore, the difference between SSLs calculated with the revised versus standard models will also vary as a function of the specific PFAS, with greater differences typically observed for longer-chain PFAS. The specific PFAS for which air-water interfacial adsorption would be comparatively insignificant will depend on site-specific conditions.

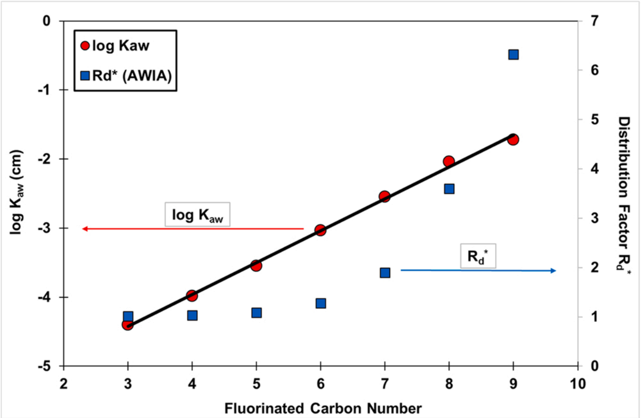

Fig. 1. Correlation of air–water interfacial adsorption coefficient (K_{aw}) and distribution factor R_d* versus fluorinated carbon number for C4-C10 perfluorocarboxylic acids (PFCAs). The asterisk denotes that this R_d accounts solely for air–water interfacial adsorption to illustrate specific impacts. Measured data from transport experiments reported in Lyu et al (Lyu et al., 2022).

It is critical to recognize that the model revision addresses only the distribution term that serves to convert soil porewater concentrations to soil concentrations. The potential impact of air-water interfacial adsorption, multi-mechanism sorption, and transformation processes on PFAS leaching and attenuation in the vadose zone is not considered. This also means that potential factors that can cause nonideal transport behavior (which may often manifest as enhanced rates of leaching), such as heterogeneity and preferential flow, rate-limited mass-transfer processes, and the impact of PFAS mixtures and co-contaminants, are not considered. This is reflected in the use of the standard EPA default assumption that there is no attenuation (AF = 1) in the vadose zone (or groundwater) for the SSL calculations. This assumption is the most conservative approach possible in terms of accounting for the impacts of retention and transformation processes on leaching in the vadose zone. Namely, this approach assumes that there is no attenuation during leaching and, therefore, that the leaching rates of the contaminant are equivalent to those of a nonreactive (conservative) solute. Hence, this approach can be considered to account for the potential impacts of nonideal transport behavior in the simplest manner possible by assuming that there is no attenuation whatsoever. The influence of retention and transformation processes on PFAS leaching can be accounted for by setting the AF to some value greater than 1. Or alternatively, through the use of advanced mathematical models.

The revised model developed in the present work serves as a first step in determining more robust SSLs that represent PFAS-specific retention and distribution behavior. It is anticipated that this revised model will improve investigations and management for PFAS-impacted sites. The limitations of the original EPA SSL model and by association the revised model are well recognized. The original model was designed for use during the early stages of site investigations, when there is typically limited information about subsurface properties and conditions (EPA, 1996a, 1996b). This provision requires that the model be relatively simple and require a minimum of site-specific information, while also being easily updatable when new information becomes available. The model achieves these goals and has become an indispensable tool for site characterization and management. However, there are certainly limitations to the effectiveness of the model. The EPA guidance explicitly discusses options for when the model-associated assumptions are likely to be invalid, noting specifically the option of using more sophisticated transport and fate models. Such models are currently being developed specifically for PFAS. For example, an analytical-solution based screening model has been published that accounts for several PFAS-specific transport and fate processes (Guo et al., 2022). In addition, advanced numerical models have been developed to simulate PFAS transport in the vadose zone (Guo et al., 2020; Silva et al., 2020; Zeng et al., 2021; Zeng and Guo, 2021; Wallis et al., 2022). These models can accurately represent more complex systems and conditions, but have greatly increased input-parameter requirements. We believe that there is value in employing multiple modeling approaches, and that the simplest

DAF models serve an important role in site characterization that is complementary to the more advanced models.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data Availability

all data are in the tables.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.hazl.2023.100077.

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