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Concepts and methods for developing site-specific soil screening levels for per and polyfluoroalkyl substances

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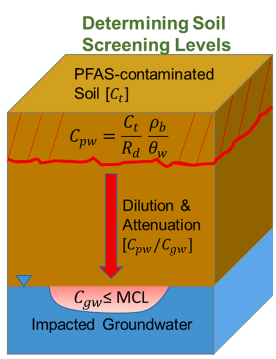
HIGHLIGHTS

- Soil screening levels are widely used to evaluate risks posed by contaminated soil.
- Porewater concentrations in soil are more complex for unsaturated conditions.
- Limitations to the use of batch leach tests are identified.
- Limitations to using field measured soil and porewater concentrations are identified.
- SSLs will vary for different PFAS.

GRAPHICAL ABSTRACT



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ABSTRACT

Soils are a primary long-term reservoir for PFAS, which poses risks to groundwater via leaching through the vadose zone. The application of soil screening levels (SSLs) is one standard, common means to determine risk-based soil concentrations that are anticipated to be protective of groundwater. As such they serve an important role in site characterization, risk assessment, and decision-making concerning the implementation of mitigation or remediation efforts. Despite their significance and widespread use, the determination of SSLs has received minimal research focus. The objective of this work was to examine the determination of SSLs specifically for PFAS-impacted sites. The conceptual basis of SSLs and of the different application methods was presented. It was demonstrated that the magnitudes of porewater concentrations in soil are more complex for unsaturated conditions, and that the difference between values for unsaturated and saturated conditions is a function of the specific PFAS as well as other factors. Methods for determining required input parameters for the SSL calculations were discussed in detail, including estimation methods, the use of laboratory measurements, and the application of field-based data. The applications and limitations of using batch leach tests and field-measured soil and porewater concentrations were specifically examined. Issues associated with data and parameter uncertainty, background concentrations, and other factors were discussed. The application of the methods is illustrated with examples for a fictitious data set and for PFAS-impacted field sites. The outcomes of this study are anticipated to provide clarity on both the conceptual and practical elements of SSL determinations, thereby leading to more robust implementations.

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1. Introduction

Per and polyfluoroalkyl substances (PFAS) have been demonstrated to be ubiquitous in the environment. Concomitantly, soils have been determined to be a primary long-term reservoir for PFAS (e.g., Anderson et al., 2019; Brusseau et al., 2020; Wang et al., 2023). One of the several concerns for sites with PFAS-impacted soil is the migration of PFAS through the vadose zone to groundwater and subsequent impacts to groundwater quality. This issue was highlighted in several early field studies that examined the impact of PFAS-contaminated soil on groundwater through a combination of site characterization and modeling (e.g., Davis et al., 2007; Shin et al., 2011; Xiao et al., 2015). The results of these initial studies demonstrated the leaching potential of PFAS and indicated that impacted soil may serve as a long-term source of contamination to groundwater. The leaching potential of PFAS was also illustrated by the results of early lysimeter leaching studies (Murakami et al., 2008; Gellrich et al., 2012; Stahl et al., 2013). Many additional laboratory, field, and modeling studies have since been conducted in the past decade that have delineated the various factors and processes that mediate PFAS migration in the vadose zone, greatly advancing our understanding (e.g., Weber et al., 2017; Brusseau, 2018; Lyu et al., 2018; Braunig et al., 2019, Brusseau et al., 2019; Dauchy et al., 2019; Brusseau, 2020; Guo et al., 2020; Silva et al., 2020; Zeng and Guo, 2021; Gnesda et al., 2022; Wallis et al., 2022; Ruyle et al., 2023; Schaefer et al., 2023; Bigler et al., 2024; Russell et al., 2025).

Determining the extent to which PFAS may leach and the anticipated magnitude of the impact to groundwater are critical to characterizing the contamination risk. This risk determination is key to exposure assessments, to decision-making concerning the implementation of mitigation or remediation efforts, and ultimately to protecting groundwater quality and human health. A common means to evaluate the risk posed to groundwater by contaminated soil is through the application of soil screening levels (SSLs). This approach produces risk-based soil concentrations that are anticipated to be protective of groundwater, to which soil concentrations measured at a given site can be compared. The SSL approach is widely used to evaluate the potential for contaminated soils to impact groundwater at a site and to assist in assessing the need for intervention. They are particularly useful for identifying which sites may experience the greatest impacts to groundwater when multiple sites are contaminated and resources for mitigation are limited.

The U.S. Environmental Protection Agency (EPA) has developed guidance for the determination of SSLs (EPA, 1996a, 1996b, 2002a). There are multiple approaches available for determining SSLs, each with associated advantages and disadvantages. In addition, parameter selection and parameter uncertainty are important elements for obtaining robust results. Despite the widespread use of the SSL approach and its central importance to site assessments, minimal research has been conducted to examine the concepts underlying the approach and the robustness of the various methods of application. Furthermore, while SSL determinations have been applied to many contaminants and for innumerable sites, its application for PFAS-impacted sites is in its infancy. It is well established that certain physicochemical properties of PFAS impart unique retention and transport behavior in soils. Currently used methods for SSL determination do not account for this unique behavior. It is therefore critical to evaluate the different approaches for SSL determination with specific consideration of PFAS retention and transport behavior in soil.

The objective of this work is to examine the determination of site-specific SSLs, with a focus on PFAS-impacted sites. The conceptual basis of the approach will be discussed along with the different application methods. A major emphasis is focused on methods for determining required input parameters. This includes estimation methods, the use of laboratory measurements, and the application of field-based data such as soil and porewater concentrations. Issues associated with data and parameter uncertainty, background concentrations, and other factors are discussed. The application of the methods is illustrated with examples, and suggested best-practices guidance is presented.

2. Background

2.1. Soil screening levels, soil cleanup levels, and groundwater vulnerability assessments

The U.S. Environmental Protection Agency (EPA) published guidance in 1996 for methods 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. The discussion herein is focused on the migration-to-groundwater pathway. The EPA SSL approach is designed for use during the early stages of site investigations, and its primary purpose is to conserve resources by identifying sites that pose the greatest concern and therefore warrant further investigation and possible intervention.

The EPA guidance presents three approaches for determining SSLs that increase in complexity, difficulty, and cost of application (EPA, 2002a). The first is to use generic values generated by a regulatory agency and reported in a reference document (i.e., "look-up" values). These are typically calculated using the EPA dilution-attenuation factor (DAF) equation, with the input parameters selected to represent a generic exposure scenario intended to be broadly protective under a wide array of site conditions. While the default scenario does not represent worst-case conditions, it is considered to be conservative, leading to comparatively conservative SSLs (EPA, 1996a, 2002a). This approach has the advantage of simplicity and ease of use, with minimal time and cost required for the effort. However, the disadvantage is that the default conditions may not represent the conditions present at the site of interest, which in turn may result in the generic SSLs being more stringent than SSLs developed using site-specific approaches (EPA 1996, 2002a).

The second approach is to use the same EPA DAF equation, but with one or more input parameters determined for the specific site of interest. There are several advantages to the site-specific DAF approach. The first is that it is simple and easy to use compared to the third option of advanced transport and fate modeling. Second, it incorporates some level of site specificity. This is anticipated to result in SSLs that are more representative of site conditions, and which may be less stringent than the generic SSLs (EPA, 1996, 2002a). The disadvantages of this approach are that additional site information and data is required to determine the selected site-specific parameters and that it is based on a number of simplifying assumptions that may not be appropriate for the target site.

The third approach is to conduct detailed mathematical modeling for the site to produce site-specific SSLs. A major advantage in general of employing transport and fate modeling is that more complex site conditions can be incorporated into the assessment. This is especially valuable for sites whose conditions deviate significantly from those assumed in the generic scenario or that cannot be addressed with the standard site-specific DAF approach. The ability to represent attenuation within the vadose zone is one factor that is likely to have a significant impact on SSL determinations. Another factor is the ability to address nonuniform soil concentrations within the vadose zone. Another major advantage of this approach is the capacity to incorporate spatial and temporal variability in processes and parameters. The use of vadose-zone attenuation factors and non-uniform soil concentrations was discussed and illustrated in Smith et al. (2024). Major disadvantages of employing advanced modeling are the time, cost, and expertise required, as well as the need for additional site characterization. These demands increase with increasing complexity of the models being applied.

It is anticipated that approaches two and three would produce more representative SSLs that more accurately represent the risks of groundwater impacts, thereby conserving resources. However, approaches two and, in particular, three will typically require increased levels of site characterization. It is therefore necessary to balance the potential cost savings accrued from possibly less stringent SSLs with the additional site-characterization costs. The choice of which approach to use is dependent upon a number of factors, including project objectives, data availability, and extant resources. Details of the concepts, framework, and methods for SSL calculations are provided in the 1996 EPA guidance documents and are discussed in Section 3. Assumptions and limitations of the approaches will be discussed in Section 6.

Preliminary remediation goals (PRGs) and soil cleanup levels (SCL) are concepts closely related to SSLs. PRGs and SCLs are risk-based site-specific concentrations established to prevent adverse effects to human health and the environment. Hence, they have similar objectives as SSLs, but are used specifically to guide cleanup efforts. While it is emphasized that SSLs are not cleanup standards, they can be used as site-specific cleanup levels under certain conditions (EPA 1996a). In addition, SSLs are often used as de facto cleanup levels or as a starting point to their development. A large body of work is available concerning the development of PRGs and SCLs, and many components and concepts are applicable to the determination of SSLs.

It is also useful to note the existence of groundwater vulnerability assessments (GVAs) and the similarities between them and SSL determinations. A primary purpose of GVAs is to assist in decision-making and conserving resources by identifying the sites upon which to focus mitigation and preventative measures (e.g., Aller et al., 1987; NRC, 1993). It is seen that primary objectives of both GVAs and SSLs are similar, to identify sites for which groundwater is anticipated to be impacted to greater extents by surface-associated contamination or activities. The former is focused on conditions prior to the proposed activities whereas the latter is focused on sites that have already been impacted. Concepts and lessons learned from VGA applications are useful for SSL determinations. For example, there is a large body of work associated with the use of screening models for conducting assessments of groundwater contamination risk posed by pesticides, fertilizers, chlorinated solvents, and fuels (e.g., Rao et al., 1985; Jury et al., 1987). Outcomes from these applications provide insight into the application of models for simulating PFAS leaching and determination of SSLs.

2.2. Fundamental relations for PFAS distribution within a soil volume

The fundamental relations for PFAS distribution in a soil volume are reviewed in the Supplemental Information (SI) file (SI-1) to establish a basis and reference framework for the upcoming discussions. This material is based on the comprehensive retention models developed by Brusseau and colleagues (Brusseau, 2018; Brusseau et al., 2019; Brusseau and Guo, 2022). To be consistent with the DAF equations used to determine SSLs, the present discussion will focus on retention associated with solid-phase adsorption, air-water interfacial adsorption, and air-water partitioning, with R_d represented as:

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

where R_d is the nondimensional distribution coefficient, K_a is the air-water partition coefficient (Henry's coefficient, -), K_{aw} is the air-water interfacial adsorption coefficient (cm^3/cm^2), K_d is the solid-phase adsorption coefficient (cm^3/g), a_{aw} is the specific air-water interfacial area (cm^2/cm^3), ρ_b is porous-medium bulk density (g/cm^3), θ_a is volumetric air content (cm^3/cm^3), and θ_w is volumetric water content (cm^3/cm^3). Air-water partitioning is included to be consistent with the EPA DAF approach discussed below, but it is assumed negligible for the present application.

With the introduction of R_d, Eq. (2) in SI-1 becomes:

$$M_t = C_{pw}\theta_w V_t R_d \tag{2}$$

where M_t is total mass in the volume of sample (M), C_{pw} is the porewater concentration (M/L^3), and V_t is the total sample volume. The total concentration of the select PFAS in the soil volume, C_t (M/M), is defined as M_t/M_s, where M_s is the mass of soil solids (M). Note it is assumed that the total concentration is equivalent to the what is commonly referred to as the soil concentration [Brusseau and Guo, 2022]. Substituting Eq. (2) into M_t/M_s gives:

$$C_t = C_{pw}\frac{\theta_w}{\rho_b}R_d \tag{3}$$

The porewater concentration of a particular PFAS is correspondingly given as:

$$C_{pw} = \frac{C_t}{R_d}\frac{\rho_b}{\theta_w} \tag{4}$$

Inspection of Eq. (4) shows that the porewater concentration is a function of the total soil concentration, soil properties, and PFAS properties. The influence of each component on the magnitude of the resultant porewater concentration is discussed in detail in SI-2. This material includes a figure illustrating the relationship between R_d and molar volume (Figure SI-1), a figure illustrating the impact of water saturation on porewater concentrations for shorter and longer-chain PFAS (Figure SI-2), and a figure illustrating the impact of water saturation on the magnitude of R_d (Figure SI-3).

The combined influence of all factors discussed in SI-2 is illustrated in Fig. 1. Values for K_{oc}, the organic-carbon normalized sorption coefficient, and K_{aw} were obtained from molar-volume based regressions reported in prior works (Brusseau, 2023a, 2024a; Brusseau and Van Glubt, 2021). K_d was determined as $K_d = K_{oc}f_{oc}$, using a fraction of organic carbon (f_{oc}) of 0.001. While the limitations of this approach for determining K_d are recognized, it is noted that the K_{oc} values obtained from the employed regression represent apparent values that incorporate the contributions of inorganic soil constituents to adsorption. Notably, the K_{oc} values are based on measurements obtained for lower f_{oc} soils. The magnitudes of the respective K_{oc} values are presented in Figure SI-4. The air-water interfacial areas were obtained from measured values for a sandy soil (Brusseau, 2023b).

Inspection of Fig. 1 shows first of all that porewater concentrations for the smallest (shorter-chain) PFAS are larger under unsaturated conditions for the same soil concentration C_t. This is due to the increase in the $\frac{\rho_b}{\theta_w}$ term as discussed in SI-2. While the decrease in θ_w under unsaturated conditions causes an increase in R_d (see Eq. (1)), this increase is outweighed by the magnitude of the increase in the $\frac{\rho_b}{\theta_w}$ term. It is also

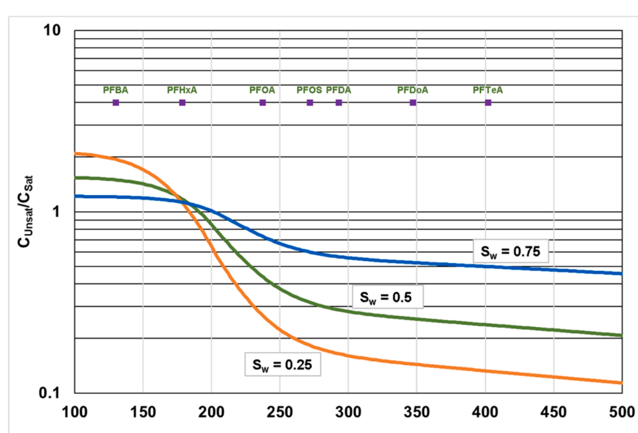

Fig. 1. The impact of unsaturated conditions on porewater concentrations as a function of PFAS size (represented by molar volume). Curves are presented for three water saturations (S_w). The small squares at the upper section of the plot are used to indicate the respective molar volumes for select representative PFAS to illustrate the size range spanned by the curves. Bulk density = 1.5 g/cm^3, porosity = 0.3, C_t = 1000 μg/kg. a_{aw} values: 912 cm^{-1} (S_w=0.25), 446 cm^{-1} (S_w=0.5), 140 cm^{-1} (S_w=0.75).

observed that the porewater concentrations for the larger PFAS (e.g., >~180 molar volume) are lower than those under saturated conditions. This is due to the factors discussed for Figure SI-2.

The ratio of total soil concentration to porewater concentration is:

$$\frac{C_t}{C_{pw}} = \frac{\theta_w}{\rho_b} R_d \tag{5}$$

Inspection of Eq. (5) reveals that R_d represents the ratio of total mass present in the soil sample to the mass present as dissolved solute in porewater. The $\frac{\theta_w}{\rho_b}$ term represents the ratio of porewater volume to soil-solids mass and as noted can be thought of as a unit conversion term. Note that the $\frac{C_t}{C_{pw}}$ term has units of L^3/M, such as L/kg. For a given soil bulk density and water content, the ratio is a function of the magnitudes of K_d and K_{aw}. As discussed in SI-2, it has been well established that the magnitudes of both parameters increase with increasing PFAS size (e.g., Guelfo and Higgins, 2013; Nguyen et al., 2020; Brusseau, 2024a), and as a consequence so does R_d. Hence, the $\frac{C_t}{C_{pw}}$ ratio is expected to be a function of PFAS size. This is illustrated in Fig. 2, which presents measured soil and porewater concentrations reported in three field studies. The measured $\frac{C_t}{C_{pw}}$ ratios are observed to be a log-linear function of molar volume. Notably, the magnitudes of the ratio vary by orders of magnitude as a function of the PFAS.

Values are observed to be less than one for the smallest PFAS. This is due to the impact of the $\frac{\theta_w}{\rho_b}$ term, which is always <1. With the default values of 1.5 kg/L and 0.3 for bulk density and porosity, respectively, assuming a water saturation of 50 % produces a $\frac{\theta_w}{\rho_b}$ value of 0.1. This may be used as a very approximate value for order-of-magnitude assessments of $\frac{C_t}{C_{pw}}$ ratios. For $\frac{\theta_w}{\rho_b}$ values close to 0.1, it is observed from Eq. (5) that the R_d term would need to be >10 for the $\frac{C_t}{C_{pw}}$ ratio to exceed 1. Based on the small magnitudes of K_d and K_{aw} typically measured for the shortest-chain PFAS, it is anticipated that their $\frac{C_t}{C_{pw}}$ ratios will often be <1. Conversely, it is anticipated that the ratios will be significantly greater than 1 for very long-chain PFAS.

3. Methods for determining site-specific SSLs

3.1. Standard and revised DAF approaches

The conceptual basis of the standard DAF approach is described in the EPA Guidance documents (EPA, 1996a, 1996b, 2002). In addition, several states have developed guidance for site-specific determination of SSLs (e.g., Wisconsin DNR, 2003; Kentucky EPPC, 2004; Florida DEP, 2008; New Jersey DEP, 2008, 2013, 2021; Ohio EPA, 2008; Nevada DEP, 20210; Minnesota PCA, 2013; Georgia DNR, 2019; Maine DEP, 2021). Contaminant concentrations are assumed to be attenuated by adsorption and degradation as leachate migrates through the vadose zone to ground water, and are subsequently diluted by mixing with groundwater at the water table and within the saturated zone during transport to the receptor point (e.g., potable-water well). This reduction in concentration can be expressed by a DAF, defined as the ratio of the soil porewater concentration to the receptor-point (groundwater) concentration. Note that while the EPA guidance uses the term "soil leachate concentration", we will use the term "soil porewater concentration" to denote concentrations in porewater present in soil that is the focus of SSL determinations (e.g., surface soil samples). The term "soil leachate concentration" will be reserved herein to refer to the aqueous concentration that is transferred from the vadose zone to groundwater at the soil-groundwater interface.

The lowest possible DAF is 1, corresponding to the situation where there is no dilution or attenuation of the contaminant concentration. In this case, the concentration in groundwater at the receptor well is equal to the porewater concentration in the soil. Conversely, high DAF values correspond to comparatively large reductions in contaminant concentrations between the soil and the receptor well due to dilution and attenuation.

The general procedure to determine SSLs with the DAF approach starts with the identification of a target concentration for groundwater that is determined to be protective with respect to the planned use. This target concentration is then multiplied by the DAF to obtain the corresponding target soil porewater concentration in the soil. In the standard DAF approach, this step accounts for dilution and attenuation of contaminant concentrations due only to mixing with groundwater and migration to the receptor well. It is specifically assumed that there is no attenuation during migration in the vadose zone or groundwater. The target porewater concentration is then multiplied by a distribution-conversion term to calculate the corresponding soil concentration. This latter step accounts for the fact that many contaminants of concern are present not only in porewater but may also be associated with soil solids and soil atmosphere. As a result, total concentrations in the soil generally differ from porewater concentrations.

The EPA DAF SSL equation is given as (EPA 1996a, 1996b):

$$SSL = C_t^T = C_{gw}^T DAF \left[K_d + (\theta_w + \theta_a K_a) \frac{1}{\rho_b} \right] \tag{6}$$

where the following relations apply:

$$C_{pw}^T = C_{gw}^T \; DAF \tag{6a}$$

and

$$C_t^T = C_{pw}^T \left[K_d + (\theta_w + \theta_a K_a) \frac{1}{\rho_b} \right] \tag{6b}$$

and where C_{gw}^T is the target groundwater concentration deemed to be protective of groundwater quality, C_{pw}^T is the target porewater concentration, and C_t^T is the target total soil concentration (i.e., the SSL). Eq. (6) can be developed and presented in a more elegant and convenient format that presents the distribution term as a nondimensional distribution factor that is essentially equivalent to the retardation factor widely used for transport and fate (Brusseau and Guo, 2022,2023). The rewritten DAF equation is:

$$SSL = C_t^T = C_{gw}^T \; DAF \; \frac{\theta_w}{\rho_b} \; R_d \tag{7}$$

with C_t defined in Eq. (3) and R_d defined as:

$$R_d = \left(1 + K_d \frac{\rho_b}{\theta_w} + K_a \frac{\theta_a}{\theta_w} \right) \tag{8}$$

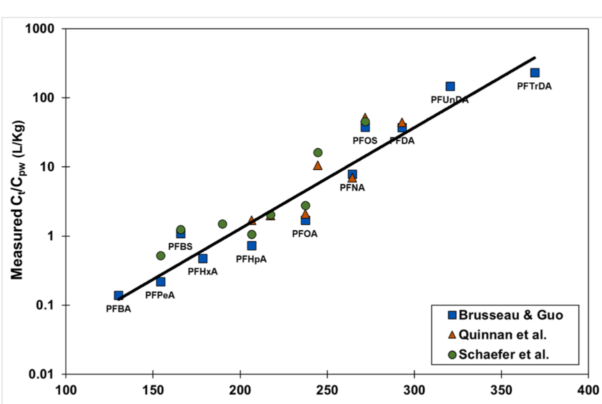

Fig. 2. Measured soil (C_t) and soil porewater (C_{pw}) concentrations for several PFAS as a function of molar volume (V_m). The three data sets represent measurements conducted for field studies. Reproduced from Brusseau (2023c).

Note that R_d in Eq. (8) is simplified from equations (1) and (SI-4).

Brusseau and Guo (2023) recently revised the EPA DAF approach to account for PFAS adsorption at the air-water interface in the distribution-conversion term used to convert porewater concentrations to total soil concentrations. The revised SSL equation in terms of the nondimensional distribution factor format is given by:

$$SSL^{Rev} = C_{gw}^{T}\ DAF\ \frac{\theta_w}{\rho_b}\ R_d^{Rev} \tag{9}$$

with the modified distribution factor for this case given by Eq. (1). The revised DAF SSL equation presented in the original EPA format is given by:

$$SSL^{Rev} = C_{gw}^{T} DAF[K_d+(K_{aw}a_{aw}+\theta_w+\theta_a K_a)\frac{1}{\rho_b}] \tag{10}$$

Comparison of Eqs. (6) and (10) shows that the revised equation differs from the original 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. Similar to the standard DAF approach, the revised approach does not account for attenuation within the vadose zone or groundwater.

One advantage of employing the revised format for the distribution-conversion term is that additional sources of retention can be readily included when relevant. This is accomplished via the comprehensive retention models and use of equation (SI-4) discussed in SI-1. The contributions to retention of all potentially relevant phases and domains within a soil sample volume are accounted for in equation (SI-4), with the exception of supramolecular structures such as micelles that may exist as a separate phase. The R_d term can be modified on a site-specific basis by employing only those terms that are relevant to PFAS retention and distribution within the soil for that site. In the present work, it will be assumed that adsorption at the air-water interface is the only additional major source of retention beyond that of solid-phase adsorption and partitioning to soil atmosphere.

3.2. Components of the DAF equation

Inspection of Eqs. (6), (7), (9), and (10) shows that the SSL consists of three components, the protective target groundwater concentration, the DAF term, and the porewater-to-soil distribution-conversion term. Regulatory or advisory limits established by a regulatory agency are often used as the target groundwater concentration. For example, maximum contaminant levels (MCLs) established under the U.S. Safe Drinking Water Act, or their equivalent in other countries, are commonly used, especially when groundwater is used as a potable water source. MCLs are currently established for two PFAS in the U.S., PFOS and PFOA, both of which are 4 ng/L.

The DAF term is the product of two components, the dilution factor (DF) and the attenuation factor (AF), i.e., DAF = DF × AF. As noted above, the standard and revised DAF approaches specifically address only contaminant dilution due to soil leachate mixing with groundwater and migration through the saturated zone. It does not account for dilution during transport in the vadose zone, nor does it account for attenuation in the vadose zone or groundwater. Hence, the AF is set by default to 1, and the DAF is equivalent to the DF for the standard and revised DAF approaches. It is important to recognize that this default assumption is the most conservative approach possible in terms of accounting for the impacts of attenuation processes on leaching in the vadose zone. As will be discussed in Sections 5 and 6, methods are available to determine AF values for use in the DAF equation.

The DF is determined by a simple mixing-zone equation derived from a mass-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 so-named Summers model (Summers et al., 1980) was one approach employed in the EPA guidance and it can be used to illustrate the development of the standard DF equation. It is given as:

$$C_{gw} = \left(\frac{Q_i}{Q_a+Q_i}\right)C_{pw} \tag{11}$$

where Q_i is the recharge from infiltration [$Q_i = I \times W \times L$, ($L^3$/T)], Q_a is groundwater flow rate [$Q_a = q \times W \times d$, ($L^3$/T)], q is Darcy flux or specific discharge (L/T), I is the annual net infiltration rate (L/T), d is the groundwater mixing-zone thickness (L), W is the width of the source zone (L), and L is the length of the source zone parallel to flow (L). Note that it is assumed for this case that there is no background contaminant in groundwater from upgradient. A more general case accounting for background concentrations is presented in Section 6.2. Inspection of Eq. (11) shows that the ratio of flow rates in parentheses serves to "dilute" the porewater concentration. This can be rewritten in terms of the porewater concentration as:

$$C_{pw} = \left(1+\frac{Q_a}{Q_i}\right)C_{gw} \tag{12}$$

Substituting the definitions for Q_a and Q_i into Eq. (13) and with the assumption of AF = 1, the following definition for DF is obtained:

$$\mathrm{DF} = \frac{C_{pw}}{C_{gw}} = 1+\frac{Q_a}{Q_i} = 1+\frac{q\ d}{I\ L} \tag{13}$$

The DF can be considered to comprise two sets of ratios, a ratio of fluxes (q/I) and a ratio of dimensions (d/L). Larger DF values represent greater reductions in porewater concentrations, and thus larger SSLs for a given target groundwater concentration and distribution-conversion term.

The term in the brackets in Eqs. (6) and (10) and the $\frac{\theta_w}{\rho_b}R_d$ term in Eqs. (7) and (9) are the respective distribution-conversion terms used to translate the porewater concentration to a total soil concentration. The distribution-conversion term is developed from a standard mass balance of contaminant distribution in a soil volume sample. Details of the development of the term are provided in the EPA document (EPA, 1996b) as well as in Section 2. The larger the distribution-conversion term, the larger the SSL will be for a given target groundwater concentration and DF.

The DAF approach implicitly captures the impact of site conditions on SSL determination via the application of the DF. This includes the impacts of soil and aquifer hydraulic properties, climate (precipitation, evapotranspiration, recharge), and source size. It is assumed that the DF is independent of the specific contaminant. The standard and revised DAF approaches incorporate contaminant specificity through the magnitudes of K_d, K_{aw}, and K_a in the distribution-conversion term and via the selected C_{gw}^{T}. AF values may also vary as a function of the contaminant. However, with the default setting of AF = 1, the DAF is independent of the contaminant and solely a function of hydraulic (dilution) factors.

3.3. Default versus site-specific parameter values for the DAF approach

The DAF equation consists of two sets of parameters, one representing hydraulic properties that influence dilution and another set that represents the distribution of solutes within the soil. The EPA guidance presents default parameter values to use with the DAF equation to determine SSLs (EPA, 1996a, 2002a). The default value for DF is 20. This results in a default DAF value of 20 with the assumption that AF = 1. This default value was determined based on a "weight of evidence" approach that incorporated results from a series of modeling simulations and from application of the DF calculation to 300 sites across the US (EPA, 1996b). An alternative default DF value of 1 was established for use at sites for which minimal dilution is anticipated (EPA, 2002a). This was stated to be relevant for sites with shallow groundwater tables, fractured media, karst topography, or source zones greater than 30 acres

(~121,000 m^2). It was stated that the use of 20 as the default DAF is considered to more accurately reflect the threat posed to groundwater for most sites compared to the value of 1 that assumes no dilution (EPA, 1996b). Some states have developed their own default DF values to be more representative of state-specific conditions (e.g., Kentucky EPPC, 2004; Maine DEP, 2021).

Default values are also provided for some of the parameters needed to calculate the distribution-conversion term (EPA, 1996a, 2002a). For example, the standard DAF approach is based on the assumption that sorption is controlled by the organic-carbon fraction of the soil. A default value of 0.002 was provided for the f_{oc}, which is used in the estimation of K_d, as will be discussed in the next subsection. Default values of 1.5 kg/L and 0.3 were provided for soil bulk density and volumetric water content (porosity), respectively.

As noted above, the EPA guidance provides the opportunity to apply the DAF equation on a site-specific basis by employing one or more site-specific parameter values. Inspection of Eqs. (6), (10), and (13) reveals that values are needed for several input parameters, specifically q, I, d, L, K_d, K_{aw}, K_a, a_{aw}, ρ_b, θ_a, and θ_w. The first four are needed to calculate the DF and hence the DAF term with AF assumed to equal 1. The latter seven terms are required for calculation of the distribution-conversion term.

A critical element in the determination of representative site-specific SSLs is the robustness of the input parameters used in the calculations. This in turn will depend upon the sources of the data and the representativeness of the values. Typically, there are multiple sources available from which to determine values for a given parameter, ranging from field-measured values to laboratory-measured values to empirical-based estimations. Using K_{sat} as an illustrative example, this parameter can be measured by conducting in-situ field tests. It can also be measured by conducting laboratory tests on samples collected from the field site, or it can be estimated based on empirical functions that employ simpler measurements such as soil texture. Finally, generic values can be used from reference documents based on soil type. These methods have increasinging levels of simplicity of application but are anticipated to have decreasing levels of representativeness. For another example, as noted, the standard DAF approach is based on the assumption that sorption is controlled by the organic-carbon fraction of the soil. Using the default value for f_{oc} along with an estimated K_{oc} represents the simplest means by which to parameterize the K_d. A common means to add site specificity in the SSL determination is to measure f_{oc} for the site soil to use in place of the default value. A more advanced site-specific approach would be to conduct laboratory experiments to measure K_d for the site soil. Finally, another alternative would be to measure a field-based "in-situ" K_d.

Standard site investigations may produce data that provide sources of values for some of the required input parameters. However, they often may comprise the application of empirical estimations that employ basic soil property measurements such as grain-size distributions. In addition, they do not typically include laboratory or field measurements of some required input parameters. While data quality is likely to be greater for measured versus estimated values, the cost of acquisition is also likely to be greater. Hence, a critical question to address for each relevant parameter is what is the lowest tier of data source (the lowest cost of acquisition) that will provide reasonably robust outcomes for SSL determinations. Methods for determining parameter values are discussed briefly in the following subsections. The options available are summarized in Table 1.

3.4. Parameter determination for the DAF approach: DAF term

The simplest means by which to parameterize the DAF equation is to employ the default values provided by the EPA. However, as discussed above, site-specific values can be used to better tailor the calculations to site conditions. These site-specific values can be determined by measurement or estimation.

The DF term can be estimated by calculation with Eq. (13). To do so requires information for four parameters, two of which are related to dimensions of the source zone and mixing zone. Source-zone dimensions are typically established through standard site investigation approaches, such as commonly employed soil sampling surveys in combination with the development of the conceptual site model and other elements. Guidance for source-zone characterization is available from multiple sources (e.g., NRC, 2005), while guidance for soil sampling specifically in relation to determination of SSLs is provided in the EPA documentation (EPA, 1996a, 1996b). However, it is important to consider the specific physicochemical properties of PFAS in site characterization efforts (ITRC, 2025).

The EPA guidance presented an equation to calculate the mixing-zone thickness:

$$d = (2\alpha_v L)^{0.5} + d_a\{1- \exp[(-LI)/(V_s n_e d_a)]\} \quad (14)$$

where α_v is vertical dispersivity, d_a is aquifer depth, V_s is horizontal groundwater velocity [$V_s = q/n_e$], and n_e is effective saturated-zone

Table 1
Methods to determine values for parameters comprising the DAF equation.

Parameter Determination Options for the SSL DAF Equation					
Parameter	Definition	Default Values	Site-Specific	Site-Specific	Site-Specific
SSL [μg/kg]	Soil screening level	Generic set value	$C_{gw}^T \times \mathrm{DF} \times \mathrm{AF} \times \mathrm{DCF}$		
C_{gw}^T [μg/L]	Protective groundwater concentration	Designated reference level	Alternative level		
DF [-]	Dilution factor	20 (1 for some cases)	$1 + \frac{q\ d}{I\ L}$	C_l^m/C_{gw}^m	
AF [-]	Attenuation factor	1	$(d_c + d_u)/d_c$	$(C_{pw}^m/C_{gw}^m)/\mathrm{DF}$	C_{pw}^m/C_l^m
DAF [-]	Dilution-attenuation factor	20 (1 for some cases)	DF × AF	C_{pw}^m/C_{gw}^m	
DCF [L/kg]	Distribution-conversion factor	$0.002K_{oc} + \frac{0.3}{1.5}$	$\frac{\theta_w}{\rho_b}R_d$	C_t^m/C_{pw}^m	
DAF × DCF [L/kg]	Combined	$20 \times [0.002K_{oc} + \frac{0.3}{1.5}]$	C_t^m/C_{gw}^m		

Notes: (1) the parameter-determination options for each parameter are independent of the options for the other parameters (the SSL can be calculated using any relevant combination of the options)
(2) the air-water mass-transfer term (Henry's coefficient) is not included in the default DCF for simplicity

C_{gw}^m = measured groundwater concentration
C_l^m = measured soil leachate concentration
C_{pw}^m = measured porewater concentration
C_t^m = measured total soil concentration
ρ_b = soil bulk density
θ_w = volumetric water content
d = groundwater mixing zone thickness
d_c = thickness of contaminated soil interval
d_u = thickness of uncontaminated soil interval
I = net infiltration (recharge)
K_{oc} = organic-carbon normalized adsorption coefficient
L = longitudinal source length
q = Groundwater specific discharge
R_d = nondimensional distribution factor

porosity. The first term on the right hand side accounts for mixing within the saturated zone due to vertical dispersivity, whereas the second term accounts for mixing due to downward flow caused by recharge. Values for L, d_a, and n_e are determined from standard site characterization, whereas I and q are determined as discussed below. The EPA guidance provided empirical relationships from Gelhar and Axness (1983) to estimate α_v as $\alpha_v = 0.056\ \alpha_L$ and $\alpha_L = 0.1$ L, where α_L is longitudinal dispersivity. Note that site-specific values can be used for α_v if available, obtained either from measurements or from other empirical relationships that may be more representative of site conditions.

While the use of Eq. (14) is the typical approach, other options are available. For example, high-resolution soil or porewater sampling of the saturated zone can be used to delineate the contaminant-impacted depth interval as a representation of the mixing-zone thickness. This approach would typically be most useful for sites with no upgradient sources. In another approach, the mixing-zone thickness can be set to a representative length of the screened interval of a potable-water supply well (e.g., Ohio EPA, 2008) or to the drawdown depth generated by a potable-water supply well (Rzepecki and Edlund, 1997), based on the concept that the pumping will mediate the mixing depth. In a third approach, mathematical-modeling simulations can be conducted to characterize a site-specific mixing-zone thickness.

The DF calculation also requires information for groundwater flow and net infiltration. Darcy flux or specific discharge can be determined for a specific site by field measurements of hydraulic conductivity (aquifer tests) and hydraulic gradient (groundwater levels). Hydraulic conductivity can also be measured in the laboratory or estimated from soil or sediment-texture correlations. Numerous references are available for determining these hydraulic parameters. The simplest approach for parameterizing net infiltration is to assume it is equivalent to annual net recharge. There are many methods available to determine net infiltration and recharge, which have been reviewed in a number of publications (e.g., Allison et al., 1994; Scanlon et al., 2002; Healy and Scanlon, 2010; Newell et al., 2023).

3.5. Parameter determination for the DAF approach: distribution-conversion term

The distribution-conversion term comprises parameters associated with properties of the soil (a_{aw}, ρ_b, θ_a, and θ_w) and properties of the contaminant (K_d, K_{aw}, K_a). Measurements of ρ_b, θ_a, and θ_w are typically made by collecting soil samples from the site and subjecting them to standard laboratory characterization. In addition, various instruments are available to measure θ_w in the field. Numerous references exist that describe these methods in detail.

The determination of values for a_{aw} is more complex than for the other soil properties. The magnitude of a_{aw} is a function of soil properties (grain-size distribution, solid surface area) and water saturation. This functionality is illustrated in Figure SI-5, which shows that a_{aw} can range over orders of magnitude depending upon site conditions. This means that the relative significance of air-water interfacial adsorption for PFAS retention and attenuation can vary from site to site. Methods are available to estimate or measure a_{aw} including integration of the soil-water characteristic curve, interfacial tracer tests, and advanced imaging methods. These have been discussed and compared in a recent review (Brusseau, 2023b). A complicating factor is that the different methods often produce different results, due in part to whether or not they characterize the contribution of microscale solid-surface roughness to interfacial area. The a_{aw} most relevant to retention and transport of PFAS in soil appear to be those measured with the interfacial tracer-test method (Brusseau and Guo, 2021). Empirical methods to estimate a_{aw} from soil properties such as grain diameter and solid surface area have been developed (Brusseau, 2023b).

There are several means by which values for K_d, K_{aw}, K_a can be estimated based on fundamental or empirical bases. One common approach is the application of quantitative-structure/property-relationship (QSPR) models or linear free-energy relationship (LFER) models. Such models have been developed to estimate several partitioning parameters specifically for PFAS, including for K_d, K_{aw}, and K_a. Additional detailed information on these methods and their efficacy is available (e.g., Arp et al., 2006; Bhhatarai and Gramatica, 2011; Kim et al., 2015; Brusseau, 2019; Lampic and Parnis, 2020; Brusseau and Van Glubt, 2021; Sosnowska et al., 2023; Brusseau, 2024b). These parameters can also be measured in the laboratory.

As noted above, the standard EPA DAF approach employs the widely used assumption that adsorption to the solid phase is governed by soil organic carbon. The K_d is thus calculated as $K_d = f_{oc}\ K_{oc}$. A default value of 0.002 was used for f_{oc} in the generic SSL calculations (EPA, 1996, 2002a). A site-specific value can be determined by measuring the f_{oc} of site soil samples. Values of K_{oc} for several PFAS measured via laboratory adsorption experiments and in-situ field tests have been compiled in a recent meta-analysis (Brusseau, 2024a). The results are illustrated in Figure SI-4.

Several methods are available to measure K_{aw} in the laboratory. The advantages and limitations of these methods as well as a comparative assessment of measurements obtained with the methods was recently discussed (Brusseau, 2025). Empirically based estimation methods have been developed that can be used to estimate K_{aw}. Example QSPR models developed for a large database of measurements compiled for many PFAS are presented in Figures SI-6 and SI-7. These figures illustrate the functional dependency of K_{aw} on PFAS molecular size. It is observed that the magnitude of K_{aw} ranges over 9 orders of magnitude as a function of molar volume. Hence, retention due to air-water interfacial adsorption can vary enormously across different PFAS, which has implications for their distribution and attenuation in soils as well as their respective SSL values.

It is noted that while many of the primary PFAS of concern have very small, essentially negligible K_a values, some PFAS have significant vapor pressures. Values for K_a have been measured for several PFAS using a number of methods. QSPR models have also been developed, with varying levels of effectiveness. The discussion herein will focus primarily on low-volatility PFAS.

A tiered approach for parameter determination specific to PFAS distribution in soil was developed and discussed by Brusseau et al. (2019). The approach was designed to provide parameter values that increase in accuracy based on the level of input information available to the user. Each input parameter has multiple sources, ranging from the most accurate being the availability of a measured value. This tiered approach is presented in Table SI-1. This approach has been supplemented and implemented into an Excel parameter selection tool (Ma et al., 2025). A link to the Excel tool is provided in the cited reference.

3.6. Parameter determination for the DAF approach: alternative methods

Standard methods to determine the input parameters for the DAF equation were discussed in the preceding subsections. There exist additional, alternative methods for parameterizing the DAF equation. One method entails the use of mathematical modeling, as will be discussed in Section 3.7. Another method employs the results from laboratory leach tests conducted using soil samples collected from the site of interest. This will be discussed in Section 4. Yet another set of methods is based on the use of field measurements of soil, porewater, and groundwater concentrations. These will be discussed in Section 5.

3.7. Transport and fate modeling

The third option for determining SSLs discussed in the EPA guidance entails the application of detailed site-specific transport and fate modeling. Several mathematical models have been developed and applied to specifically simulate PFAS transport in the vadose zone (e.g., Guo et al., 2020; Silva et al., 2020; Zeng and Guo, 2021; Zeng et al., 2021; Wallis et al., 2022; Arshadi et al., 2024; Russell et al., 2025). These model-based studies have simulated PFAS migration and leaching under different scenarios, with the results demonstrating air-water interfacial adsorption and solid-phase adsorption to generally be critical retention processes that can contribute to significant attenuation within the vadose zone. These results suggest that obtaining representative SSLs for PFAS may in many cases require site-specific determinations that account for attenuation.

The models that have been developed range in complexity from fully 3-D complex models to 1-D screening-type models. There are advantages and disadvantages to each type of model. More complex models may more accurately represent site conditions and processes, but have greater input requirements. Conversely, screening-type models are easier to use and require fewer input, but may not provide as accurate representations. There is use for all ranges of model complexity, which can be matched to the goals and available resources of the project.

A key element to employing mathematical modeling is to ensure that the available input supports the level of model complexity selected. Another important element is to implement robust calibration and validation steps. A third is to characterize and quantify the presence and impact of uncertainty in both inputs and outputs. Numerous publications are available that discuss the application of mathematical modeling for simulating contaminant transport and fate.

4. Application of leach-test measurements

4.1. Approach

The 1996 EPA guidance allows for the use of leach tests as an alternative for determining the distribution-conversion term in the DAF equation. This is codified per the quoted statements from the guidance document- "A leach test may be used instead of the soil/water partition equation. If this option is chosen, soil parameters are not needed for this pathway. However, a dilution factor must still be calculated" (EPA 1996a). Note that the "soil/water partition equation" referenced in the guidance is referred to herein as the "distribution-conversion" term.

The synthetic precipitation leaching procedure (SPLP) test (EPA, 1994) was mentioned as the suggested method. This and other batch-mode leach tests contact a contaminated soil sample with a volume of aqueous solution, after which the aqueous concentrations are measured. These concentrations are considered to represent the porewater concentrations that would be established in equilibrium with the concentrations in the soil sample. They therefore may provide site-specific information on expected porewater concentrations that can be used in SSL determinations.

It is important to note that the SPLP test and most other batch leach tests are conducted under water-saturated conditions using a typically comparatively large liquid-to-solids ratio. They therefore do not reflect the typical soil conditions present in the vadose zone, which are rarely fully saturated. This means that the measured porewater concentrations do not represent the impact of air-water interfacial adsorption and other factors on PFAS distribution. As has been discussed in Section 2, porewater concentration under unsaturated conditions may vary significantly from those under saturated conditions. As a result, the measured porewater concentrations may often not be representative of in-situ concentrations. This potential limitation should be kept in mind when applying the results of batch leach tests, and is discussed in more detail in the following subsection.

4.2. Comparison of SPLP and in-situ porewater concentrations

Batch leach tests are typically conducted using specific masses of soil and volumes of solution. For example, the SPLP test uses a 20:1 liquid-to-solids (L:S) ratio. An important factor relevant for assessing the use of SPLP or other leach-test results is the impact of L:S ratios on porewater concentrations. In addition, some of the methods discussed in SI-3 were developed in response to the use of a 20:1 ratio in the SPLP test. The impact of the L:S ratio on measured aqueous concentrations is a function of the magnitude of contaminant retention (which is a function of contaminant and soil properties), the mass of contaminant present in the soil, the nature of the extractant solution, and the timescale of the extraction. This has been discussed in prior works (e.g., Townsend et al., 2006; Thompson et al., 2024; Kleja et al., 2025). The SPLP test has prescribed extractant solutions and timeframes, so the discussion will focus on the first two elements.

Consider as a limiting case a contaminant that has a very large K_d and that is present at a very large soil concentration. Inspection of Eq. (4) shows that porewater concentrations are anticipated to be comparatively small for contaminants with large K_d and R_d values. The mass of PFAS present in porewater will represent a very small fraction of the total mass for cases with large K_d values and large initial soil masses. In such a case, the measured aqueous concentration would be similar to the resident porewater concentration. In other words, there would be minimal dilution of the concentration due to the leach-test procedure. In contrast, for a contaminant with small K_d values and small soil masses, the mass of PFAS removed in the extraction may represent a large portion of the initial mass. In this case, the measured porewater concentration would at some point be an inverse function of the L:S ratio. This relationship is illustrated in Fig. 3 for several K_d values and a fixed C_t. It is observed for example that the leach-test concentration is <10 % of the in-situ concentration for K_d values less than approximately 2 cm^3/g. The impact of the L:S ratio on solution concentrations can be evaluated if desired by conducting the leach tests with different volumes of solution.

As discussed in the preceding subsection, the SPLP test is conducted under saturated conditions, whereas soils are typically not fully saturated. As such, the solution concentrations measured in the test may not be representative of in-situ soil porewater concentrations. The porewater concentration under unsaturated conditions is influenced by several factors as discussed in Section 2. As a result, the relationship between SPLP solution concentrations and in-situ porewater concentrations is more complex for unsaturated conditions. This is illustrated in Fig. 4 wherein the divergence of the two concentrations is presented as a function of PFAS molar volume.

First, the leach-test solution concentrations are significantly less than the in-situ concentrations for the intermediate- and short-chain PFAS. This is a result of the dilution effect discussed above. Conversely, the leach-test solutions concentrations under unsaturated conditions are larger than the in-situ porewater concentrations for the longer-chain PFAS. This is due to the lower porewater concentrations associated

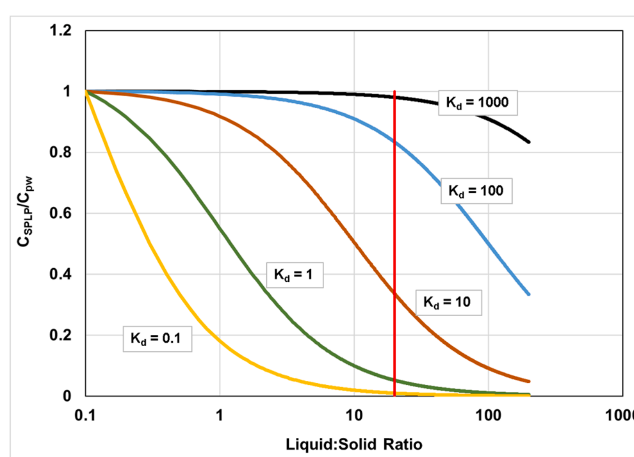

Fig. 3. The impact of the liquid-to-solid ratio on the divergence between solution concentrations obtained from a leach test (C_{SPLP}) and in-situ porewater concentrations (C_{pw}). Note that this analysis is for water-saturated conditions only. The vertical red bar denotes the 20:1 ratio used in the standard SPLP test. Bulk density = 1.5 g/cm^3, porosity = 0.3.

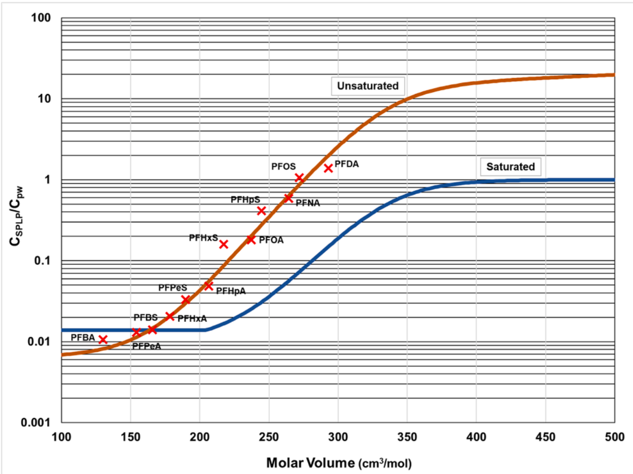

Fig. 4. Comparison of solution concentrations obtained from a leach test (C_{SPLP}) and in-situ porewater concentrations (C_{pw}) for saturated and unsaturated conditions as a function of PFAS molar volume. The two curves represent theoretical calculations using an example set of parameter values as used for Fig. 1. A L:S ratio of 20 is used to represent the SPLP test. Also included are compiled measured data from two field studies, Quinnan et al. (2021) and Brusseau et al. (2026).

with unsaturated conditions (Fig. 1), which lead to larger C_{SPLP}/C_{pw} ratios. Second, the concentration ratios are higher for unsaturated versus saturated for a given molar volume, except for the shortest PFAS. The leach-test solutions concentrations are lower than the in-situ porewater concentrations for the unsaturated conditions due to the L:S dilution effect, just as they are for saturated conditions. However, the curve for the unsaturated condition is shifted to the left of the saturated-condition curve as a result of the impacts discussed in association with Figure SI-2 and Fig. 1, wherein porewater concentrations are lower under unsaturated conditions (except for the shortest-chain PFAS). The results presented in Fig. 4 illustrate that solution concentrations obtained from leach tests may often not be representative of in-situ concentrations. Furthermore, the relationship between the two concentrations can be complex, especially for unsaturated conditions.

SPLP concentrations have been compared to paired lysimeter porewater concentrations for two published field studies (Quinnan et al., 2021; Brusseau et al., 2026). The reported concentration data were used herein to calculate C_{SPLP}/C_{pw} ratios for the PFAS that have sufficient data to compare results. The ratios are plotted in Fig. 4. The magnitudes of the measured ratios vary by PFAS, with the lowest ratio corresponding to the PFAS (PFBS) with the smallest molar volume. Conversely, the highest ratio corresponds to the PFAS (PFDA) with the largest molar volume. These results are consistent with the predicted behavior.

4.3. Methods for using leach-test data

The methods of applying and interpreting the results of SPLP or other leach tests vary across different guidance documents and studies. One primary reason for this variability is the use of a 20:1 L:S ratio for the SPLP test and differing perceptions of the consequences. Note that the different methods in some manner make use of the relationships between soil and porewater concentrations illustrated in Eqs. (3)-(5). For example, the test data can be used to determine a C_t^m/C_{pw}^m ratio, where the superscript m represents measured values, which serves to parameterize the distribution-conversion term as: $SSL = C_{gw}^T\ DAF\ C_t^m\ /C_{pw}^m$. This is demonstrated by inspection of Eqs. (5) and (6), which shows that the C_t^m/C_{pw}^m ratio corresponds to the $\frac{\theta_w}{\rho_b}R_d$ term in Eq. (5) or to the term in brackets in Eq. (6).

As discussed in SI-4, there are multiple methods by which the results of leach tests have been used in the determination of SSLs. Some are consistent with the original EPA guidance while others are not. The use of leach-test data for SSL determinations is mediated by the two critical issues discussed above. Thus, a relevant question is it possible and worthwhile to determine representative correction factors to account for the fact that leach-test solution concentrations may often not be representative of in-situ field porewater concentrations. This could be done via laboratory measurements, but this would be costly and time consuming. Another option would be to use the results presented in Fig. 4 to estimate an approximate PFAS-specific correction factor to scale the results of a SPLP test. This scaling would account for the impacts of both unsaturated conditions and dilution effects. The representativeness of the estimates would depend upon the degree of representativeness of the underlying correlations used to develop the figure, as well as the representativeness of the air-water interfacial areas employed (which represent a sandy soil in Fig. 4).

Based on these issues, the most robust approach is to use SPLP results to directly determine K_d values (Brusseau et al., 2026). An advantage of this approach is that it eliminates concerns about the use of a specific L:S ratio in the test. It also eliminates the issue that the SPLP test is conducted under saturated conditions. Notably, using the results of a leach test in this manner is essentially equivalent to conducting a laboratory sorption/desorption measurement. However, the methodology of the SPLP test represents a simplest version of such measurements, and more involved methods may be employed if desired or necessary. For example, experiment parameters such as L:S ratio, solution chemistry, and equilibration time can be changed to suit the extant properties and conditions of the samples. The use of leach tests to determine K_d or K_{oc} values for PFAS is discussed in recent works (Thompson et al., 2024; Kleja et al., 2025; Brusseau et al., 2026).

5. Application of field-measured soil, porewater, and groundwater concentrations

5.1. Approach

The sampling and analysis of porewater to determine PFAS concentrations in soil porewater is becoming more prevalent for PFAS-impacted sites. The methodology, advantages, and limitations of porewater sampling for PFAS have been discussed in detail and are not repeated herein (e.g., Quinnan et al., 2021; Anderson, 2021; Rayner et al., 2024; Costanza et al., 2025). These data can be combined with more commonly measured soil and groundwater concentration data to support SSL determinations (Brusseau et al., 2026). Specific examples of how porewater data can be employed for SSL determination are discussed below. These applications may be viable for an increasing number of sites as porewater sampling becomes more routine.

5.2. Determining DAF, DF, and AF terms

An alternative, field-based approach to determining the DAF term is to make use of the relation $DAF = C_{pw}^m/C_{gw}^m$. This is based on the assumption that the ratio of measured porewater concentrations to measured groundwater concentrations can be used as a measure of contaminant dilution and attenuation occurring between the soil and groundwater at the site. This assumption is anticipated to be reasonable if the measured concentrations are representative of the target zones, and they represent long-term stable, equilibrium conditions. The influence of different factors on the porewater concentration was discussed in Section 2.2. Note that the relation presented here differs from that provided in subSection 3.1 and Eq. (13), where DF equals the $\frac{C_{pw}}{C_{gw}}$ ratio. This is due to the assumption of AF = 1 in the standard DAF approach.

This application of porewater concentrations is of course based on several additional assumptions and limitations, most of which apply to the DAF approach as a whole and will be discussed in Section 6. An additional factor of importance for this approach is the determination of representative groundwater concentrations to use in the analysis. One element to this is typical spatial variability that may be present, with groundwater concentrations varying across the site. Another element is ensuring that the groundwater sampled is representative of the zone of influence impacted by mass discharge from the targeted soil source zone. A third element is identifying if other, upgradient sources may be impacting the target groundwater zone, which would potentially reduce the representativeness of the analysis.

An alternative for determining the DF term separately from DAF is based on measuring porewater concentrations near the saturated zone, which are presumed to be equivalent to the soil leachate concentration. These concentrations can then be compared to groundwater concentrations to assess the magnitude of dilution, where DF = C_l^m/C_{gw}^m and C_l^m is the soil leachate concentration.

The C_{pw}^m/C_{gw}^m ratio analysis can also be used to estimate AF values. This is based on the relations C_{pw}^m/C_{gw}^m = DAF = DF × AF. With DAF determined from the ratio and DF determined from Eq. (13), AF can be estimated where AF = (C_{pw}^m/C_{gw}^m)/DF. Such an analysis would provide insight into the relative magnitude of contaminant attenuation occurring at the site compared to dilution. This approach is subject to the same limitations noted above.

Yet another approach for determining AF values is based on measuring porewater concentrations at two depths for a number of locations. Specifically, for each location, porewater samples would be collected from the highest soil-concentration interval (presumably nearer the surface) and from near the bottom of the vadose zone (C_l^m). The AF would then be determined as AF = C_{pw}^m/C_l^m. It is anticipated that this approach would often be more robust than using the above C_{pw}^m/C_{gw}^m ratio analysis given that there is likely to be much less uncertainty in the source-specific representativeness of C_l^m compared to C_{gw}^m.

5.3. Determining the distribution-conversion term

An alternative field-based approach to determine the distribution-conversion term in the SSL equations is to use field-measured data to calculate ratios of total soil concentrations and soil porewater concentrations, C_t^m/C_{pw}^m, or to determine associated correlation functions. Similar to the SPLP case, the application of measured soil and porewater concentrations is based on the relationship between C_t, C_{pw}, and $\frac{\theta_w}{\rho_b}R_d$. Methods that have been proposed for analyzing soil and porewater data for SSL determination are discussed in SI-5.

The efficacy of this approach is based on an assumption that both the measured soil and porewater concentrations represent stable long-term conditions. A potential advantage of using field-measured porewater concentrations is that they may be more representative of actual in-situ concentrations if the samples are collected such that the operative processes influencing PFAS distribution are preserved. A recent study employed field-measured paired soil and porewater concentration data to successfully determine SSLs for select PFAS (Brusseau et al., 2026). This will be illustrated in Section 7.

5.4. Determining combined DAF and distribution-conversion terms

The two approaches discussed in the preceding two subsections can be combined. In this case, the measured C_{pw}^m/C_{gw}^m ratios are used to determine DAF and measured C_t^m/C_{pw}^m ratios are used to determine the $\frac{\theta_w}{\rho_b}R_d$ (distribution-conversion) term. This provides field-measured values for both terms.

Alternatively, soil and groundwater concentration data can be combined if available to provide field-based values for both parameters in the SSL equation. This is illustrated by:

$$SSL^{Rev} = C_{gw}^T\ C_{pw}^m \Big/ C_{gw}^m \times C_t^m \Big/ C_{pw}^m = C_{gw}^T\ C_t^m \Big/ C_{gw}^m \tag{15}$$

Thus, the ratio of soil to groundwater concentrations can be used to estimate both the DAF and the distribution-conversion term. Based on the relations and discussions presented in the preceding sections, soil concentrations are expected to generally be larger than groundwater concentrations, particularly for larger PFAS. However, this may not be the case under certain conditions. For example, under conditions with low dilution (C_{pw}^m/C_{gw}^m ratios close to 1), groundwater concentrations may exceed soil concentrations for smaller PFAS given that they may have C_t^m/C_{pw}^m ratios <1 (Fig. 2).

6. Assumptions, limitations, and additional concerns

6.1. Attenuation

One major assumption employed in the standard and revised DAF approaches as noted above is that contaminant attenuation is not considered. The approach considers only dilution, and specifically only dilution that occurs from mixing at the soil-groundwater interface and within the saturated zone. This assumption was justified in the original development based in part on another major assumption, that the contaminant is present at a uniform soil concentration from the ground surface to the bottom of the unsaturated zone. In such cases, there would be no attenuation due to physical processes. However, this does not account for the impact of transformation/degradation processes.

The assumption of a uniform soil concentration spanning the entire vadose zone may be a particularly limiting assumption, especially for PFAS. Many field studies have demonstrated nonuniform distributions of PFAS soil concentrations, with the highest concentrations often nearer to the surface. This is illustrated in Figure SI-8 in SI-6, which represents data aggregated from 30 AFFF-impacted source areas (Brusseau et al., 2020). This nonuniform distribution has important ramifications for the magnitudes of attenuation that may impact PFAS leaching. Attenuation may be significant in particular for sites wherein extensive sections of the vadose zone have minimal or no contamination.

The magnitude of attenuation experienced by a compound is a function of several factors, including the physicochemical properties of the compound (retention propensity), physical and geochemical properties of the soil (retention capacity), and the depth to groundwater from the bottom of the contaminated soil interval. Depth to groundwater is not considered in the DAF approach, again due to the assumption of a uniform distribution of concentrations across the vadose zone. This may be a significant limitation for many PFAS-impacted sites.

One method to incorporate attenuation in the determination of SSLs is to conduct transport and fate modeling. For example, Smith et al. (2024) employed the analytical solutions of Guo et al. (2022) to compute site-specific vadose-zone attenuation factors. The vadose-zone attenuation factor AF is defined as the ratio between the maximum porewater concentration of PFAS in the soil and the maximum PFAS concentration in the leachate discharged to groundwater over the entire leaching period. This approach to compute the AF and the derivation of site-specific SSLs has been implemented in the PFAS-LEACH Tier 3&4 Excel tool (Ma et al., 2025). A distinct advantage of this approach is that it can account for nonuniform soil concentrations and PFAS transport in the vadose zone. It can also incorporate the impacts of transformation explicitly.

There are also other methods available to estimate attenuation factors. One involves the use of measured porewater and groundwater concentrations as discussed in subSection 5.2. This approach is subject to the availability of porewater data and to the uncertainties discussed. However, it does implicitly account for the impacts of transformation.

Another approach is available when the soil contamination is distributed nonuniformly, with an uncontaminated or minimally contaminated interval of soil present between an upper contaminated zone and the saturated zone (e.g., Minnesota PCA, 2013). The attenuation factor is based on a simple assumption of mass redistribution from the initial contaminated zone to the entire vadose zone (Connor et al., 1997). The attenuation factor is calculated from the ratio of depth intervals as:

$$AF = C_{pw1}/C_{pw2} = (d_c + d_u)/d_c \tag{19}$$

where C_{pw1} is the porewater concentration at the bottom of the interval that is initially contaminated, C_{pw2} is the porewater concentration at the bottom of the vadose zone, d_c is the thickness of the initially contaminated zone, and d_u is the thickness of the uncontaminated section of vadose zone. While there are multiple assumptions and limitations associated with this approach, it does provide a simple means to account for the presence of nonuniform soil concentrations, which as discussed above is often observed for PFAS. However, it does not account for compound-specific attenuation associated with retention processes nor the impacts of transformation.

Some PFAS have sufficiently high vapor pressures that partitioning to the vapor phase may significantly influence their distribution in soil. The impacts of vapor-phase transport and retention processes should be considered in such cases (Brusseau and Guo, 2024). For example, vapor-phase transport in the vadose zone can be significantly more rapid than aqueous-phase transport, which would reduce the magnitude of overall attenuation. Such impacts would need to be considered in the determination of SSLs.

6.2. Background concentrations

Many studies have documented the presence of PFAS in soil at sites that are far removed from any identified source, which in some cases likely originated from long-term atmospheric transport. The ubiquitous distribution of PFAS has resulted in anthropogenic background concentrations of PFAS that may be present at a particular site of interest. It is therefore important to account for this background when conducting SSL determinations. A detailed discussion of PFAS background concentrations is presented in Bryant et al. (2022).

There may also be background concentrations in groundwater at the site of interest, originating from upgradient sources. The presence of background concentrations can have a significant impact on SSLs depending upon the background levels and the magnitudes of soil concentrations and dilution/attenuation impacting porewater concentrations at the target site. In such cases, the SSLs would need to be lower than they would be in the absence of a background concentration to meet the same target groundwater concentration.

The Summers model provides a simple mass-balance based approach for estimating the impact of background groundwater concentrations (Summers et al., 1980; Georgia DNR, 2019). The equation is given as:

$$C_{gw} = \left(\frac{Q_i}{Q_a + Q_i}\right) C_{pw} + \left(\frac{Q_a}{Q_a + Q_i}\right) C_b \tag{20}$$

where C_b is the background groundwater concentration. This can be rewritten in terms of the porewater concentration as:

$$C_{pw} = \left(1 + \frac{Q_a}{Q_i}\right) C_{gw} - \left(\frac{Q_a}{Q_i}\right) C_b = DF\ C_{gw} - (DF - 1) C_b \tag{21}$$

This modified porewater concentration can be used in the SSL calculation to account for the presence of background concentrations in groundwater.

Note that when DF is significantly greater than 1, Eq. (21) simplifies to $DF = C_{pw}/(C_{gw}\text{-}C_b)$. Field-measured porewater and groundwater concentrations can be used with this simplification to estimate a DAF value (not DF) as discussed in subSection 5.2, in this case corrected for the presence of a background groundwater concentration. However, it is important to recognize the impact of the simplifying assumption on error in the estimated DAF. The error is a function of the magnitude of DF and the magnitude of the difference between C_{gw} and C_b. An analysis indicates that the error is <10 % for all C_{gw}/C_b ratios >2 when the DF >10. The error is also <10 % for all DF values when the C_{gw}/C_b ratio is >10.

6.3. Spatial and temporal variability

One issue common for any site characterization effort is that of spatial variability. Soil and porewater concentrations may vary across the site due to multiple factors. In addition, soil heterogeneity may exist at the site, leading to spatially variable values for some of the input parameters used in the distribution-conversion term for site-specific SSL determinations. These include K_d, a_{aw}, θ_w, and ρ_b. The representativeness of the samples and associated measurements must therefore be considered. The issue of spatial variability has been addressed in numerous publications and is not elaborated upon herein. While parameters associated with the DF term (i.e., q and I) may also be spatially variable, it is typically assumed that they are constant over the area being addressed in the SSL determination.

Temporal variability is also an issue to consider for some of the SSL parameters. Both q and I are likely to exhibit temporal variability for the DAF term. In addressing this issue, it is important to recognize that the SSL concept is based on the long-term disposition of the site. The SSL is not meant to represent the impact of any singular leaching event. Rather, it represents some form of representative behavior averaged over some extensive timeframe. As a result, the most representative values to use for q and I would typically be averages determined from a long period of historical records (Brusseau and Guo, 2023).

For the distribution-conversion term, a_{aw} and θ_w can exhibit significant temporal variability, whereas K_d and ρ_b can typically be assumed to be effectively constant. As discussed previously, the magnitude of a_{aw} is a function of θ_w. This elicits the question of which θ_w and corresponding a_{aw} to use in the revised DAF calculations. The application of the distribution-conversion term in the standard and revised DAF approaches is based on the long-term equilibrium distributions of contaminant within the soil volume. Hence, θ_w and a_{aw} values that represent the long-term equilibrium distribution of water and interfacial area values should be used (Brusseau and Guo, 2023). In this case, the vadose zone is treated as being under quasi steady-state conditions, and water saturations and air-water interfacial areas representative of long-term status are selected for use in the SSL calculation. The adequacy of assuming steady-state conditions for assessing long-term leaching behavior of PFAS in the vadose zone has been demonstrated with modeling simulations (Guo et al., 2022).

6.4. Uncertainty

Uncertainty is a critical issue to address in the determination of robust SSLs. There is uncertainty in the measurements or estimates of input parameter values for all approaches. There is also uncertainty associated with spatial and temporal variability of site properties and conditions as discussed in the preceding subsection. In many cases, measurement and estimation uncertainty may often be less than uncertainty due to spatial/temporal variability. Sources of potential uncertainty are listed in Table SI-2 (NRC, 1993). All of these contribute to uncertainty in the SSLs determined. It is therefore important to incorporate characterizations of uncertainty in the determination of SSLs. The impact of input-parameter variability and measurement uncertainty on the resultant uncertainty in SSLs was examined in a study that determined SSLs for a PFAS-impacted site (Brusseau et al., 2026). This will be discussed further in Section 7.3.

7. Illustrative applications

7.1. Example applications of measured soil and porewater concentration data

Two examples are presented illustrating the use of C_t^m/C_{pw}^m data obtained from a laboratory leach test or obtained from field measurements to determine the distribution-conversion term for the DAF equation. The first example is presented for an ideal synthetic data set. Two methods for application of the data will be illustrated. The first is to directly tabulate C_t^m/C_{pw}^m values for all samples and to use some corresponding representative value, such as the mean value as input into the SSL calculation. The second method is to create a regression plot of the data, which may be useful for example in cases where the measured concentrations range over several orders of magnitude. In this case, the regression would typically be conducted using log-transformed values as discussed in SI-5.

The application of these approaches is illustrated in Fig. 5 and Table 2. The regression analysis is conducted as described in Method 2 in SI-5. The slope of the regression is observed to be 1, as expected in this case. The intercept is 0.99, which represents the magnitude of log ($\frac{\theta_w}{\rho_b}$ R_d), resulting in ~10 for ($\frac{\theta_w}{\rho_b}$ R_d). This value is then used in Eqs. (6), (7), (9), or (10) along with values for DAF and C_{gw}^T. A representative C_t^m/C_{pw}^m value can also be used from the data set to determine the distribution-conversion term. The SSLs calculated for this example are presented in Table 2.

The slopes of the regressions should equal 1 for ideal data sets for which adsorption processes are linear and effectively instantaneous, and for which other factors such as spatial variability of air-water interfacial areas are not significant. In such cases, the two regression approaches from Method 2 and the regression approach from Method 3 will produce very similar absolute values of the intercept and thus consistent SSLs. However, slopes will deviate from 1 when adsorption is nonlinear, with the degree of deviation a function of the degree of nonlinearity. In addition, nonlinear regressions may result from an inconsistent data set. It is therefore good practice to analyze each data set with both regression approaches presented in Method 2 and use the one that produces the most robust results (Brusseau et al., 2026).

The second example comprises the application of SPLP tests and soil and porewater sampling to help determine site-specific SSLs for four PFAS-impacted installations (Brusseau et al., 2026). Data sets with at least 6 paired samples were included in the analysis, resulting in data reported for 11 PFAS. The combined data represent 594 individual paired samples for the field measurements and 742 for the SPLP tests. An example of the measured data sets is presented in Fig. 6.

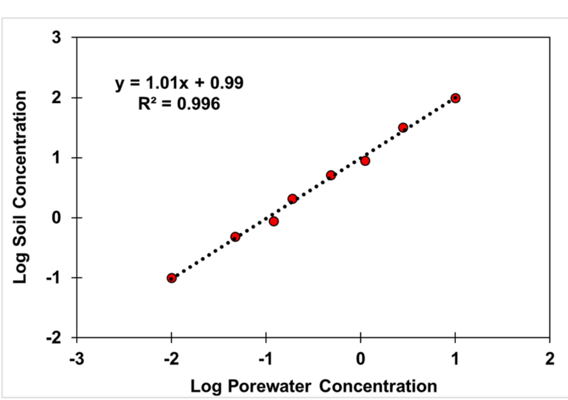

Fig. 5. The application of measured soil and porewater concentrations for determining the distribution term in the DAF equation. The measured data may originate from a laboratory leach test or from field measurements. Concentrations represent any set of consistent units such as μg/kg and μg/L.

Table 2
Values for illustrative SSL calculation example for data presented in Fig. 5.

Parameter	Value
C_{gw}^T	0.01
DAF	10
$C_{pw}^T = C_{gw}^T$DAF	0.1
Regression intercept [($\frac{\theta_w}{\rho_b}$ R_d)] (non-log)	9.8
Regression SSL	0.98
C_t^m/C_{pw}^m Geomean [($\frac{\theta_w}{\rho_b}$ R_d)]	9.8
Geomean SSL	0.98

Both data sets were subject to regression analysis following Method 2 in SI-5. The concentrations spanned 3–5 orders of magnitude. The results of the regression analyses showed that the slopes were close to 1 for all regressions, except for a few cases for the shorter-chain PFAS. This indicates that both solid-phase and air-water interfacial adsorption are effectively linear under the site conditions for the PFAS characterized.

Inspection of Fig. 6 shows that PFPeS SPLP concentrations are much lower than the corresponding porewater concentrations for a given soil concentration. In contrast, PFOS SPLP and porewater concentrations are similar. This aspect was further examined by direct comparisons of paired SPLP and porewater concentrations. Significant differences were observed between the two sets of concentrations, with the magnitude of the difference a function of the specific PFAS. The differences result from the 20–1 dilution and saturated conditions used in the SPLP test as discussed in Section 4. The concentration ratios are plotted in Fig. 4 as discussed in that section.

7.2. Application of the PFAS-LEACH platform

Here we illustrate the application of the simpler model tiers (i.e., Tiers 3 and 4) of the PFAS-LEACH platform for deriving site-specific SSLs. The PFAS-LEACH Tiers 3 and 4 models have been implemented in an Excel tool (Ma et al., 2025). The Tier 3 model combines a set of analytical solutions for PFAS transport in the vadose zone (Guo et al., 2022) and EPA's dilution factor model to derive a site-specific SSL (Smith et al., 2024). The Tier 4 model implements the revised EPA SSL approach (Brusseau and Guo, 2023) described above. The Excel tool also implements the standard EPA DAF approach for comparison.

We consider an AFFF-impacted site located at the Joint Base McGuire-Dix-Lakehurst, which was contaminated by PFAS due to foam formulation testing. No AFFF was applied at the site after approximately

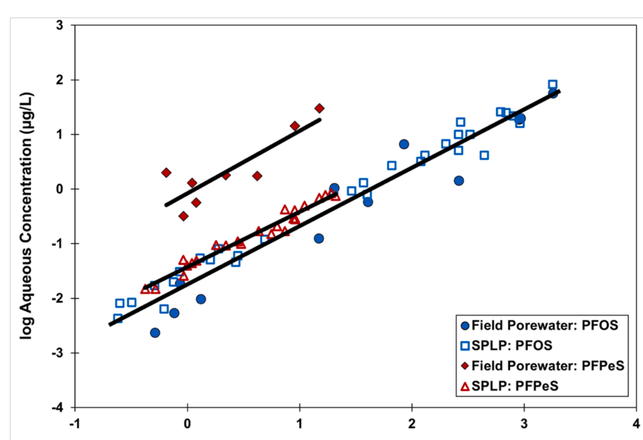

Fig. 6. Comparison of paired samples of field-measured soil and porewater concentrations and soil-SPLP concentrations for PFOS and PFPeS for Installation 2. Reproduced from Brusseau et al. (2026).

1997. PFAS concentrations in soil and porewater were presented in prior studies (Schaefer et al., 2022,2023; Russell et al., 2025). See Fig. 7 for a schematic of the site and the experimental installations. Table 3 summarizes the input parameters for applying the PFAS-LEACH Tiers 3 and 4 models, which are based on site-specific information reported in the cited studies and are discussed in the following paragraph. PFOS is used as the illustrative PFAS.

Net infiltration is obtained by multiplying the annual rainfall rate by 0.47 (Schaefer et al., 2023). Water content is an average value determined from time-domain reflectometry measurements of soil moisture over a two-month period. The air-water interfacial area is estimated by the PFAS-LEACH Excel tool using the thermodynamic approach with an empirical scaling factor equation (Brusseau, 2023b). Soil bulk density, saturated water content, d50, and the solid-phase sorption coefficient were determined in the lab using soil samples collected from the site (Schaefer et al., 2022). Air-water interfacial adsorption coefficient was determined from surface tension data measured at an ionic strength representative of the porewater at the site (0.01 mol/L) (Brusseau and Van Glubt, 2021). The other parameters were estimated based on site-specific information.

PFAS concentrations were measured from multiple soil borings at the site. The soil boring with the highest data resolution (Soil boring #5 in Russell et al., 2025) is used for the simulation, which has PFAS soil concentrations for each 0.25 feet (7.6 cm) interval. Providing the site-specific input parameters for PFOS to the PFAS-LEACH Excel tool yields the SSL values in Table 4. The computed dilution factor (DF) is 212.7 and the attenuation factor (AF) derived from PFAS-LEACH-Analytical is 6.8. The same dilution factor is applied to all three approaches to derive the SSLs. The acceptable concentration in groundwater is assumed to be the MCL of 0.004 ug/L for PFOS.

Inspection of the SSLs derived by the three approaches shows that the SSL derived from the PFAS-LEACH-Analytical model (Tier 3) is the largest, followed by that derived by the PFAS-LEACH-DAF model (Tier 4). The SSL derived by the standard EPA DAF approach is much smaller, approximately 1/50 and 1/7 of the SSLs derived by the PFAS-LEACH Tiers 3 and 4 models, respectively. Given that the DF is the same for all three calculations, these results demonstrate two important observations. First, the only difference in the calculations of the Tier 4 and standard SSL values is that the former includes air-water interfacial adsorption in the distribution term. Thus, the factor of 7 difference indicates the significant contribution of that process to PFOS distribution in the soil. Second, the Tier 3 SSL is 6.8-times larger than the Tier 4 SSL, which corresponds to the calculated AF. This indicates that attenuation within the vadose zone is significant for PFOS in this system. The differences between the 3 SSL determinations are a function of site conditions and the specific PFAS (Brusseau and Guo, 2023).

An SSL was also calculated using the measured soil and porewater concentrations reported for PFOS in the original study (Schaefer et al., 2022). The mean values determined from all samples were used for both concentrations, as the soil and porewater data do not represent paired

Table 3
Site-specific input parameters for applying the PFAS-LEACH Tiers 3 and 4 models.

Parameter	Value
Site area	400 m^2
Annual net infiltration	55 cm
Soil bulk density	1.63 g/cm^3
Saturated water content	0.344
d50	0.035 mm
Vadose-zone longitudinal dispersivity	10 cm
Water content	0.14 cm^3/cm^3
Air-water interfacial area	588.6 cm^2/cm^3
Solid-phase sorption coefficient	6.9 cm^3/g
Groundwater darcy flux	1095 m/year
Air-water interfacial adsorption coefficient	0.118 cm^3/cm^2
Lateral side width	20 m
Saturated zone thickness	6.43 m
Groundwater vertical dispersivity	0.11 m
Mixing zone thickness	1.06 m

Table 4
SSL values for PFOS derived by the PFAS-LEACH Tiers 3 and 4 models and the standard EPA DAF approach. Also included in an SSL calculated using measured soil and porewater data.

Soil screening levels	Value
PFAS-LEACH-Analytical (Tier 3)	289 μg/kg
PFAS-LEACH-DAF (Tier 4)	42.4 μg/kg
Standard EPA DAF	5.9 μg/kg
Field measured C_t/C_{pw}	101 μg/kg

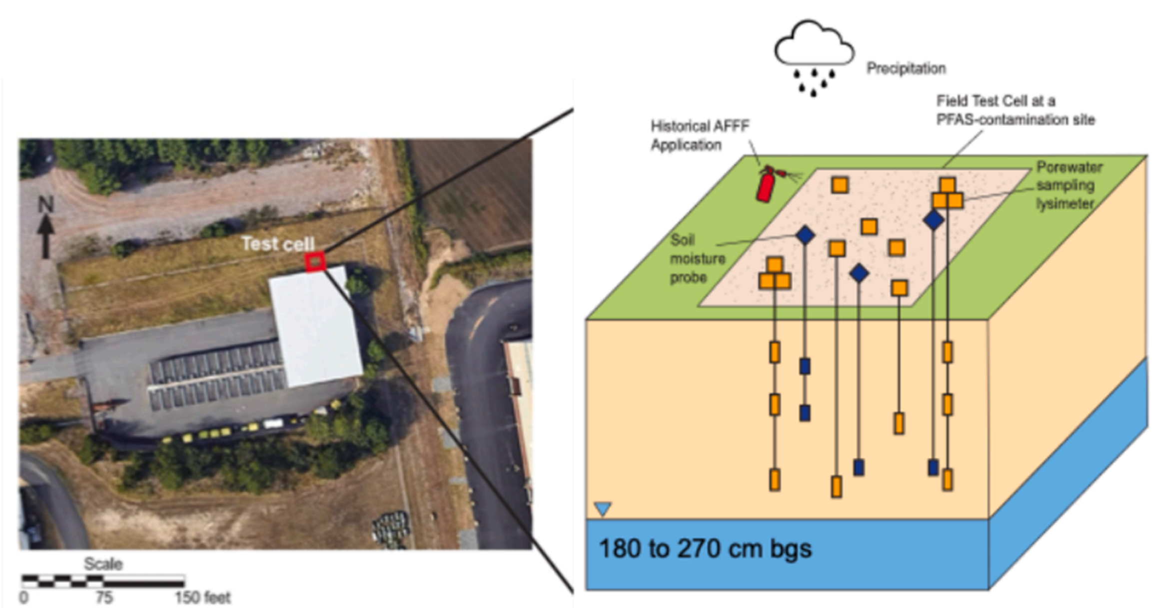

Fig. 7. Schematic for the AFFF-impacted site and the experimental installation reported in Schaefer et al. (2022,2023). The sketch of the installation is from Russell et al. (2025).

sets. Note that the mean soil concentration was calculated using all values to a depth of 6 feet, to correspond to the placement of the sampling lysimeters (the deepest was 5 feet BGS). A C_t/C_{pw} ratio of 119 L/kg is obtained from the mean soil (1249 μg/kg) and porewater (10.5 μg/L) concentrations. Using the same DF as above produces an SSL of 101 μg/kg. Notably, this value is within the range of the values determined with the Tier 3 and 4 models, and similarly is significantly larger than the SSL determined with the standard EPA DAF approach.

These data can also be used to demonstrate the difference between field "K_d" and actual K_d values determined from C_{SPLP}/C_{pw} ratios as described in SI-4. A K_d of 6.9 cm^3/g was measured for PFOS in a batch desorption experiment conducted using soil from the field site (Schaefer et al., 2022). This value is 17-times smaller than the C_{SPLP}/C_{pw} ratio (i.e., the field "K_d").

7.3. Framework for site-specific SSL determination

Brusseau, Guo, and colleagues have demonstrated the application of a framework for determining site-specific SSLs at four AFFF-impacted installations (Brusseau et al., 2026). The framework, based on the PFAS-LEACH platform, consists of a tiered approach for the application of methods to determine SSLs and a corresponding tiered approach for the determination of input parameters. The framework was applied at four PFAS-impacted installations to determine site-specific SSLs. The application comprised multiple parts, with the first consisting of detailed mathematical modeling conducted at one site to delineate the relevant transport processes and determine the most representative input parameters in support of the use of simpler methods for determining SSLs. A simplified analytical-solution based screening model and the revised DAF equation that are available as a user-friendly Excel tool within PFAS-LEACH were then used to determine site-specific SSLs for three PFAS for the four installations. A decision tree was developed to help in the selection of an application method most relevant to project objectives and site conditions Fig. 8.

The SSLs determined with the site-specific approach were a factor of three to more than two orders-of-magnitude larger than generic EPA screening values. The disparities were shown to result from the consideration of PFAS retention and attenuation in the vadose zone and in particular the impact of air-water interfacial adsorption. The SSLs determined for PFOS were larger than those for PFOA and PFHxS due to the greater retention properties of PFOS. The influence of input-parameter uncertainty was assessed using a Monte Carlo analysis, producing a factor of four range in SSLs. This is a relatively modest range considering the input-parameter variability included.

The impact on SSLs of possible ranges in values for various input parameters was also assessed in the study. For example, sites located in more humid climatic zones may have higher mean soil-water contents, larger magnitudes of recharge, and shallower groundwater compared to an arid site. These conditions would likely result in lower DF and AF values. For another example, soils at a particular site may be coarser grained and have low organic-carbon and metal-oxide contents, which would likely result in lower retention and correspondingly smaller magnitudes for AF and the distribution-conversion term.

A Monte-Carlo sensitivity analysis was conducted to illustrate the impact of a broad range of possible site conditions on SSLs, using PFOS as an example. Note that this is separate from the site-specific uncertainty analysis discussed above. The magnitudes of infiltration rate and groundwater flux were varied, producing DF values that ranged from close to 1 (minimal dilution) to >3-times greater than the EPA default of 20. Parameters mediating the magnitude of air-water interfacial area were also varied to produce air-water interfacial retardation factors ranging from close to 1 to almost 200-times larger. These parameter ranges resulted in SSLs that ranged by more than two orders of magnitude. This highlights the large range over which SSLs can potentially vary, and the benefits of accounting for site-specific conditions when determining SSLs.

A large body of work exists with respect to determining most of the parameters needed for SSL calculations, such as groundwater recharge and discharge (flow), solid-phase adsorption coefficients, and standard soil hydraulic parameters. However, much less is available for the determination of air-water interfacial areas. In addition, air-water interfacial areas can exhibit spatial and temporal variability due to spatial variability of soil properties and spatial and temporal variability of water contents, the latter which mediates the magnitude of air-water interfacial area for a given soil. Furthermore, water contents are not typically measured as part of standard site investigations. Thus, parameterizing the air-water interfacial adsorption component of the distribution-conversion term is likely to be a primary limiting factor for many SSL applications. Prior research has demonstrated that air-water interfacial adsorption typically contributes minimally to the retention of very short-chain PFAS. In such cases, it may be excluded in some cases without significant impact to the SSL calculations (Brusseau et al., 2026). However, air-water interfacial adsorption is likely to be relevant under many conditions for intermediate and longer-chain PFAS and therefore important to incorporate into SSL determinations.

The use of field-measured paired soil and porewater concentration data to determine the distribution-conversion term is of particular advantage in cases for which air-water interfacial adsorption is important, as they characterize the contribution of all relevant retention processes to PFAS distribution. For example, such data were used

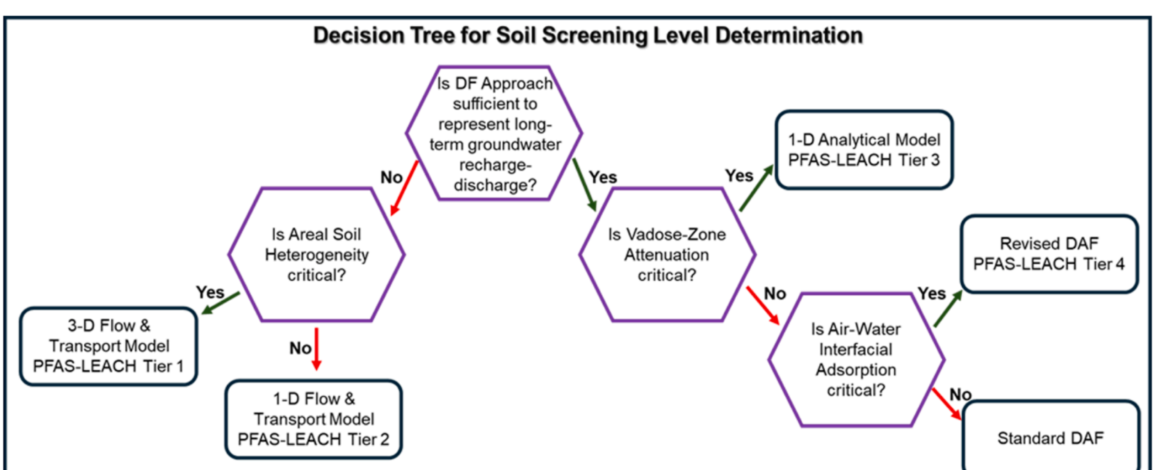

Fig. 8. Decision tree for selection of methods for SSL determination. Reproduced from Brusseau et al. (2026).

successfully to determine SSLs that were consistent with those calculated using independently determined input parameters (Brusseau et al., 2026). There are several best-practice elements to maximize the robustness and usefulness of porewater sampling. One is to collect paired soil samples from the same location as the porewater sampling. These soil samples should be characterized for PFAS concentrations, moisture content, and soil properties such as texture and organic-carbon content. If possible, it would be useful to collect samples from different depths across the vadose zone, including near the top of the saturated zone. When applying the regression analyses, both regression approaches should be applied and data quality should be assessed based on the range of concentrations characterized and the slope linearity in addition to goodness-of-fit metrics.

8. Conclusions

This work provided an overview and detailed discussion of the concepts and methods underlying the site-specific determination of SSLs for PFAS. It is anticipated that site-specific SSLs would often be more representative and less stringent than generic reference values due to the consideration of site-specific conditions. However, site-specific applications require increased levels of site characterization. It is therefore necessary to balance the potential cost savings accrued from less stringent SSLs with the additional site-characterization costs. While there are multiple assumptions and limitations associated with the determination of site-specific SSLs, they are a key tool in cost-effective, risk-based management of PFAS-impacted sites.

An important factor to consider is the fact that SSLs are likely to exhibit a range in values, possibly over orders of magnitude, for different PFAS at the same site. This is due to the functional dependency of retention processes on PFAS size, which influences the distribution-conversion term in the DAF approach and attenuation processes in transport and fate modeling. Thus, smaller SSLs may generally be anticipated for shorter-chain versus longer-chain PFAS. However, this disparity will be impacted by the potential existence of different protective target groundwater levels for different PFAS. The presence of multiple PFAS in soils at most sites therefore elicits the possibility that measured soil concentrations may exceed SSLs for some PFAS but not for others. This possibility needs to be considered in site characterization and decision-making.

CRediT authorship contribution statement

Mark L. Brusseau: Writing – original draft, Conceptualization, Writing – review & editing, Funding acquisition, Formal analysis, Data curation. **Bo Guo:** Writing – review & editing, Funding acquisition, Formal analysis, Data curation.

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.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.watres.2026.125386.

Data availability

This is a review article and all data are from the literature

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