User Guide: Excel tool for Tiers 3 and 4 models of PFAS-LEACH (PFAS-LEACH-Analytical and PFAS-LEACH-DAF)

Version 1.0

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Disclaimer

The Excel tool for the PFAS-LEACH Tiers 3 and 4 models (PFAS-LEACH-Analytical and PFAS-LEACH-DAF) is distributed in the hope that it will be useful, but without any warranty; without even the implied warranty of merchantability or fitness for a particular purpose. Information in this document is subject to change without notice. Application of this Excel tool and interpretation of the computed results are the sole responsibility of the user.

Acknowledgment

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How to cite

The Tier 3 PFAS-LEACH-Analytical tool was built upon Guo et al. (2022) and Smith et al. (2024) and the Tier 4 PFAS-LEACH-DAF tool was based on Brusseau and Guo (2023). If you use the Tier 3 and/or Tier 4 models, please cite the following respective references.

- Ma, M., Smith, J., Brusseau, M. L., & Guo, B. (2025). User guide: Excel tool for Tiers 3 and 4 models of PFAS-LEACH (PFAS-LEACH-Analytical and PFAS-LEACH-DAF). University of Arizona. Tucson, Arizona.
- Smith, J., Brusseau, M. L., & Guo, B. (2024). An integrated analytical modeling framework for determining site-specific soil screening levels for PFAS. *Water Research*, 121236.
- Guo, B., Zeng, J., Brusseau, M. L., & Zhang, Y. (2022). A screening model for quantifying PFAS leaching in the vadose zone and mass discharge to groundwater. *Advances in Water Resources*,160, 104102.
- Brusseau, M.L. and Guo, B. (2023). Revising the EPA dilution-attenuation soil screening model for PFAS. *Journal of Hazardous Materials Letters*, 4, 100077.

The Excel tool

Link to download the Excel tool: https://github.com/GuoSFPLab/PFAS-LEACH-Tier-3-4

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Contents

1 Quick-start Guide

How can I get started with the Excel tool?

To get started with the Excel tool, users are recommended to first go through 1) the Q&A in this Quick-start guide and 2) the examples in Section 3. When running their own simulations, users can refer to Section 2 for additional guidance.

What does the Excel tool include?

This Excel tool includes implementations of the Tiers 3 and 4 models (PFAS-LEACH-Analytical and PFAS-LEACH-DAF) of PFAS-LEACH.

PFAS-LEACH is a comprehensive decision support platform for predicting PFAS leaching in source zones. It is comprised of four tiers of models at different levels of model complexity. In addition to the simplified Tiers 3 and 4 models documented here, PFAS-LEACH also includes two more sophisticated models (Tiers 1 and 2). The Tier 1 model incorporates a comprehensive representation of flow, transport, and transformation processes in three dimensions (3D), referred to as PFAS-LEACH-COMP (Guo et al., 2020; Zeng and Guo, 2021). The Tier 2 model (PFAS-LEACH-HYDRUS) incorporates a set of simplifications to focus on one-dimensional leaching along the vertical direction (Zeng et al., 2021) and is implemented within a modified opensource version of the widely used industry-standard software, HYDRUS-1D. The codes for Tiers 1 and 2 models are being finalized and we hope to release the beta version soon.

What is PFAS-LEACH-Analytical?

The core of PFAS-LEACH-Analytical is a set of analytical solutions that solve the partial differential equations for the leaching of PFAS in the vadose zone (Guo et al., 2022). The vadose-zone analytical solutions are also coupled to a simple groundwater dilution factor model (Smith et al., 2024; USEPA, 1996), which allows for computing PFAS concentration in a receptor well and deriving site-specific soil screening levels (SSLs) for a given acceptable groundwater PFAS concentration. Figure 1 is a conceptual diagram that shows the PFAS-LEACH-Analytical model representations of PFAS leaching in the vadose zone and dilution in groundwater. The process-based vadose-zone analytical solutions represent a set of PFAS-specific attenuation processes during transport through the unsaturated zone, including air–water interfacial adsorption and rate-limited solid-phase sorption.

The PFAS-LEACH-Analytical model allows one to compute, over time, the spatial profiles of PFAS concentration in the vadose zone, mass discharge rates to groundwater, and the groundwater PFAS concentration in a receptor well at the edge of the contaminated site. Additionally, given an acceptable PFAS concentration in groundwater, PFAS-LEACH-Analytical derives a site-specific soil screening level for a specific PFAS. The mass discharge rates computed from PFAS-LEACH-Analytical can also be imported to more sophisticated groundwater flow and transport models (e.g., MODFLOW/MT3D-USGS (Bedekar et al., 2016)) to simulate PFAS transport in the saturated zone.
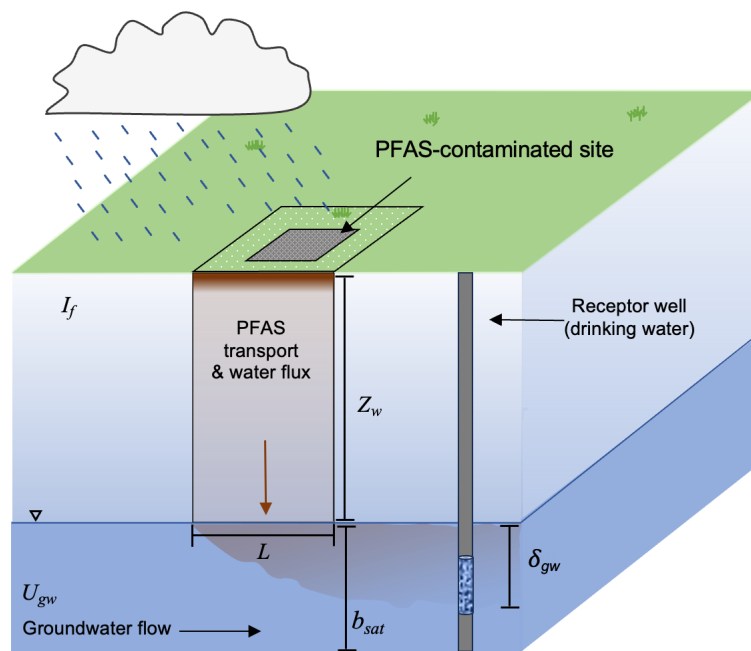
Figure 1: Conceptual diagram of the PFAS-LEACH-Analytical model presentation of PFAS leaching in the vadose zone and dilution in groundwater (modified from Smith et al., 2024).

What is PFAS-LEACH-DAF?

PFAS-LEACH-DAF is a revision to the widely used dilution attenuation factor (DAF) approach in the USEPA SSL framework (USEPA, 1996) for determining SSLs for PFAS (Brusseau and Guo, 2023). The revised PFAS-specific DAF approach considers the adsorption of PFAS at the air–water interfaces when converting the porewater concentration to a soil concentration. PFAS-LEACH-DAF is a simple algebraic model to compute site-specific SSLs for PFAS. It does not represent any transport processes in the vadose zone (e.g., attenuation) and does not generate any space- or time-dependent results.

What can I use the Excel tool for?

Here are some example uses of PFAS-LEACH-Analytical:

- Evaluate groundwater contamination risks by providing mass discharge rates to groundwater and groundwater concentration in a receptor well.
- Derive site-specific SSLs for a given acceptable groundwater concentration.
- Evaluate remedial objectives, e.g., by computing mass discharge rates to groundwater and groundwater concentration in a receptor well for different scenarios of PFAS mass removal in the vadose zone.
- Provide mass discharge rates for further analysis in the saturated zone, e.g., as input for groundwater flow and transport models such as REMFluor (Newell, 2025), ATRANS (SSPA, 2025), and MODFLOW/MT3D-USGS (Bedekar et al., 2016).

Compared to PFAS-LEACH-Analytical, PFAS-LEACH-DAF is substantially simpler. Its primary use is to algebraically derive site-specific SSLs for a given acceptable groundwater

concentration.

What input data do I need?

PFAS-LEACH-Analytical requires parameters related to soil properties and site conditions, PFAS properties, and groundwater dilution. While a number of parameters are needed for each of these categories, many parameters can be estimated if no measured values are available. For example, van Genuchten parameters (α and *n*) for soil water characteristics are needed for estimating air–water interfacial area, but soil water characteristics parameters are usually not part of standard site characterizations. In this case, the van Genuchten parameters can be estimated using pedotransfer function tools (e.g., Rosetta 3 (Zhang and Schaap, 2017)) with basic soil texture information (i.e., sand, silt, and clay fractions) and/or soil bulk density. Descriptions for systematic estimation of the input parameters are presented in Section 2.

What are Module 0, Module 1, and Module 2 of the Excel tool?

The Excel tool includes three modules: *Module 0*, *Module 1*, and *Module 2*. Module 0 provides the basic functionalities for quantifying PFAS leaching and deriving SSLs. Module 1 adds an additional capability of parameter sensitivity analysis, and Module 2 allows for Monte Carlo simulations for uncertainty quantification. Each module includes an Input tab and an Output tab as user interfaces.

What are the limitations of the PFAS-LEACH-Analytical and PFAS-LEACH-DAF models?

PFAS-LEACH-Analytical is based on analytical solutions that employ a number of simplifying assumptions listed below.

- One-dimensional, steady-state water infiltration.
- Homogeneous, uniformly unsaturated vadose zone.
- Linear and instantaneous adsorption at air–water interfaces.
- Linear and rate-limited sorption at solid–water interfaces.
- Partitioning to the air phase is neglected.
- PFAA precursor transformation is not yet directly accounted for.
- The receptor well is at the edge of the contaminated site.

Despite these assumptions, PFAS-LEACH-Analytical represents a set of PFAS-specific retention processes and has been demonstrated to be an effective tool for providing order-of-magnitude estimates of PFAS mass discharge to groundwater and for deriving site-specific soil screening levels at PFAS-contaminated sites (Guo et al., 2022; Smith et al., 2024).

PFAS-LEACH-DAF is a direct revision of the standard USEPA DAF approach to derive site-specific SSLs, it therefore shares similar advantages and limitations of the USEPA's DAF approach as documented in USEPA (1996).

How do I leverage suction lysimeter porewater concentration data?

Porewater concentration sampled by suction lysimeters have become available at many PFAS-contaminated sites (e.g., Anderson, 2021; Quinnan et al., 2021; Schaefer et al., 2022; Anderson et al., 2022; Schaefer et al., 2023). PFAS-LEACH-Analytical and PFAS-LEACH-DAF can directly take porewater concentrations as input parameters to estimate or constrain air–water interfacial area, which represents one of the parameters involving the greatest uncertainties. The underlying theory and specific steps for approximating A_{aw} from lysimeter porewater data have been reported in Russell et al. (2025). In this user guide, the approach of using lysimeter porewater concentration data to estimate air–water interfacial area is summarized in Table 1 in Section 2.2.1.

2   Tool User Guide

2.1   User interface

This tool consists of three modules: Module 0, Module 1, and Module 2. Module 0 provides the basic simulation functions. Module 1 and Module 2 share the same interface structure as Module 0 but include additional capabilities. Specifically, Module 1 enables parameter sensitivity analysis, while Module 2 allows for Monte Carlo simulations to support uncertainty quantification.

2.1.1   Overall structure of the user interface

All three modules have a tab for input (e.g., "Module0_Input") and a tab for output (e.g., "Module0_Output"). In addition, Module2 includes an auxiliary tab ("Module2_ParaToolkit") that allows users to visualize parameter distributions for the Monte Carlo sampling. The *Input Screen* tab includes five input boxes to specify the input parameters for soil properties and site conditions, PFAS properties, groundwater dilution, initial PFAS soil concentration profile and lysimeter porewater concentration, and simulation information. Users should work through these five boxes *sequentially* as entries in the later boxes may depend on those in the earlier boxes. One exception is the lysimeter porewater concentration table in Box 4, which will be required to compute the air–water interfacial area scaling factor in Box 1 if the user selects to use lysimeter porewater data to estimate the scaling factor. We briefly introduce the five boxes below.

- *Box 1 (Soil Properties and Site Conditions)* asks for basic site information (e.g., contaminated area, depth to groundwater, net infiltration) and parameters about the soil physical properties (e.g., bulk density and soil hydraulic parameters).
- *Box 2 (PFAS Properties)* seeks input for the physicochemical parameters of the PFAS to determine their partitioning to air–water interfaces and solid–water interfaces.
- *Box 3 (Groundwater Dilution)* asks for site-specific parameters to determine the extent of dilution after PFAS discharge to groundwater. The set of parameters here are identical to those used in the USEPA's DAF approach for computing a site-specific dilution factor.
- *Box 4 (Initial PFAS Soil Concentration Profile and Lysimeter Porewater Concentration)* specifies the initial concentration distribution of the PFAS in the soil profile and lysimeter

porewater concentration. The initial soil concentration data can be arbitrary and with any spatial resolution. The lysimeter porewater concentration data are *optional*; they are only required when the user wants to use them to constrain the air–water interfacial area.

- *Box 5 (Simulation Information)* inputs information to set up the simulation (e.g., simulation time, output time interval, output time point, and acceptable groundwater concentration).

2.1.2   Cell types for input parameters

Cells in the *Input Screen* tab are color-coded to indicate their types.

- Gray Cells

  These cells are locked and are not supposed to be interacted with by users.

- Blue Cells

  These cells can be manually entered by the user. If the values are not available, these cells can be populated with reference values by a drop-down menu (e.g., by selecting a reference soil or PFAS type).

- *White Cells*

  These cells can be manually entered by the user. When the values are not available, these cells can be estimated using the assistive functional buttons (by clicking the gray button to the right of the white cells that provides methods for parameter calculation or estimation). This serves as an auxiliary tool for users when measurements are unavailable.

  If the blue-cell parameters used to estimate a white-cell parameter are updated, users need to apply (i.e., "click") the functional button again to update the white-cell parameter. In general, users are recommended to apply the functional buttons to re-estimate all the white-cell parameters if any of the blue-cell parameters are updated. This would ensure that all the estimated white-cell parameters are updated.

- Yellow Cells

  These cells are only present in Module 1 and are for the user to input or adjust the parameter ranges for the sensitivity analysis.

- Orange Cells

  These cells are only present in Module 2 and are used to input the coefficient of variation (CV) for the Monte Carlo simulation. Orange cells are divided into *dark* orange and *light* orange. Dark orange cells must be populated by the user. If the user does not have information about the coefficient of variation, a default value of "0" can be entered (assuming negligible variability). The light orange cells are more involved. When left blank, the variability of the parameter will be accounted for internally using the variability of the relevant blue-cell parameters (i.e., coefficient of variation in the relevant dark orange cells) following the assistive estimation function. When a value is given, it will be directly used as coefficient of variation. For the light orange cells, if the user does not have information about the uncertainty, they may give a coefficient of variation of 0 (assuming negligible variability) or leave it blank (relying on the variability determined internally by the assistive estimation functions).

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2.1.3   Toolkit for visualizing parameter distribution — Module 2

The Module2_ParaToolkit tab provides an auxiliary interface that helps users 1) visualize the distribution of input parameters under normal and log-normal distributions, and 2) convert the mean (μ) and standard deviation (σ) (for log-normally distributed parameters) between linear space and log space. We briefly introduce the functionalities below.

- *Normal Distribution*

  Users input a positive mean (μ) and two non-negative coefficients of variation (CV). The mean needs to be positive because the parameter value has to be physically meaningful. By clicking the *"Plot"* button, users can generate probability density curves for the normal distribution under the two given CV scenarios. The dashed vertical lines denote the range of $\mu \pm \sigma$, and the probability within this range is displayed. This visualization enables users to compare how changes in CV affect the distribution's spread.

- *Log-10 Normal Distribution*

  This box enables users to explore log-normal distributions. After providing a positive mean (μ) and two non-negative CV values in the linear space, clicking the *"Plot"* button generates probability density curves for the log-normal distributions (with a base of 10). The curves illustrate how the skewness and spread depend on the given μ and CV parameters. The dashed vertical lines denote the range of $\mu \pm \sigma$, and the probability within this range is displayed.

- *Conversion between Linear and Log-Normal Parameters*

  In the log-normal distribution box, it also provides the capability to convert the mean and standard deviation between linear and log spaces. Users can convert between (μ, σ) in the linear space and (μ_{10}, σ_{10}) in the log space. For example, before inputting the mean and standard deviation in the linear space to Module 2, users can use this feature to get a sense of the mean and standard deviation in the log space. Or, when the mean and standard deviation are given in the log space (e.g., estimates from Rosetta 3), users can use this functionality to obtain the mean and standard deviation in the linear space.

2.2   Description of input parameters

Below we elaborate on the input parameters in each of the five Boxes in the Input tabs. After that, we introduce the sensitivity analysis parameters in Module 1 and the Monte-Carlo related parameters (i.e., mean and coefficient of variation) in Module 2.

2.2.1   Soil properties and site conditions

Table 1: Input parameters for soil properties and site conditions

Parameter	Description
Depth to groundwater Z_w (cm)	The depth of the vadose zone at the contaminated site. If the groundwater table fluctuates (e.g., seasonal fluctuation), it is recommended to use the shallowest water table depth to be conservative for quantifying PFAS leaching to groundwater (Zeng et al., 2024).
Contaminated site area A (m²)	PFAS-LEACH-Analytical is a 1D model, thus the computed mass discharge rate needs to multiply the lateral area of the contaminated site that the 1D model represents. Alternatively, the user can also set a unit area (i.e., 1 m²) if desired, for example, when the mass discharge rates computed from PFAS-LEACH-Analytical are used as input for a gridded groundwater flow and transport model (e.g., MODFLOW/MT3D-USGS (Bedekar et al., 2016)).
Temperature T (°C)	A representative temperature in the vadose zone of the contaminated site used to compute the air–water interfacial adsorption coefficient (K_{aw}). The Kelvin temperature is used to compute K_{aw}, thus K_{aw} is generally not very sensitive to temperature variabilities at a site.
Net infiltration rate I_f (cm/yr)	The portion of water infiltration available for groundwater recharge per year, accounting for losses between the land surface and the water table (e.g., evapotranspiration and runoff). A variety of approaches spanning different levels of complexity and data availability for estimating net infiltration are reported in the literature (e.g., Scanlon et al., 2002; Healy, 2010), including a recent review by Newell et al. (2023) in the context of quantifying PFAS mass discharge from unsaturated source zones. For example, following a simple scaling equation suggested by Stephens et al. (1996) and Connor et al. (1997), one could estimate the net infiltration rate as $I_f = 0.0018p^2$ (cm/yr), where p is net annual precipitation (cm/yr).
Soil bulk density ρ_b (g/cm³)	The mass of oven-dry soil per unit volume of bulk soil, including both soil particles and pore spaces. If no measured values are available, ρ_b can be estimated by selecting a soil from the list of the twelve reference soil types.

Parameter	Description

Saturated hydraulic conductivity K_{sat} (cm/day)	If no measured values are available, K_{sat}, θ_r, θ_s, and n can all be estimated using pedotransfer function tools (e.g., Rosetta 3 (Zhang and Schaap, 2017)) with basic soil texture information (i.e., sand, silt, and clay fractions) and/or bulk density.
	    Various versions of the Rosetta model can be found in the following link: https://soil-modeling.org/resources-links/model-portal/rosetta
	    K_{sat}, θ_r, θ_s, and n are used to estimate θ for a given net infiltration. θ_r, θ_s, α, and n are used to estimate A_{aw} with the thermodynamic-based method.

Residual water content θ_r (cm³/cm³)	See notes in the entry for "K_{sat}" for how to estimate if no measured values are available.
Saturated water content θ_s (cm³/cm³)	See notes in the entry for "K_{sat}" for how to estimate if no measured values are available.
Median grain diameter d_{50} (cm)	The particle size of a soil sample at which 50% of the particles are smaller and 50% are greater. d_{50} is used in one of the methods for estimating the A_{aw} scaling factor SF.
Organic carbon fraction f_{oc} (%)	The fraction of organic carbon that contributes to the solid-phase sorption of PFAS. f_{oc} is used to estimate solid-phase sorption coefficient K_d.
van Genuchten parameter α (1/cm)	An empirical parameter of the van Genuchten model for soil-water characteristics. See notes in the entry for "K_{sat}" for how to estimate if no measured values are available.
van Genuchten parameter n ($-$)	An empirical parameter of the van Genuchten model for soil-water characteristics. See notes in the entry for "K_{sat}" for how to estimate if no measured values are available.
Longitudinal dispersivity α_L (cm)	An empirical parameter that represents the spreading of PFAS along the direction of flow due to variations of water velocity in space. α_L needs to be estimated. The Excel tool has an option to approximate it using an empirical model (Xu and Eckstein (1995); Al-Suwaiyan (1996)), i.e., $\alpha_L = 0.82[log(Z_w/100)]^{2.446}$ where Z_w (cm) is the depth to groundwater. Note that this empirical model was developed based on datasets collected for saturated zones and as a result does not consider the dependence of α_L on water saturation.

Parameter	Description
Water content θ (cm^3/cm^3)	Representative θ in the vadose zone, which may be measured by moisture probes such as time-domain reflectometer probes or estimated from soil samples collected at the site.
	If no measured values are available, the Excel tool estimates θ by assuming unit gradient flow $I_f = k_r(\theta)K_{sat}$, where k_r is the relative permeability that is a function of the water content via the van Genuchten–Mualem model. Note that this estimated θ will have substantial uncertainties due to the use of the van Genuchten–Mualem model for the relative permeability, especially when the van Genuchten parameters are also estimated (e.g., by pedotransfer functions). This uncertainty should be accounted for when conducting simulations using PFAS-LEACH-Analytical (e.g., by conducting sensitivity analysis using Module 1 or Monte-Carlo analysis using the Module 2).

Parameter	Description
Air–water interfacial area scaling factor SF (−)	An empirical parameter to account for the additional air–water interfacial area not represented by the thermodynamic-based approach, e.g., due to the impact of microscale surface roughness of soil grains or other field-specific factors.
	The Excel tool provides an option to estimate the scaling factor caused by microscale surface roughness using an empirical equation reported by Brusseau (2023),
	$$SF = (-0.65S_w + 1.33)(-0.45d_{50} + 5),$$
	where $S_w = \theta/\theta_s$ is water saturation and d_{50} (cm) is the soil median grain diameter. Note that the above empirical equation for SF was derived from air–water interfacial area datasets obtained for three sandy soils (Brusseau, 2023), which may have greater uncertainties when applied to finer-grained soils with greater microscale surface roughnesses (e.g., soils with greater clay and/or silt fractions).
	Alternatively, the scaling factor can be estimated by leveraging lysimeter porewater concentrations via mass balance. The approach assumes that the soil PFAS concentration remains unchanged during the sampling period and it consists of PFAS in the aqueous, solid phase, and air–water interface, i.e., $C_{\text{soil}}^{\text{V}} = \theta C_{\text{aq}} + \rho_b K_d C_{\text{aq}} + K_{aw} C_{\text{aq}} A_{aw}$ (Russell et al., 2025). As such, A_{aw} can be estimated as
	$$A_{aw} = \frac{C_{\text{soil}}^{\text{V}} - \theta C_{\text{aq}} - \rho_b K_d C_{\text{aq}}}{K_{aw} C_{\text{aq}}},$$
	where $C_{\text{soil}}^{\text{V}} = \rho_b C_{\text{soil}}^{\text{M}}$ (μg/dm^3) is PFAS mass per unit bulk soil volume, where $C_{\text{soil}}^{\text{M}}$ (μg/kg) is PFAS mass per unit soil mass. θ is volumetric water content (cm^3/cm^3), C_{aq} is porewater PFAS concentration (μg/L), ρ_b is soil bulk density (g/cm^3), K_d is solid-phase adsorption coefficient (cm^3/g), and K_{aw} is air–water interfacial adsorption coefficient (cm^3/cm^2). This approach assumes all of the parameters in the equation are available or can be estimated, and A_{aw} is the only unknown parameter.

Parameter	Description
Air–water interfacial area scaling factor SF $(-)$	The air–water interfacial area A_{aw} estimated above corresponds to a specific water content (i.e., water saturation). The scaling factor is then estimated by taking the ratio between the porewater-estimated A_{aw} and that estimated by the thermodynamic-based approach. Because the scaling factor estimated above leverages *in situ* data in the field, it provides a means to potentially account for the various factors not represented in the A_{aw} estimated by the thermodynamic approach (e.g., the impact of microscale surface roughness or other factors). Solid-phase desorption at legacy PFAS-contaminated sites is often rate-limited. If the time scale of desorption is much greater than the residence time of porewater, the rate-limited fraction of the solid-phase adsorption may be excluded when applying the approach described above. For a conservative assessment of risks (i.e., overestimating PFAS leaching) at the contaminated site, users can assume that SF equals to 1.
Air-water interfacial Area A_{aw} (cm^2/cm^3)	The total area of the air–water interfaces per unit bulk volume of the soil. One of the approaches implemented in the Excel tool is the revised thermodynamic-based method that estimates the specific air–water interfacial area A_{aw} using the soil water characteristics (Leverett, 1941; Morrow, 1970) scaled by the scaling factor SF that accounts for the impact of microscale surface roughness (Zeng et al., 2021; Guo et al., 2022; Brusseau, 2023) or other factors as $$A_{aw} = SF \frac{\phi}{\sigma_0} \int_{S_w}^{1} p_c \mathrm{d}S_w,$$ where $S_w = \theta/\theta_s$ is water saturation. $\phi = \theta_s$ is soil porosity. σ_0 is the surface tension of porewater when no PFAS are present. p_c (cm) is capillary pressure, which is a function of water saturation via the van Genuchten model $p_c(S_w) = \frac{1}{\alpha}\left[\left(\frac{S_w - S_r}{S_s - S_r}\right)^{-\frac{1}{1-\frac{1}{n}}} - 1\right]^{\frac{1}{n}}$, where $S_r = \theta_r/\theta_s$. Note that the standard thermodynamic-based approach (Leverett, 1941; Morrow, 1970) does not account for the impact of microscale surface roughness or other factors (i.e., $SF = 1$).

2.2.2 PFAS properties

Table 2: Parameters for PFAS properties

Parameter	Description
Surface tension parameter a (mg/L)	A fitting parameter of the Szyszkowski equation that describes the surface tension as a function of PFAS concentration in the aqueous solution. a, b, and σ_0 are used to determine the air–water interfacial adsorption coefficient K_{aw}. The Excel tool provides reference values for the three surface tension parameters for a list of PFAS that can be selected using the drop-down menu *"PFAS type"*. The PFAS are ordered alphabetically. There are some PFAS on the list where no surface tension parameters are available. For those PFAS, users can select the QSPR method to estimate the K_{aw} values.
Surface tension parameter b ($-$)	A fitting parameter of the Szyszkowski equation that describes the surface tension as a function of PFAS concentration in the aqueous solution. See notes in the entry for "a" for how this parameter is used.
Surface tension parameter σ_0 (dyn/cm)	Surface tension of the porewater when no PFAS is present. See notes in the entry for "a" for how this parameter is used.
Molar Mass M (g/mol)	Mass per mole of a given PFAS.
Molecular diffusion coefficient D_0 (cm^2/s)	Molecular diffusion coefficient of a given PFAS in the free porewater. When D_0 is not available, it can be estimated empirically based on the molar volume (Wilke and Chang, 1955) $$D_0 = \frac{7.4 \times 10^{-8} \, (\psi M_s)^{0.5} \, T}{\eta V_m^{0.6}}$$ where D_0 is the diffusion coefficient (cm^2/s), ψ is the association factor of the solvent (dimensionless), M_s is the molecular weight of the solvent (g/mol), T is the absolute temperature (K), η is the solvent viscosity (cP), and V_m is the molar volume of PFAS (cm^3/mol). ψ = 2.6, M_s = 18 g/mol, T = 293.15 K, and η = 1.002 cP (Schaefer et al., 2019) are used to compute the diffusion coefficient of the PFAS for which no measured D_0 is available .
Molar volume V_m (cm^3/mol)	The volume occupied by one mole of a given PFAS. It is equal to the molar mass divided by the mass density.

Parameter	Description
Organic carbon-water partition coefficient K_{oc} (cm^3/g)	Normalized linear solid-phase sorption coefficient of organic carbon for a given PFAS, which is used to estimate $K_d = f_{oc}K_{oc}$ when K_d is not available and hydrophobic interaction is the main mechanism for solid-phase sorption. K_{oc} can be estimated using the QSPR approach when no measured valeus are available (Brusseau, 2024). Additional details for estimating K_{oc} are provided in Table 7. While it has been recognized that $f_{oc}K_{oc}$ may estimate K_d when hydrophobic interaction is not the primary solid-phase adsorption mechanism, the K_{oc} values provided for the list of PFAS indirectly accounts for non-hydrophobic interactions particularly for the shorter-chain PFAS.
Solid-phase sorption coefficient K_d (cm^3/g)	Linear solid-phase sorption coefficient. K_d can be estimated from f_{oc} and K_{oc} as $K_d = f_{oc}K_{oc}$ assuming that hydrophobic interaction is the primary mechanism for solid-phase sorption.
Air-water interfacial adsorption coefficient K_{aw} (cm^3/cm^2)	When the surface tension parameters (a, b, and σ_0) are available, K_{aw} can be estimated by the Langmuir isotherm as $K_{aw} = \frac{1}{RT}\frac{\sigma_0 b}{a+C_r}$, where C_r is a representative porewater concentration provided by the user. Note that the units for the various parameters need to be consistent when computing K_{aw} (e.g., the molar mass may need to be used to convert the units). For most contaminated sites and PFAS, it is usually a good approximation to use $C_r = 0$ when estimating K_{aw}. The Excel tool provides reference values for the surface tension parameters for a subset of PFAS. When no surface tension parameters are available, the Excel tool has the option to estimate K_{aw} using the QSPR method based on the molar volume of PFAS (Brusseau and Van Glubt, 2021). Because the QSPR method is an empirical correlation equation with the parameters fitted from the available data for a limited range of PFAS, it may introduce errors especially when it is extrapolated to estimate PFAS beyond the range used to fit the parameters. Therefore, we recommend that users use surface tension parameters to estimate K_{aw} whenever they are available.
Instantaneous solid-phase sorption fraction F_s (−)	F_s is the fraction of sorbent for which sorption is instantaneous. F_s and α_s can be determined by batch desorption experiments, if kinetic desorption is of interest.
Kinetic solid-phase sorption rate constant α_s (1/hour)	The first-order rate constant for kinetic solid-phase sorption.

2.2.3 Groundwater dilution calculation

Table 3: Parameters for groundwater dilution calculation. The approach to determine these parameters follows the USEPA technical document for determining soil screening levels (USEPA, 1996).

Parameter	Description
Groundwater darcy flux U_{gw} (m/yr)	Darcy flux of the groundwater beneath the contaminated site.
Lateral site width L (m)	The lateral width of the contamination site parallel to the groundwater flow. Here, it is assumed that the source area is a square. When deriving soil screen levels, this may be conservative for sites with their longer dimensions perpendicular to groundwater flow or nonconservative for sites with their longer dimensions parallel to groundwater flow (USEPA, 1996). Under those conditions, the source length may be calculated as the square root of the source area.
Saturated zone thickness b_{sat} (m)	The saturated thickness of the water-bearing unit.
Vertical dispersivity α_v (m)	α_v can be estimated as α_v = 0.0056L.
Mixing zone thickness δ_{gw} (m)	Computed estimate for the thickness of the groundwater mixing zone (m), which is calculated using the following equation $$\delta_{gw} = \sqrt{2\alpha_v L} + b_{sat}\left[1 - \exp\left(\frac{-I_f L}{U_{gw}b_{sat}}\right)\right].$$ By definition, δ_{gw} cannot exceed b_{sat}. Note that the unit for I_f needs to be converted to m/yr to be consistent with the other parameters when applying the equation above.
Dilution Factor DF (−)	It is used to estimate the extent to which contaminants leached from soil are diluted after entering groundwater, which is calculated by the following equation $$DF = 1 + \frac{U_{gw}\delta_{gw}}{I_f L}.$$

2.2.4 Initial PFAS soil concentration profile and lysimeter porewater concentration

Initial PFAS soil concentration

To evaluate the PFAS mass discharge rates to groundwater and the contamination risks, it is critical to know the amount of initial mass and its vertical distribution in the source

vadose zone. This information needs to be provided to the Excel tool as the initial PFAS soil concentration profile (e.g., PFAS soil concentration (μg/kg) as a function of the depth (cm)).

In practice, soil samples are typically collected at only a limited number of depths. The Excel tool provides four columns where users can enter up to 38 depth–concentration sets. PFAS soil concentrations can be specified independently for each depth—there is no need to follow a particular order (e.g., shallow to deep). Entered depths are automatically rounded to the nearest centimeter, and the discrete concentration values are then spatially interpolated to generate an approximate soil concentration profile at 1-cm resolution. Two methods are provided for the spatial interpolation (piecewise constant and piecewise linear). Users can select which interpolation method to use via the drop-down menu of "Interpolation methods". Whenever the soil PFAS concentration table is updated, the user needs to re-apply the interpolation method to obtain an updated interpolation.

Please note the following when entering the soil concentration data:

- Depth below land surface should not exceed the total depth to groundwater (Z_w).
- Users are recommended to input soil PFAS concentrations at $z = 0$ and $z = Z_w$. If they are not available, users can provide estimates. If no values are provided by the user, soil PFAS concentrations at $z=0$ and $z = Z_w$, by default, will be assigned a concentration of the data point closest to them.
- If a soil PFAS concentration data point represents the average concentration over an interval, the user should input the depth location of the center of the interval.
- Users can provide up to 38 depth-discrete PFAS soil concentration data points.
- Users can enter measurement data at any depths independently without following a particular order, e.g., shallow to deep. Blank rows between depth entries are also acceptable, though we do not recommend doing so.

Lysimeter porewater concentration

Lysimeter porewater concentration data up to 10 sets can be provided. The input table is located at the bottom-right of Box 4 of the Excel input interface. Each concentration–depth set is independent. For example, two different lysimeter porewater concentration data can have the same depth (e.g., they were collected at the same depth at different locations at the site). The datasets will be used to constrain the air–water interfacial area A_{aw} (by estimating the air–water interfacial area scaling factor SF). For each row, the depth and concentration must be provided. The water content in the third column is optional; when it is not provided, the water content value from Box 1 of the Excel input interface will be used. Rows without depth or concentration will be ignored. Users can click the button "Estimate local SF" in the top-right corner to estimate the local scaling factor in the fourth column using the values from the first three columns (or the first two columns and the water content value from Box 1 if it is not provided in the third column). Note that if any of the related input data in the previous boxes are updated, users need to click the button again to re-estimate the local scaling factor. When multiple concentration–depth sets are provided, the arithmetic mean of the computed local scaling factors will be used in Box 1 when Method 2 is selected to estimate the scaling factor. The user can also make their own estimate of the scaling factor (e.g., other than the arithmetic mean) based on the local scaling factor values, and then manually input that in Box 1.

For Module 1, in the bottom-right table of Box 4, if only the median water content is

entered in column T for a row, that single value is used to compute all three scaling factor values—left bound, median, and right bound. To examine sensitivity to water content, users can also additionally provide a left bound (smaller) and a right bound (greater) value for the water content. The corresponding left bound and right bound of the scaling factor will be computed after clicking the button "Estimate local SF". Because the left bound is defined such that they generate a smaller leaching, the left bound of the scaling factor will be greater than the median while the right bound will be smaller than the median. The arithmetic mean of the left and right bounds of the local scaling factors will be used respectively as the left and right bounds in Box 1. If no water content is provided (or incomplete for the three values) in the lysimeter data table in Box 4, the water content values from Box 1 (including left bound, median, and right bound) will be used.

2.2.5 Simulation information

Table 4: Parameters for simulation information

Parameter	Description
Simulation time (time series) t (yr)	Total simulation time. To derive SSLs, the simulation time should be sufficiently long such that the vadose-zone leachate concentration (or the mass discharge rate to groundwater) reaches the maximum.
Output time interval (time series) dt (yr)	The temporal resolution of the output time series (e.g., groundwater mass discharge rate).
Output time points (profiles) t_p (yr)	The time points at which PFAS concentration profiles are output. In Module 0 and Module 1, multiple time points can be entered at once, separated by commas (e.g., "10,20"). In Module 2, only a single time point can be entered for each run.
Acceptable groundwater concentration $C_{gw,a}$ (μg/L)	Acceptable groundwater concentration at a receptor point (e.g., a groundwater well). The receptor well is assumed to be at the edge of the contaminated site.

2.2.6 Input parameters for Module 1 sensitivity analysis

Module 1 allows for most of the input parameters (soil properties and site conditions, PFAS properties, and groundwater dilution) to be perturbed from the median value to conduct a sensitivity analysis. Users can set the left and right bounds of parameters by specifying the relative or absolute deviation (if one of them is specified, the other will be computed automatically). Users can choose to perturb multiple parameters simultaneously or one single parameter at a time.

NOTE: The *"left"* (or *"right"*) bound of the input parameters is defined such that they generate *smaller* (or *greater*) leaching. Therefore, the "left" bound of the parameter may not always be smaller than the median, depending on whether the parameter positively or

negatively correlate with leaching. For example, the "left" bound for A_{aw} is greater than the median while the right bound is smaller than the median. In this case, the relative deviations for both the left and right bounds are negative.

If the user employs Rosetta 3 to obtain the van Genuchten parameters (e.g., θ_r, θ_s, α, n, K_{sat}) from a specified soil type, the estimated parameter values represent the median values for that soil type.

2.2.7 Input parameters for Module 2 Monte Carlo analysis

Module 2 allows for most of the input parameters (soil properties and site conditions, PFAS properties, and groundwater dilution) to be assigned a *mean* and a *coefficient of variation* to perform Monte Carlo simulations. In these simulations, parameters are sampled from either a log-normal distribution (base 10) or a normal distribution (See Table 5).

Below are instructions for the input of the mean and coefficient of variation values (columns F and G). Regardless of the distribution type, the values entered in the mean and CV columns are physically meaningful quantities in the linear space. For log-normally distributed parameters, if users have the mean and CV values expressed in the log-normal space (base 10), they can use the Module2_ParaToolkit to convert them into linear-space values.

Mean (column F): Since the inputs represent physically meaningful quantities, these values should in principle be positive.

- *Blue cells*: Values can be populated from the drop-down menu (reference values) or entered manually by the user.
- *White cells*: They can be estimated by the assistive functional button or manually entered by the user. If any blue-cell parameter used by an assistive functional button is updated, the user should apply the functional button again to re-estimate the dependent parameters.

Coefficient of Variation (column G): The coefficient of variation is defined in the linear space regardless of whether the parameter follows a normal and a log-normal distribution. The CV values must be non-negative, which defines the range of variability for the random sampling.

- *Dark-orange cells (required)*: The user must assign a non-negative coefficient of variation (CV) to these cells. If the user does not have information about the variability, a default value of "0" may be used (i.e., assuming negligible variability).
- *Light-orange cells (optional)*: When the cell is left blank, it activates *function-based sampling*, whereby the variability is accounted for internally using the variability of the *blue-cell* parameters via the built-in estimation functions. Users can also provide CV values to the light-orange cells manually. If the user does not have information about the parameter's variability, a default value of "0" may be assigned (assuming no variability). When left blank, the CV values estimated by the built-in functions will be automatically written back to the empty CV cells after the calculation is completed.
- For a normal distribution, CV describes how tightly the values cluster around the mean: A small CV (e.g., 0.1) means values are tightly concentrated and a larger CV (e.g., 0.5) means values are more widely spread. For a log-normal distribution, CV reflects the degree of skewness and the heaviness of the right tail: A small CV means the distribution

is close to symmetric and concentrated and a large CV means most values are small, but there is a higher chance of occasional very large values.

Table 5: Assumed probability distributions for model parameters

Normal distribution	**Log-normal distribution (base 10)**
A variable X is normally distributed, i.e., $$X \sim \mathcal{N}(\mu, \text{SD}^2),$$ where μ is the arithmetic mean and SD is the standard deviation. The coefficient of variation (CV) is defined as $$\text{CV} = \frac{\text{SD}}{\mu}.$$	Let $Y = \log_{10} X$, where $Y \sim \mathcal{N}(\mu_{10}, \text{SD}_{10}^2)$. Here, μ_{10} and SD_{10} are the mean and standard deviation of Y. The corresponding mean and standard deviation of X in the linear space can be expressed as $$\mu = 10^{\mu_{10}} \cdot \exp\left(\tfrac{1}{2}(\ln 10)^2 \, \text{SD}_{10}^2\right),$$ $$\text{SD} = \mu \cdot \sqrt{\exp\left((\ln 10)^2 \, \text{SD}_{10}^2\right) - 1}.$$ The coefficient of variation (CV) is defined in the linear space as $$\text{CV} = \frac{\text{SD}}{\mu} = \sqrt{\exp\left((\ln 10)^2 \, \text{SD}_{10}^2\right) - 1}.$$
• Soil bulk density (ρ_b) • Residual water content (θ_r) • Saturated water content (θ_s) • Water content (θ) • Surface tension parameters (a, b) • Molecular diffusion coefficient (D_0) • Lateral site width (L) • Saturated zone thickness (b_{sat}) • Mixing zone thickness (δ_{gw})	• Net infiltration (I_f) • Saturated hydraulic conductivity (K_{sat}) • Median grain size (d_{50}) • Organic carbon fraction (f_{oc}) • Van Genuchten parameters (α, n) • Longitudinal dispersivity (α_L) • Air–water interfacial area scaling factor (SF) • Air–water interfacial area (A_{aw}) • Organic carbon–water partition coefficient (K_{oc}) • Solid-phase adsorption coefficient (K_d) • Air–water interfacial adsorption coefficient (K_{aw}) • Groundwater darcy flux (U_{gw}) • Vertical dispersivity (α_v) • Dilution factor (DF)

When Rosetta 3 is used to estimate VG parameters, it may provide parameter *means*

and *standard deviations* either in the linear space or in the log-10 space, depending on the parameter's assumed distribution (normal vs. log-normal). Because the Module 2 interface requires all inputs to be in the linear space, if Rosetta provides (μ_{10}, SD_{10}) for a parameter assumed log-normal, use the Module2_ParaToolkit to convert (μ_{10}, SD_{10}) to the linear-space mean μ and standard deviation *SD*. Then compute the linear-space coefficient of variation as CV = SD/μ. Enter μ into the *Mean* column (F) and CV into the *CV* column (G). If Rosetta already provides linear-space (μ, SD) for a normally distributed parameter, you may directly compute CV = SD/μ and input them into columns F and G.

The sampled parameters for the Monte Carlo realizations need to be physically meaningful. Table 6 summarizes the allowed ranges for the parameters and the basis for determining them. These ranges would apply to any Monte Carlo realization regardless of the mean and coefficient of variation assigned to the parameters.

Table 6: Constrained ranges for the CV values in Module 2

Parameter (Unit)	Range	Description
I_f (cm/yr)	$(0, 200]$	A maximum of 200cm/yr is assumed for the net infiltration to cover extremely humid regions with highly permeable vadose zones.
ρ_b (g/cm^3)	$[1, 2]$	Physical range for typical soil bulk density.
K_{sat} (cm/day)	$[0.019, 27600]$	Soil saturated conductivity bounded by values compiled from the unsaturated soil hydraulic database (UNSODA) (Nemes et al., 2015).
θ_r (cm^3/cm^3)	$(0, 0.357]$	Residual water content bounded by values compiled from the UNSODA database (Nemes et al., 2015).
θ_s (cm^3/cm^3)	$[0.2078, 0.66]$	Saturated water content bounded by values compiled from the UNSODA database (Nemes et al., 2015).
d_{50} (cm)	$[0.001, 0.05]$	Median particle size that covers different soil types.
f_{oc} (%)	$[0, 20]$	Soil organic carbon fraction covering typical field values.
α (cm^{-1})	$[0.000347, 0.261]$	van Genuchten empirical parameter bounded by values compiled from the UNSODA database (Nemes et al., 2015).
n $(-)$	$[1.01, 6.39]$	van Genuchten pore-size distribution parameter bounded by values compiled from the UNSODA database (Nemes et al., 2015). A lower bound of 1.01 is set to avoid numerical convergence issues.
α_L (cm)	$[10, 446.82]$	Longitudinal dispersivity bounded by estimated values for a vadose zone depth of 1 m and 100 m.
θ (cm^3/cm^3)	$[\theta_r, \theta_s]$	Soil water content bounded by residual and saturated values.
SF $(-)$	$(0, 100]$	Scaling factor for interfacial area bounded based on empirical estimates.
A_{aw} (cm^2/cm^3)	$(0, 10000]$	Air–water interfacial area bounded based on empirical estimates.
a (mg/L)	$(0, 30000]$	Surface tension parameter bounded by reported values for a wide range of PFAS.
b $(-)$	$(0, 1]$	Surface tension parameter bounded by reported values for a wide range of PFAS.
D_0 (cm^2/s)	$[10^{-7}, 10^{-4}]$	Aqueous diffusion coefficient bounded by estimated values for a wide range of PFAS.
K_{oc} (cm^3/g)	$[0.1, 2 \times 10^7]$	Organic carbon–water partition coefficient bounded by estimated values for a wide range of PFAS.

2.3 Functional Buttons

The Excel tool has implemented a few functional buttons for estimating parameters, including longitudinal dispersivity α_L, soil water content θ, air–water interfacial area scaling factor SF, air–water interfacial area A_{aw}, solid–phase sorption coefficient K_d, air–water interfacial adsorption coefficient K_{aw}, and three parameters related to groundwater dilution (α_v, δ_{gw}, DF). We elaborate on these functional buttons below.

- Module 0: The gray button computes values in the white cells.
- Module 1: The gray button computes the white cells together with their corresponding left and right boundary values in the yellow cells (three columns).
- Module 2: The gray button computes only the mean values in white cells; coefficient of variation values are not computed—they need to be manually input by the user.

Table 7: Functional Buttons

Functional Button	Required Parameters	Description
Estimate α_L Estimate α_L	Z_w	α_L is approximated using an empirical model (Xu and Eckstein, 1995; Al-Suwaiyan, 1996), i.e., $\alpha_L = 0.82[\log(Z_w/100)]^{2.446}$ where Z_w (cm) is the depth to groundwater. The empirical model was developed based on datasets collected for saturated zones and does not consider the dependence of α_L on water saturation.
Estimate θ Estimate θ	θ_r, θ_s, I_f, K_{sat}, n	θ is estimated inversely from the net infiltration rate by assuming unit gradient flow $I_f = k_r(\theta)K_{sat}$, where k_r is the relative permeability that is a function of the water content via the van Genuchten–Mualem model. Users should note that the inversely estimated θ relies on the van Genuchten parameter n that may also be estimated (e.g., from pedotransfer functions like Rosetta 3). Therefore, the estimated θ may involve substantial uncertainties, which need to be accounted for, e.g., by sensitivity (Module 1) or Monte-Carlo analysis (Module 2).

Name	Required Parameters	Description
Estimate *SF* Estimate *SF*	*Approach 1*: Water saturation $S_w = \theta/\theta_s$ and d_{50}; *Approach 2*: C_{soil}, C_{aq}, Depth, θ, ρ_b, K_d, K_{aw}.	The A_{aw} scaling factor approximates the impact of microscale grain surface roughness on air–water interfacial area. **Approach 1**: The scaling factor is estimated using an empirical equation reported by Brusseau (2023), $$SF = (-0.65S_w + 1.33)(-0.45d_{50} + 5),$$ where d_{50} is the soil median grain diameter (cm). **Approach 2**: This method requires users to input lysimeter-sampled porewater concentrations and corresponding water content values. The input table is located at the bottom-right of Box 4 of the Excel input interface. For each concentration–depth set, an *SF* value is computed following the approach described in the entry for "Air–water interfacial area scaling factor *SF*" in Table 1 (Russell et al., 2025). When multiple concentration-depth sets are provided, the arithmetic mean of the computed scaling factors will be used in Box 1 of the Excel input interface.
Estimate A_{aw} Estimate A_{aw}	θ_r, θ_s, n, θ, α, σ_0, *SF*	A_{aw} is approximated by the thermodynamic-based method using the soil water characteristics (Leverett, 1941; Morrow, 1970) scaled by the scaling factor *SF* that accounts for the impact of microscale surface roughness (Brusseau, 2023) as $$A_{aw} = SF\frac{\phi}{\sigma_0}\int_{S_w}^{1} p_c dS_w,$$ where $S_w = \theta/\theta_s$ is water saturation. $\phi = \theta_s$ is soil porosity. σ_0 is the surface tension of porewater when no PFAS are present. p_c (cm) is capillary pressure, which is a function of water saturation via the van Genuchten model. The standard thermodynamic-based approach (Leverett, 1941; Morrow, 1970) does not account for the impact of microscale surface roughness (i.e., *SF* = 1).

Name	Required Parameters	Description
Estimate K_d `Estimate $K_d$`	f_{oc}, K_{oc}	Linear solid-phase sorption coefficient. In the current version, K_d is estimated as $K_d = f_{oc}K_{oc}$ assuming that hydrophobic interaction is the primary mechanism for solid-phase sorption. In the next version, we plan to generalize the estimation function to incorporate the contribution of other solid-phase adsorption mechanisms such as the interaction between PFAS and soil constituents other than organic carbon (e.g., metal oxides and clay minerals).
Estimate K_{aw} `Estimate $K_{aw}$`	T, M, V_m, a, b, σ_0, a representative pore-water concentration C_r	When the surface tension parameters (a, b, and σ_0) are available, K_{aw} is estimated by the Langmuir isotherm as $K_{aw} = \frac{1}{RT}\frac{\sigma_0 b}{a+C_r}$, where C_{rep} is a representative porewater concentration. Note that the units for the various parameters need to be consistent when computing K_{aw}. For most contaminated sites and PFAS, it is usually a good approximation to use $C_{rep} = 0$ when estimating K_{aw}. When no surface tension parameters are available, the Excel tool has the option to estimate K_{aw} with the QSPR method based on molar volume V_m: $K_{aw} = 0.019V_m - 7.1$ (Brusseau and Van Glubt, 2021).

Name	Required Parameters	Description
Estimate α_v, δ_{gw}, DF Estimate α_v, δ_{gw}, *DF*	I_f, U_{gw}, L, b_{sat}	The dilution factor (USEPA, 1996) can be computed as $$DF = 1 + \frac{U_{gw}\delta_{gw}}{I_f L},$$ where U_{gw} is the groundwater darcy flux (m/yr). I_f (m/yr) represents annual net infiltration. L (m) is the lateral width of the contamination site along the groundwater flow direction. Here, it is assumed that the source area is a square. When deriving soil screen levels, this may be conservative for sites with their longer dimensions perpendicular to groundwater flow or nonconservative for sites with their longer dimensions parallel to groundwater flow (USEPA, 1996). Under those conditions, the source length may be calculated as the square root of the source area. δ_{gw} represents a computed estimate for the thickness of the groundwater mixing zone (m), which is calculated using the following equation $$\delta_{gw} = \sqrt{2\alpha_v L} + b_{sat}\left[1 - \exp\left(\frac{-I_f L}{U_{gw} b_{sat}}\right)\right],$$ where the vertical groundwater dispersivity α_v is estimated as $0.0056L$, and b_{sat} represents the saturated thickness of the water-bearing unit (m). Note that the unit for I_f has the unit of m/yr to be consistent with the other parameters when applying the equation above. By definition, δ_{gw} cannot exceed b_{sat}.
Estimate local SF Estimate local *SF*	C_{soil}, C_{aq}, $Depth$, θ, ρ_b, K_d, K_{aw}.	Click this button to automatically calculate the local scaling factor based on the entered depth, concentration, and (optional) water content data. If multiple datasets are provided, local scaling factors will be calculated for all valid rows. The results will be filled in the fourth column, and you need to click the button again to refresh the results whenever the input data are updated.

Name	Required Parameters	Description
Basic solver Basic Solver	For *Module 0* and *Module 1*, it needs parameters with an asterisk (and optionally other parameters). For *Module 2*, it requires all the input parameters except the ones in cells with light-orange color.	The basic solver assumes equilibrium solid-phase sorption. After clicking the "Basic Solver" button, the bottom left corner of the Excel user interface will display the calculation progress as *"Simulation progress: X% completed"*.
Advanced solver Advanced Solver	For *Module 0* and *Module 1*, it needs parameters with an asterisk (and optionally other parameters). The advanced solver is not available for Module 2.	The advanced solver accounts rate-limited solid-phase sorption using a two-site model. As a rule of thumb, it is not necessary to use the advanced solver when the half-life of kinetic desorption (estimated as $\sim 1/\alpha_s$) is significantly less than the residence time of PFAS in the vadose zone (e.g., smaller than $0.1\times$ residence time) due to the negligible impact of kinetic solid-phase sorption. If the user thinks that rate-limited solid-phase sorption may be important at the site, we recommend to first use the basic solver (assuming equilibrium solid-phase sorption) to estimate the residence time ($T_{\text{residence}} \sim \min(RZ_w\theta/I_f, RZ_w^2\theta/I_f/\alpha_L)$) and compare with the half-life of kinetic desorption ($\sim 1/\alpha_s$) to assess if it is necessary to use the advanced solver. The residence time of PFAS in the vadose zone is provided in the Excel output interface. Similar to the basic solver, after clicking the "Advanced Solver" button, the bottom left corner of the Excel user interface will display the calculation progress as *"Simulation progress: X% completed"*.

2.4 Navigating the Outputs

Module 0 provides the basic simulation functions. Module 1 and Module 2 have the additional capability to conduct sensitivity analysis and Monte Carlo simulations. Their Output tabs ("Module0_Output" ,"Module1_Output" and "Module2_Output") also present the results from the basic simulation, the sensitivity analysis, and Monte Carlo simulations. Each Output tab includes two parts.

The **first** part consists of five variables computed by PFAS-LEACH-Analytical:

- Vadose-zone mass discharge rate of the entire contaminated site (μg/year) or the mass discharge rate of a unit area if the contaminated site area is set to 1 m². It is computed by multiplying the mass discharge rate per unit area with the area of the contaminated site (or a unit area of 1 m²). Here, the site is assumed to be homogeneous laterally.
- Mass remaining in the vadose zone (as % of the initial PFAS mass in the vadose zone).
- PFAS concentration in a receptor well (μg/L) at the edge of the contaminated site.
- Soil concentration profiles in the vadose zone (μg/kg), showing the spatial variation of total soil PFAS concentrations at specified times (the initial profile is displayed as a reference).
- Aqueous concentration profiles in the vadose zone (μg/L), showing the spatial variation of PFAS concentrations in porewater at specified times.

These results are displayed graphically and can be viewed using the drop-down menu below *"Select what to plot"*. The datasets can also be downloaded as .csv files (by clicking the button *"Download data"*) for further analysis or other applications. The mass discharge rate divided by the water flow rate can be interpreted as the undiluted concentration exiting the bottom boundary of the vadose zone. In contrast, the receptor well groundwater concentrations reflect the diluted concentration in the underlying saturated zone. The Excel tool employs the simple dilution factor approach reported in the US EPA soil screening level guidance (USEPA, 1996) to estimate the receptor well groundwater concentration. However, the mass discharge rates data can also be used as input in sophisticated models such as 3D groundwater flow and transport models (e.g., analytical models like ATRANS and numerical models such as MODFLOW/MT3D-USGS) to more accurately simulate PFAS transport in the *saturated* zone. The mass discharge rate and receptor well groundwater concentrations were computed directly from the analytical solutions. The mass remaining in the vadose zone was obtained via numerical integration of the mass discharge rate over time, which may involve numerical errors due to time discretization. For an output timestep size of 1 year, the error can be up to one or two percent (i.e., the mass remaining can go slightly negative). The .csv output file only shows positive values for the mass remaining in the vadose zone.

For the visualization of profiles, Module 0 allows plotting a single profile or several profiles at multiple times for users to observe how the profiles evolve over time. Module 1 plots three profiles, corresponding to the left bound (less leaching), the mean, and the right bound (greater leaching), but only at one time. Module 2 also only plots one time, but can plot up to 200 realizations from the Monte Carlo sampling. Three percentiles are highlighted: 5th percentile, median, and 95th percentile. For the vadose-zone results (4 of the 5 plots), the percentiles are obtained by ranking the realizations based on a leaching-risk metric ($\frac{C_{soil,max}*I_f}{AF*R*\theta/\rho_b}$) in ascending order, such that lower percentiles represent smaller leaching risk and higher percentiles represent greater leaching risk. For the receptor well concentration results (1 of the 5 plots), the percentiles are obtained using the metric of $1/\text{SSL}_{\text{Tier 3}}$ such that lower percentiles have greater SSL values (hence smaller leaching risks) and higher percentiles have smaller SSL values (hence greater leaching risks).

The **second** part presents the SSLs derived via three methods:

- $\text{SSL}_{\text{Tier 3}}$ (μg/kg) is the SSL derived from the Tier 3 model PFAS-LEACH-Analytical. It accounts for the attenuation of PFAS in the vadose zone and dilution in groundwater.

The SSL can be written as

$$SSL_{\text{Tier 3}} = C_{gw,a} \times AF_{\text{vz}} \times DF \times [K_d + (K_{aw}A_{aw} + \theta_w)\frac{1}{\rho_b}], \tag{1}$$

where the vadose-zone attenuation factor (AF_{vz}) is defined as the ratio between the maximum porewater concentration of PFAS in the vadose zone and the maximum PFAS concentration in the leachate discharged to groundwater over the entire leaching period, which represents the PFAS-specific attenuation processes in the vadose zone. $C_{gw,a}$ (μg/L) is an acceptable concentration in a groundwater receptor well, DF (-) is the dilution factor in groundwater, K_d (cm^3/g) is the solid-phase sorption coefficient , K_{aw} (cm^2/cm^3) is the air–water interfacial adsorption coefficient, A_{aw} (cm^3/cm^2) is the specific air–water interfacial area, θ_w (cm^3/cm^3) is volumetric water content , and ρ_b (g/cm^3) is the soil bulk density. The terms in the brackets serve to convert the porewater concentration to the soil concentration based on equilibrium mass partitioning between the porewater, solid surface, and air–water interfaces (Brusseau and Guo, 2023).

- $SSL_{\text{Tier 4}}$ (μg/kg) is derived using the Tier 4 model PFAS-LEACH-DAF reported by Brusseau and Guo (2023) that revises the USEPA SSL approach to include the mass partitioning of PFAS at the air–water interfaces when converting the porewater concentration to the soil concentration. The revised SSL approach has the following form

$$SSL_{\text{Tier 4}} = C_{gw,a} \times DF \times [K_d + (K_{aw}A_{aw} + \theta_w)\frac{1}{\rho_b}] \tag{2}$$

- SSL (USEPA standard DAF) is derived using the USEPA standard SSL approach

$$SSL_{\text{EPA standard}} = C_{gw,a} \times DF \times [K_d + \theta_w\frac{1}{\rho_b}] \tag{3}$$

Additionally, the second part presents the retardation, attenuation, and dilution factors computed from the Tier 3 model PFAS-LEACH-Analytical that may help users understand relative contributions of the various factors to the derived PFAS-LEACH-Analytical-derived SSL. It also reports the estimated residence time of PFAS in the vadose zone and the duration over which the groundwater concentration at the receptor well exceeds the acceptable concentration (computed from PFAS-LEACH-Analytical). The descriptions for these variables are elaborated below:

- Air–water interfacial retardation $R_{aw} = K_{aw}A_{aw}/\theta$ represents the retardation due to air–water interfacial adsorption.
- Solid–water interfacial retardation $R_s = \rho_b K_d/\theta$ represents the retardation due to solid-phase adsorption.
- Total retardation factor $R = 1+R_{aw}+R_s$ represents the retention from solid-phase adsorption and air–water interfacial adsorption.
- Vadose-zone attenuation factor AF_{vz} is defined as the ratio between the maximum porewater concentration of PFAS in the vadose zone and the maximum PFAS concentration in the leachate discharged to groundwater, which represents the PFAS-specific attenuation processes in the vadose zone. Mathematically, $AF_{vz} = C_{\text{porewater,max}}/C_{\text{leachate,max}}$. Here, $C_{\text{porewater,max}}$ is the maximum porewater concentration of PFAS within the unsaturated zone, and $C_{\text{leachate,max}}$ represents the peak PFAS concentration in the aqueous phase at

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the bottom boundary of the vadose zone (i.e., the leachate that would enter the ground-water), derived from the simulation results over the entire leaching period. To obtain an accurate value for AF_{vz}, it is important to select a simulation time that is sufficiently large such that the vadose-zone leachate concentration reaches the maximum, i.e., $C_{\text{leachate,max}}$.

- Dilution factor DF is the ratio between the PFAS concentration in the vadose-zone leachate and the groundwater concentration at a receptor point (e.g., a drinking water well).
- Estimated residence time of PFAS in the vadose zone. The residence time is estimated from the basic solver (assuming equilibrium solid-phase sorption) as $t_{\text{residence}} \sim \min(RZ_w\theta/I_f, RZ_w{}^2\theta/I_f/\alpha_L)$.
- Duration exceeding the acceptable groundwater concentration, which is the time period during which the groundwater concentration in the receptor well exceeds $C_{gw,a}$.

The Output Tab of Module 1 ("Module1_Output") presents the results computed using the left and right bounds of the input parameters. Because the left (or right) bound of the input parameters is defined such that they generate smaller (or greater) leaching. Therefore, the left bound of the computed SSLs, retardation factors, attenuation and dilution factors is greater than their median, while the right bound is smaller than their median.

The Output Tab of Module 2 ("Module2_Output") presents the results from the Monte Carlo simulations, representing the 5th percentile, the median, and the 95th percentile. The percentiles are obtained by ranking the Monte Carlo realizations. The soil screening levels (SSLs) derived using three approaches (PFAS-LEACH-Analytical, PFAS-LEACH-DAF, and the USEPA standard method) decrease from the 5th percentile to the 95th percentile, reflecting greater leaching risk at higher percentiles. The key transport-related parameters from PFAS-LEACH-Analytical, including retardation, attenuation, dilution factors, residence time, and the duration of exceedance in groundwater illustrate the uncertainty ranges of the underlying physical processes. For instance, R_{aw}, R_s, and the total retardation factor R decrease with percentile, showing that higher-risk realizations correspond to weaker retardation. Similarly, DF decreases from low to high percentiles, reflecting smaller dilution under a greater contamination risk. T_R also decreases from low to high percentiles, reflecting shorter residence times under more severe leaching conditions.

3 Examples

Before using the Excel tool, users should do the following to set up the Excel environment:

- Change "macro" security to either "Enable all macros" or "Disable all macros with notification" (you need to enable macro for the Excel tool when asked). Instructions for how to do this (Windows users, Mac users).
- Enable "automatic calculation" via "Formulas"->"Calculation Options"->"Automatic".

We present three examples (one example for each module) to illustrate how to use Module 0, Module 1, and Module 2. The same case is used for all modules, with Module 1 and Module 2 including additional sensitivity analysis and Monte Carlo simulations.

We consider a legacy site to which aqueous film forming foam (AFFF) products were

applied over a couple of decades due to fire training activities. We assume that the site has very limited datasets available. We have basic soil characterization data (e.g., soil texture, organic carbon fraction) and concentrations for a list of PFAS at a few discrete depths from a soil core. We also have some site information such as the size of the contaminated area, depth to groundwater, and annual precipitation. One of the goals of using the Excel tool is to provide a screening level analysis and identify the priority of additional data collection for the next step. For illustrative purposes, we use PFOA as an example PFAS.

3.1 Example for Module 0

3.1.1 Inputs

① **Soil Properties and Site Conditions**			Parameter Values	Set Default Values
Depth to groundwater*	Z_w	cm	300	
Contaminated site area (or unit area)	A	m^2	2500	Soil Type 👆
Temperature	T	℃	20.00	User defined
Net infiltration*	I_f	cm/yr	25.92	
Soil bulk density*	ρ_b	g/cm^3	1.53	
Saturated hydraulic conductivity	K_s	cm/day	44.87	
Residual water content	θ_r	cm^3/cm^3	0.064	
Saturated water content*	θ_s	cm^3/cm^3	0.370	
Median grain size	d_{50}	cm	0.005	
Organic carbon fraction	f_{oc}	%	0.41	
van Genuchten parameter	α	cm^{-1}	0.018	
van Genuchten parameter	n	(-)	1.51	
Longitudinal dispersivity*	α_L	cm	13.42	Estimate α_L
Water content*	θ	cm^3/cm^3	0.219	Estimate θ
Air–water interfacial area scaling factor	SF	(-)	4.7	Estimate SF
Air–water interfacial area*	A_{aw}	cm^2/cm^3	753.9	Estimate A_{aw}

Figure 2: Module 0 input. Parameters for soil properties and site conditions.

For soil properties and site conditions, we have directly available values for the following parameters: Z_w, A, T, ρ_b, d_{50}, f_{oc}. Additionally, the annual precipitation at the site is p = 120 cm, and the soil texture in the vadose zone was measured from soil samples (70% sand, 20% silt, 10% clay).

We estimate I_f, K_s, θ_r, θ_s, α, n, α_L, θ, SF, and A_{aw} as follows:

- Following the approach described in Table 1, we estimate the net infiltration as I_f = $0.0018p^2$ = 25.92 cm/yr.
- With the soil texture of 70% sand, 20% silt, 10% clay, and bulk density ρ_b = 1.53 (g/cm^3), we use Rosetta 3 to estimate K_s = 44.87 (cm/day), θ_r = 0.064 (cm^3/cm^3), θ_s = 0.37 (cm^3/cm^3), α = 0.018 (1/cm), n = 1.51 (−). Note that the parameter values estimated from Rosetta 3 are the median values for the given soil texture.

- α_L, θ, *SF*, and A_{aw} can be estimated using the functional buttons on the right (details of the functions are presented in Table 7). If the blue-cell parameters used to estimate a white-cell parameter are updated, users need to apply (i.e., click) the functional button again to update the white-cell parameter. In general, users are recommended to apply the functional buttons to re-estimate all the white-cell parameters if any of the blue-cell parameters are updated. This would ensure that all the estimated white-cell parameters are updated.

② PFAS Properties			Parameter Values	
Surface tension parameter	*a*	mg/L	62.1	
Surface tension parameter	*b*	(-)	0.19	PFAS Type 👆
Surface tension parameter	σ_0	dyn/cm	71.0	PFOA
Molar mass*	*M*	g/mol	414.07	
Molecular diffusion coefficient*	D_0	cm^2/s	4.90E-06	
Molar volume	V_m	cm^3/mol	237.20	
Organic carbon-water partition coefficient	K_{oc}	cm^3/g	136.2	
Solid–phase adsorption coefficient*	K_d	cm^3/g	0.56	Estimate K_d
Air–water interfacial adsorption coefficient*	K_{aw}	cm^3/cm^2	3.69E-03	Estimate K_{aw}
NOTE: Fs and α$_s$ are only needed for using the advanced solver.				
Instantaneous solid-phase sorption fraction*	F_s	(-)	0.50	
Kinetic solid-phase sorption rate constant*	α_s	1/hour	1.00E-04	

Figure 3: Module 0 input. Parameters for PFAS properties.

We do not have directly available values for any of the parameters for PFAS properties. We obtain the surface tension parameters *a*, *b*, σ_0, and other PFAS-specific parameters by selecting "PFOA" from the drop-down button ("PFAS Type"). We estimate K_d and K_{aw} using the functional buttons on the right, following the approach described in Table 2. We do not have any information about F_s and α_s. To understand the potential impact of kinetic solid-phase sorption, we set F_s = 0.5 and α_s = 1/10,000 hour^{-1}. These two parameters will be used when we run the "advanced solver".

③ Groundwater Dilution			Parameter Values	
Groundwater darcy flux	U_{gw}	m/yr	365.00	
Lateral site width	*W*	m	3.00	
Saturated zone thickness	b_{sat}	m	0.35	
Vertical dispersivity	α_v	m	0.02	
Mixing zone thickness	δ_{gw}	m	0.32	Estimate α$_v$, δ$_{gw}$, *DF*
Dilution Factor*	*DF*	(-)	151.0	

Figure 4: Module 0 input. Parameters for groundwater dilution.

For the parameters related to groundwater dilution, we estimate the groundwater darcy flux U_{gw}, lateral site width *L*, and saturated zone thickness b_{sat} based on information collected

at the site. Following the approach described in Table 7, α_v, δ_{gw}, and DF are estimated using the functional button on the right.

Depth (cm bgs)	PFAS soil conc. (ug/kg)	Depth (cm bgs)	PFAS soil conc. (ug/kg)
0	100		
10	100		
50	30		
100	10		
150	2		
250	1		
300	0.5		

④ **Initial PFAS Soil Conc. & Lysimeter Porewater Conc.**

Interpolation Method

Piecewise Linear Interpolation

Re-apply interpolation whenever datapoints are updated.

I_f = 25.92 cm/yr

PFAS transport & water flux

Receptor well (drinking water)

Z_w = 300 cm

L = 3.00 m

δ_{gw} = 0.32 m

U_{gw} = 365 m/yr
Groundwater flow

b_{sat} = 0.35 m

Lysimeter Data
(for estimating A_{aw} scaling factor in Box ①)

Estimate Local SF

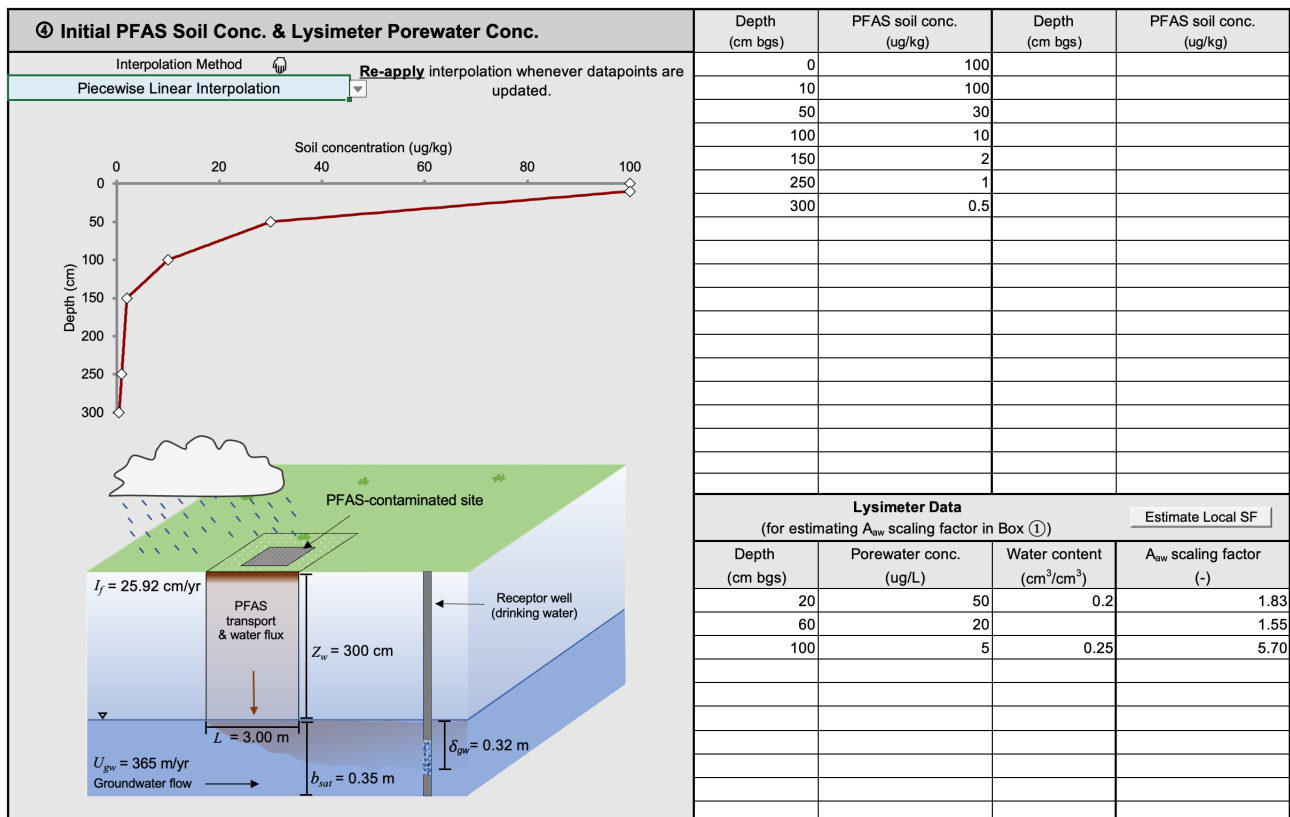| Depth (cm bgs)	Porewater conc. (ug/L)	Water content (cm³/cm³)	A_{aw} scaling factor (-)
20	50	0.2	1.83
60	20		1.55
100	5	0.25	5.70

Figure 5: Module 0 input. Initial PFAS soil concentration profile and lysimeter porewater concentration profile.

We have PFOA soil concentrations measured at 5 depth locations (z = 10, 50, 100, 150, 250 cm). The PFOA concentration at z = 0 cm is approximated as 100 μg/kg by assuming that it is the same as the concentration at z = 10 cm. We obtain the PFOA concentration at z = 300 cm (0.5 μg/kg) by linearly extrapolating from the two concentrations at z = 250 cm and z = 150 cm. Note that if we do not do this extrapolation, the Excel tool will assign the concentration at z = 300 cm the same concentration at z = 250 cm, i.e., 1 μg/kg. Similarly, if we do not provide a concentration to z = 0 cm, the Excel tool will assign to it the concentration of the shallowest depth by default. After entering the depth-discrete concentrations, we select "Piecewise Linear Interpolation" to obtain the approximated soil PFOA concentration profile. The discrete concentration values and the interpolated approximate soil PFOA concentration profile are presented in Figure 5.

If lysimeter data are used to estimate the scaling factor (SF), the parameters described in Table 1 that are required to compute SF must first be provided in Box 1, together with an initial soil concentration profile. Before using the "Estimate SF" functional button with "Method 2" in Box 1, we first need to enter the information in the "Lysimeter Data" table at the bottom right of Box 4. Rows with both depth and porewater concentration are available are treated as valid inputs. Among the three effective depths (z = 20, 60, 100 cm bgs), both z = 20 cm and z = 100

cm have measured water contents, so all three columns (depth, porewater concentration, and water content) are used directly to calculate the scaling factor. At the intermediate depth (z = 60 cm bgs), no water content measurement is available; in this case, the water content in cell "F20" is used as an approximation. Finally, the local scaling factors at the three valid depths (fourth column) are computed. If the user selects "Method 2" under the "Estimate SF" option in Box 1, the arithmetic mean of these local SF values is returned in cell "F21".

We simulate 100 years of PFOA leaching and output the time series annually (see Figure 6). As mentioned in Table 4, to derive SSLs, the simulation time should be sufficiently long such that the mass discharge rate to groundwater reaches the maximum. In addition, concentration profiles at selected time points (t_p = 5, 10, 30, and 50 years) can also be generated, allowing for the evaluation of vertical leaching dynamics throughout the vadose zone. The acceptable groundwater concentration is set as $C_{gw,a}$ = 0.004 μg/L. We first conduct the simulations using the basic solver, and then employ the advanced solver to assess the potential impact of kinetic solid-phase sorption on PFOA leaching at the site.

⑤ Simulation Information			Parameter Values		
Simulation time (time series)*	t	yr	100		Basic Solver
Output time interval (time series)*	dt	yr	1		(Equilibrium solid-phase sorption)
Output time points (profiles)*	t_p	yrs	5,10,30,50		Advanced Solver
Acceptable groundwater concentration*	$C_{gw,a}$	ug/L	0.004		(Kinetic solid-phase sorption)

Figure 6: Module 0 input. Parameters for simulation information.

3.1.2 Results

We first go over the results computed by the basic solver that assumes equilibrium solid-phase sorption.

In the Output tab ("Module0_Output"), we can use the drop-down menu to view the 1) vadose-zone mass discharge rate of the entire contaminated site (μg/year) or the mass discharge rate of a unit area if the contaminated site area is set to 1 m^2, 2) mass remaining in the vadose zone (as % of the initial PFAS mass in the vadose zone), 3) PFAS concentration in a receptor well (μg/L) at the edge of the contaminated site. 4) Soil concentration profiles in the vadose zone, showing vertical distributions of PFAS total soil concentration at selected time points. 5) Aqueous concentration profiles in the vadose zone, showing vertical distributions of PFAS porewater concentration at selected time points. A screenshot for the plotted vadose-zone mass discharge rate is shown in Figure 7, while the soil concentration profile output is shown in Figure 8. Tabulated data of the results can also be downloaded as a .csv file by clicking "Download data".

NOTE: The mass discharge rate and receptor well groundwater concentrations were computed directly from the analytical solutions. The mass remaining in the vadose zone was obtained via numerical integration of the mass discharge charge over time, which may involve numerical errors due to time discretization. For an output timestep size of 1 year, the error can be up to one or two percent (i.e., the mass remaining can go slightly negative). The .csv output file only shows positive values for the mass remaining in the vadose zone.
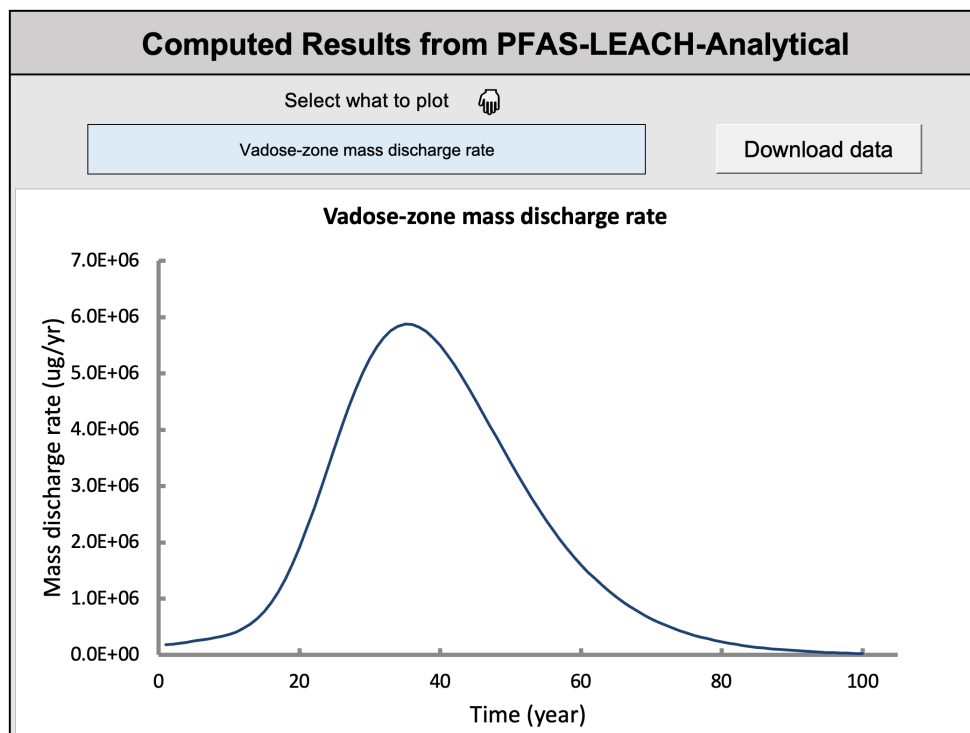
Figure 7: Module 0 output. Mass discharge rate computed from PFAS-LEACH-Analytical (basic solver). Users can use the drop-down menu to also display mass remaining in the vadose zone and PFAS concentration in a receptor well.
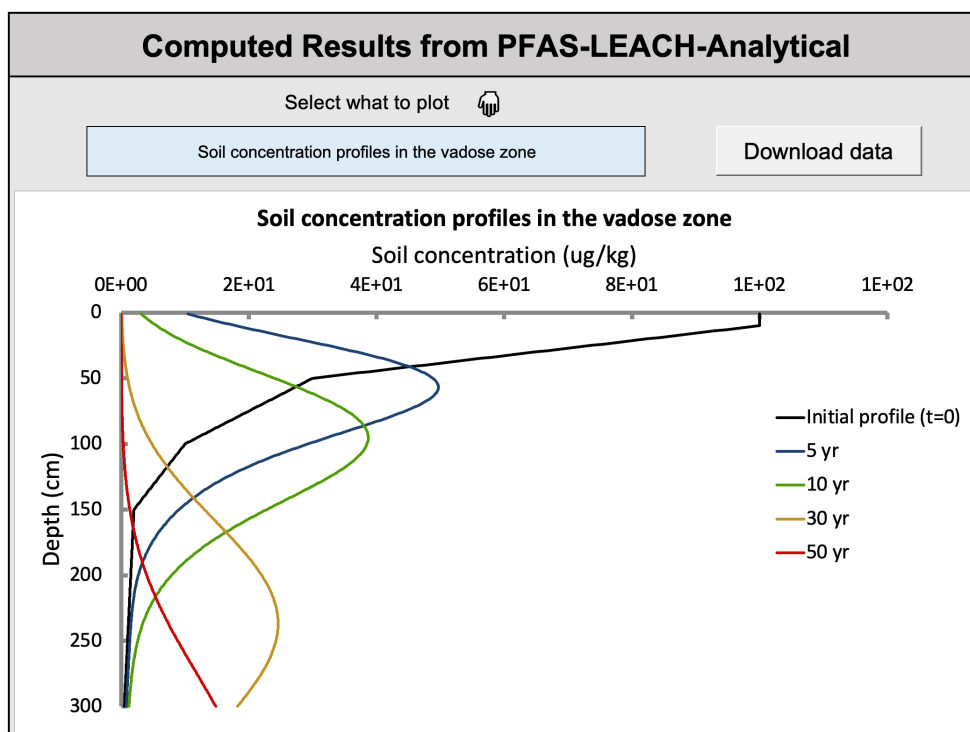

Figure 8: Module 0 output. PFAS soil concentration profiles at selected time points from PFAS-LEACH-Analytical (basic solver). Users can use the drop-down menu to also display PFAS aqueous concentration profiles in the vadose zone.

Soil Screening Levels			Values
Soil screening level (PFAS-LEACH-Analytical)	SSL_{Tier3}	ug/kg	6.66
Soil screening level (PFAS-LEACH-DAF)	SSL_{Tier4}	ug/kg	1.52
Soil screening level (USEPA Standard DAF)	$SSL_{EPA\ standard}$	ug/kg	0.42
Retardation, attenuation, and dilution factors (PFAS-LEACH-Analytical)			
Air–water interfacial retardation	R_{AW}	(-)	12.7
Solid–water interfacial retardation	R_S	(-)	3.9
Total retardation factor	R	(-)	17.6
Vadose-zone attenuation factor	AF_{VZ}	(-)	4.4
Dilution factor	DF	(-)	151.0
Estimated PFAS residence time	T_R	yr	44.6
Duration exceeding the acceptable groundwater concentration	$t_{gw,e}$	yr	64.0

Figure 9: Module 0 output. SSLs computed from PFAS-LEACH-Analytical (basic solver), PFAS-LEACH-DAF, and USEPA Standard DAF, and other important variables computed from PFAS-LEACH-Analytical (basic solver).

Additionally, the Output tab presents the PFOA SSLs computed from three approaches (Tier 3 model PFAS-LEACH-Analytical, Tier 4 model PFAS-LEACH-DAF, and USEPA standard DAF). The Excel tool also presents other important variables computed from the Tier 3 model PFAS-LEACH-Analytical, including the retardation, attenuation, and dilution factors, the estimated residence time for PFOA, and the duration over which the groundwater concentration at the receptor well exceeds the acceptable concentration. A screenshot of the results is presented in Figure 9.

Now, we run the advanced solver with kinetic solid-phase sorption. However, because the residence time of PFOA ($t_{\text{residence}} \sim \min(RZ_w\theta/I_f, RZ_w^2\theta/I_f/\alpha_L)$ = 44.6 years) is much greater than the half-life of kinetic solid-phase desorption $\sim 1/\alpha_s$ = 10,000 hours = 416.7 days, the results accounting for kinetic solid-phase sorption are only slightly different from those computed assuming equilibrium solid-phase sorption (Figure 10). Note that the advanced solver may be substantially slower than the basic solver. Users can monitor the simulation progress at the bottom left corner of the Excel user interface, which should display "Simulation progress: X% completed".
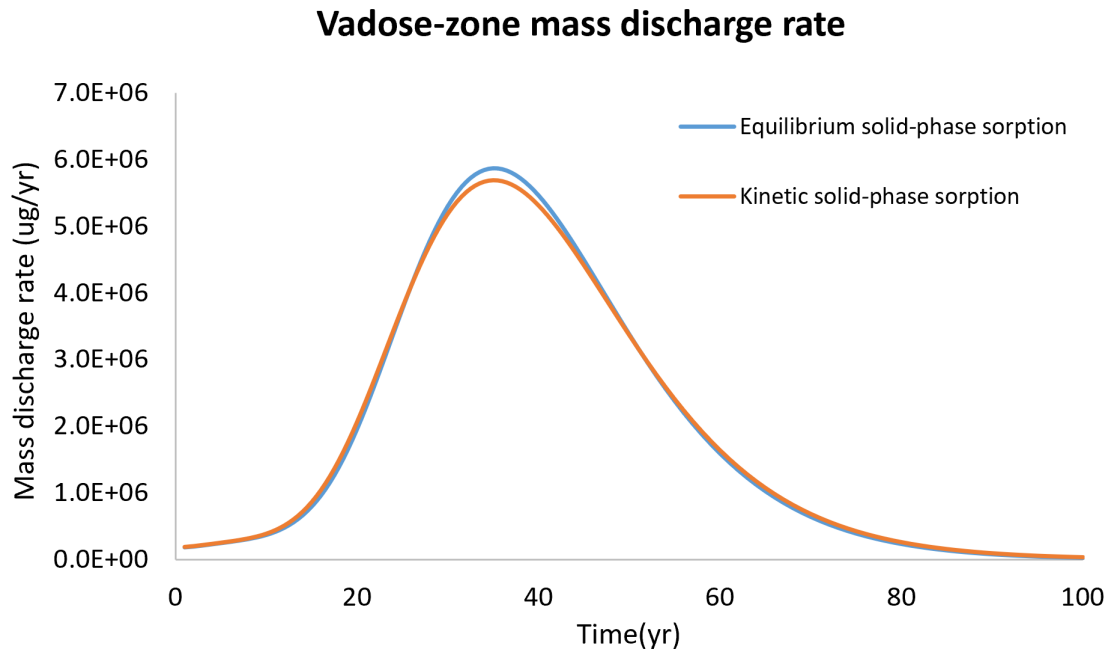
Vadose-zone mass discharge rate

Figure 10: Module 0 output. Simulated vadose-zone mass discharge rate by PFAS-LEACH-Analytical (equilibrium [basic solver] vs. kinetic solid-phase sorption [advanced solver]).

3.2 Example for Module 1

3.2.1 Inputs

Because we simulate the same case, all the input parameters are the same as those presented in Section 3.1 for Module 0. The only additional input information needed for Module 1 is the left and right bounds of the parameters.

For soil properties and site conditions, we assign 30% relative deviation for I_f and 15% relative deviation for n. Because we would like the left bound of the parameter to introduce smaller leaching rates and the right bound to introduce greater leaching rates, the left bound is set to n = 1.74 and the right bound is set to n = 1.28, i.e., the deviation is −15%. To focus on the sensitivity of these two parameters, we do not perturb the other parameters for soil properties and site conditions. The deviation for α_L, θ, SF, and A_{aw} is automatically computed from their estimation functions, in response to the deviation of I_f and n. Figure 11 shows a screenshot of the parameters for the soil properties and site conditions. However, users can also manually set the deviation for α_L, θ, SF, and A_{aw}, i.e., they do not have to be coupled with the deviation of the other blue-cell parameters. In fact, any of the input parameters can be perturbed independently to examine their impact on the final results.

For the parameters related to PFAS properties, we only perturb K_{aw} and we do so by manually setting the left bound to K_{aw} = 4.8 × 10^{-3} cm (i.e., smaller leaching) and the right bound to K_{aw} = 2.58 × 10^{-3} cm (i.e., greater leaching). In this case, the relative deviation is −30% for both bounds. Alternatively, users can set deviations for a, b, and σ_0, which will automatically compute a deviation for K_{aw}.

The parameters for groundwater dilution and simulation are kept unchanged, i.e., they

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are the same as those in the example in Module 0, except for *DF*. *DF* is a function of the net infiltration. The left bound is *DF* = 214.9 and the right bound is *DF* = 116.6. Because the Module 0 example showed that kinetic solid-phase sorption had a negligible impact on PFAS leaching in the vadose zone, here we focus on applying the basic solver that assumes equilibrium solid-phase sorption.

① Soil Properties and Site Conditions			Left bound		Median value	Right bound		Set Default Values
			% deviation from mean	value	median	value	% deviation from mean	
Depth to groundwater*	Z_w	cm			300			
Contaminated site area (or unit area)	A	cm^2			2500			
Temperature	T	°C			20.00			Soil Type
Net infiltration*	I_f	cm/yr	30	18.14	25.92	33.70	30	User defined
Soil bulk density*	ρ_b	g/cm^3	0	1.53	1.53	1.53	0	Set default deviation: 0%
Saturated hydraulic conductivity	K_s	cm/day	0	44.87	44.87	44.87	0	
Residual water content	θ_r	cm^3/cm^3	0	0.064	0.064	0.064	0	
Saturated water content*	θ_s	cm^3/cm^3	0	0.370	0.370	0.370	0	
Median grain size	d_{50}	cm	0	0.005	0.005	0.005	0	
Organic carbon fraction	f_{oc}	%	0	0.41	0.41	0.41	0	
van Genuchten parameter	α	cm^{-1}	0	0.018	0.018	0.018	0	
van Genuchten parameter	n	(-)	-15	1.74	1.51	1.28	-15	
Longitudinal dispersivity*	α_L	cm	0	13.42	13.42	13.42	0	Estimate α_L
Water content*	θ	cm^3/cm^3	19	0.178	0.219	0.280	28	Estimate θ
Air–water interfacial area scaling factor	SF	(-)	-8	5.08	4.73	4.19	-11	Estimate SF
Air–water interfacial area*	A_{aw}	cm^2/cm^3	-41	1060.9	753.9	342.4	-55	Estimate A_{aw}

Figure 11: Module 1 input. Parameters for soil properties and site conditions with left, median, and right bounds.

3.2.2 Results

Figure 12 shows a screenshot of the computed vadose-zone mass discharge rate of the entire contaminated site (μg/year) or the mass discharge rate of a unit area if the contaminated site area is set to 1 m^2, including the results computed from the left bound, median, and right bound of the parameter sets. The left-bound case (blue) represents sustained low leaching rates over a long period, indicating limited PFAS migration from the vadose zone. In contrast, the right-bound case (green) shows rapid leaching with an early sharp peak in mass discharge. The median case (yellow) falls between these two, with a moderate peak followed by a gradual decline. Figure 13 illustrates soil concentration profiles in the vadose zone after 10 years. In the left-bound case (blue), concentrations remain in the shallow depth and migrate very slowly. The right-bound case (green) reveals faster downward transport and leaching to deeper depth, while the median case (yellow) lies between the two, reflecting intermediate leaching behavior.
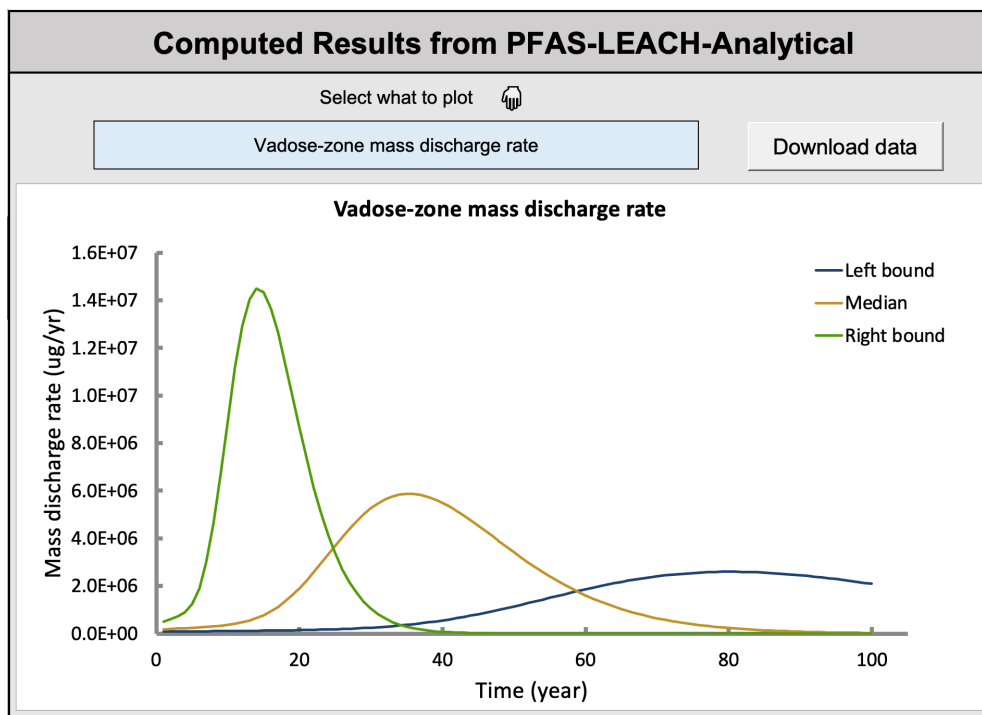
Figure 12: Module 1 output. Vadose-zone mass discharge rate computed from PFAS-LEACH-Analytical (basic solver). The three curves represent left-bound (blue), median (yellow), and right-bound (green) parameter sets.
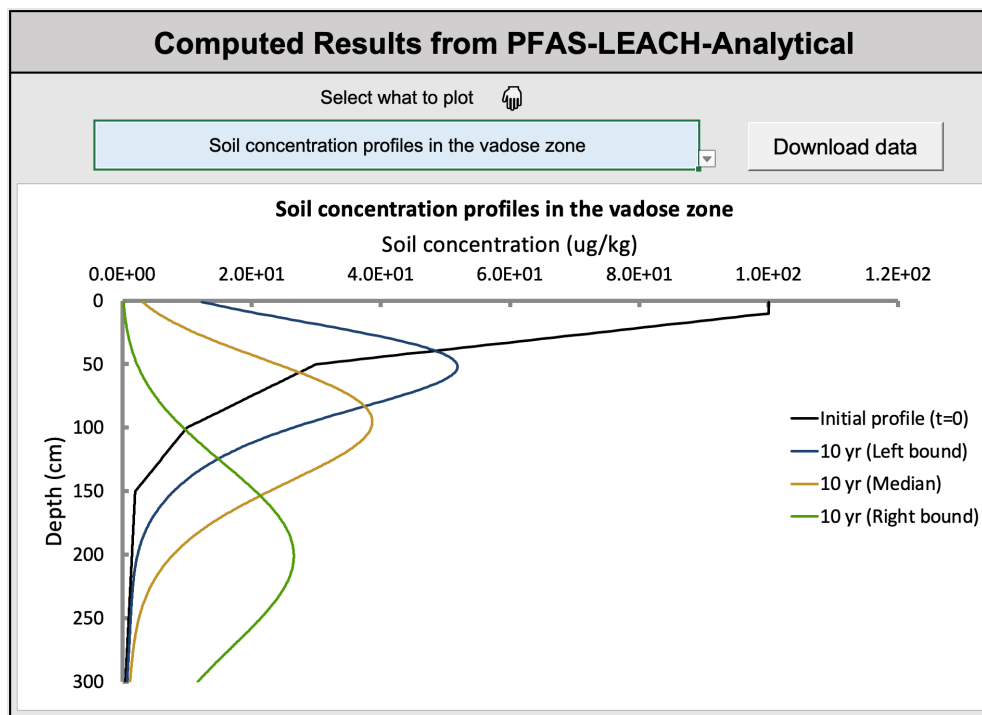

Figure 13: Module 1 output. Soil concentration profiles in the vadose zone after 10 years, computed from PFAS-LEACH-Analytical (basic solver). The three curves represent left-bound (blue), median (yellow), and right-bound (green) parameter sets.

Soil Screening Levels			Left bound	Median	Right bound
Soil screening level (PFAS-LEACH-Analytical)	SSL_{Tier3}	ug/kg	15.02	6.66	2.71
Soil screening level (PFAS-LEACH-DAF)	SSL_{Tier4}	ug/kg	3.44	1.52	0.62
Soil screening level (USEPA Standard DAF)	$SSL_{EPA\ standard}$	ug/kg	0.58	0.42	0.35
Retardation, attenuation, and dilution factors (PFAS-LEACH-Analytical)					
Air–water interfacial retardation	R_{AW}	(-)	28.6	12.7	3.2
Solid–water interfacial retardation	R_S	(-)	4.8	3.9	3.1
Total retardation factor	R	(-)	34.4	17.6	7.2
Vadose-zone attenuation factor	AF_{VZ}	(-)	4.4	4.4	4.4
Dilution factor	DF	(-)	214.9	151.0	116.6
Estimated PFAS residence time	T_R	yr	101.3	44.6	18.0
Duration exceeding the acceptable groundwater concentration	$t_{gw,e}$	yr	62.0	66.0	34.0

Figure 14: Module 1 output. SSLs computed from PFAS-LEACH-Analytical (basic solver), PFAS-LEACH-DAF, and USEPA Standard DAF, and other important parameters computed from PFAS-LEACH-Analytical (basic solver).

Figure 14 shows a screenshot of the derived SSLs and the other variables computed from PFAS-LEACH-Analytical. Note that because the left (or right) bound of the input parameters is defined such that they generate smaller (or greater) leaching (see discussion in Section 2.4), the "left bound" of the computed SSLs, retardation factors, attenuation and dilution factors is greater than their "median", while the "right bound" is smaller than their "median".

3.3 Example for Module 2

3.3.1 Inputs

For Module 2, users specify the "mean" and the "coefficient of variation" for each input parameter, based on prior knowledge, site-specific information, or published literature. CV is defined in the linear space regardless of whether the parameter follows a normal and a log-normal distribution. CV must be non-negative by definition. Together, these two sets of values form the basis for Monte Carlo sampling in Module 2 (Figures 15, 19, and 20). In this example, the mean values are set equal to those used in Module 0, except for the K_s, α, and n. The means and standard deviations for these three parameters were obtained from Rosetta using the same soil texture (70% sand, 20% silt, 10% clay) as in Module 0, and then converted from log space to linear space. In this way, the medium of K_s, α, and n in the Monte Carlo realizations would correspond to the values used in Module 0 and Module 1.

① Soil Properties and Site Conditions			Probability Distribution	Mean Values	Coefficient of Variation	Set Default Values
Depth to groundwater	Z_w	cm		300		
Contaminated site area (or unit area)	A	m^2		2500	Set Default CV	Soil Type
Temperature	T	°C		20.0		User defined
Net infiltration	I_f	cm/yr	Log$_{10}$ N	25.92	0.20	
Soil bulk density	ρ_b	g/cm^3	N	1.53	0.10	
Saturated hydraulic conductivity	K_s	cm/day	Log$_{10}$ N	45.36	0.15	
Residual water content	θ_r	cm^3/cm^3	N	0.064	0.12	
Saturated water content	θ_s	cm^3/cm^3	N	0.370	0.02	
Median grain size	d_{50}	cm	Log$_{10}$ N	0.005	0.20	
Organic carbon fraction	f_{oc}	%	Log$_{10}$ N	0.41	0.20	
van Genuchten parameter	α	cm^{-1}	Log$_{10}$ N	0.018	0.17	
van Genuchten parameter	n	(-)	Log$_{10}$ N	1.51	0.04	
Longitudinal dispersivity	α_L	cm	Log$_{10}$ N	13.42		Estimate α_L
Water content	θ	cm^3/cm^3	N	0.219		Estimate θ
Air–water interfacial area scaling factor	SF	(-)	Log$_{10}$ N	4.7		Estimate SF
Air–water interfacial area	A_{aw}	cm^2/cm^3	Log$_{10}$ N	753.9		Estimate A_{aw}

Figure 15: Module 2 input. Parameters for soil properties and site conditions with mean values and coefficient of variations.

For soil properties and site conditions (Figure 15), the coefficient of variation is given for I_f, ρ_b, K_s, θ_r, θ_s, d_{50}, f_{oc}, α, n, α_L. For θ, SF and A_{aw}, the coefficient of variation values are left blank, which automatically activates the built-in estimation function to compute their variabilities from the sampled values of the dark-orange soil parameters. The computed coefficient of variation value for θ, SF and A_{aw} will be returned after running the simulation.

To better understand and prepare parameter inputs, the Module2_ParaToolkit can be used to visualize sampling distributions. For example, when the mean and CV of θ_s and K_s are entered into the toolkit, the resulting probability density functions are shown in Figures 16 and 17, visualizing how the parameters are distributed under normal and log-normal distributions given the mean and CV values. In addition, the mean and standard deviation for some parameters may be reported in the log$_{10}$ space (e.g., some of the van Genuchten parameters estimated from Rosetta 3) in the literature. The conversion function provided in the toolkit (Figure 18) allows users to convert the mean and standard deviation values between log$_{10}$

and linear spaces, so that the linear-space parameters can be obtained and entered into the Module 2 input interface.
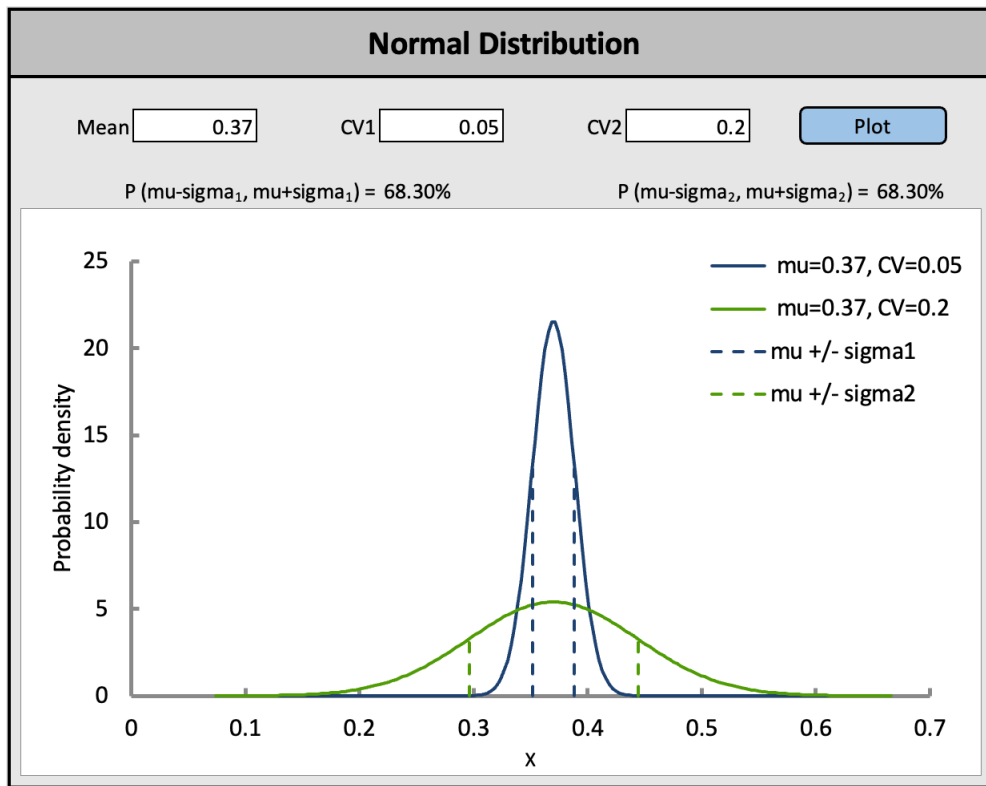

Figure 16: Visualization of the sampling distribution for θ_s under a normal distribution.
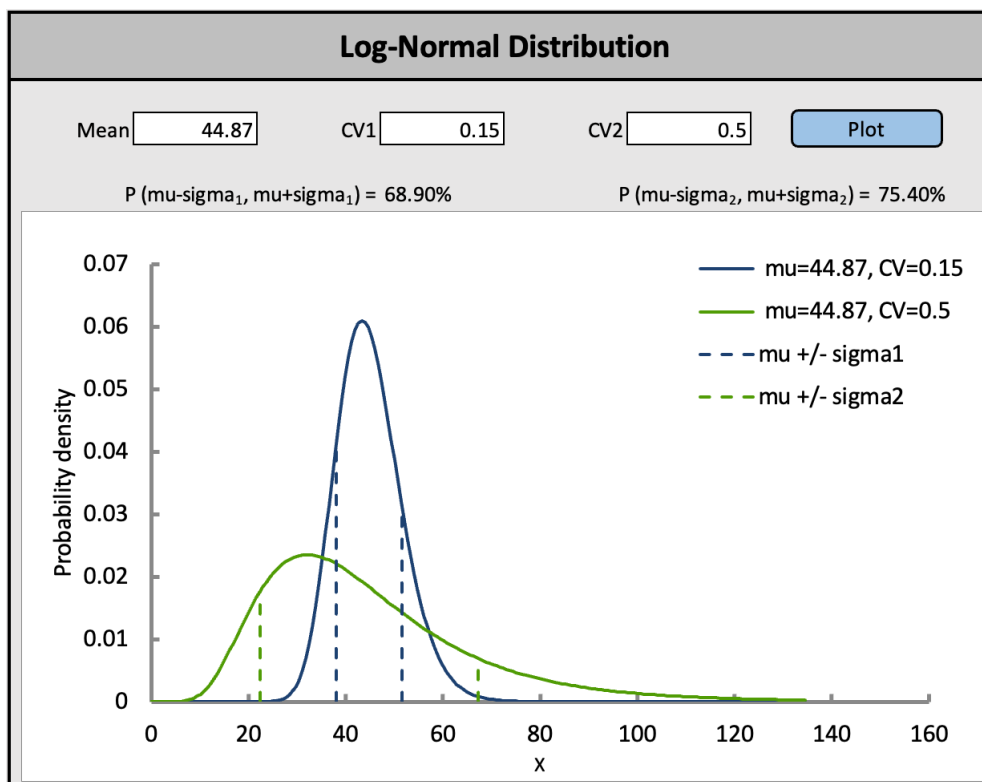
Log-Normal Distribution

Mean [44.87]   CV1 [0.15]   CV2 [0.5]   [Plot]

P (mu-sigma$_1$, mu+sigma$_1$) = 68.90%   P (mu-sigma$_2$, mu+sigma$_2$) = 75.40%

Legend:
— mu=44.87, CV=0.15
— mu=44.87, CV=0.5
– – mu +/- sigma1
– – mu +/- sigma2

Figure 17: Visualization of the sampling distribution for K_s under a log-normal distribution.

Conversion between (mu, sigma) and (mu$_{10}$, sigma$_{10}$)

Linear space

mu
[44.87]

sigma
[0.15]

CV
[0.003343]

$$\mu_{10} = (\ln(\mu) - (1/2)\ln(1 + \sigma^2/\mu^2))/\ln(10)$$

$$\sigma_{10} = \sqrt{\ln(1 + \sigma^2/\mu^2)}/\ln(10)$$

[(mu, sigma) -> (mu$_{10}$, sigma$_{10}$)]

[(mu, sigma) <- (mu$_{10}$, sigma$_{10}$)]

$$\mu = 10^{\mu_{10}}\exp(0.5(\sigma_{10}\ln(10))^2)$$

$$\sigma = \mu\sqrt{\exp((\sigma_{10}\ln(10))^2) - 1}$$

Log-Normal space

mu$_{10}$
[1.6519536]
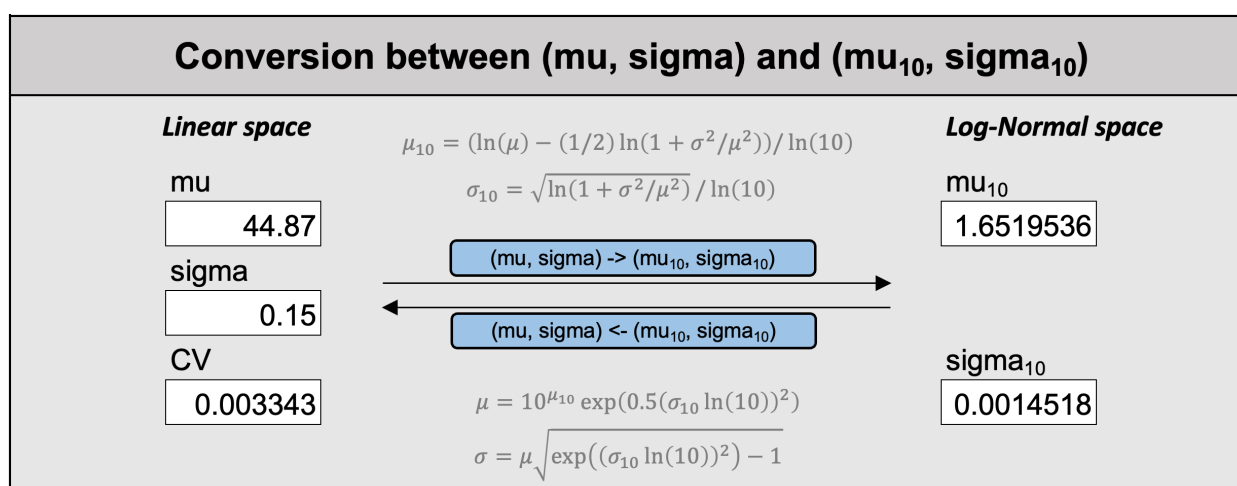
sigma$_{10}$
[0.0014518]

Figure 18: Conversion tool for translating parameter statistics between linear space and log$_{10}$-normal spaces.

For PFAS properties (Figure 19), CV values are assigned to a, b, D_0, and K_{oc}, and are left blank for K_d, and K_{aw}. Module 2 employs the basic solver (assuming equilibrium solid-phase sorption), so the values for F_s and α_s are not needed. Other parameters such as σ_0, M, and V_m are not assigned CV values, as they are treated as constants assuming negligible variability.

② PFAS Properties			Probability Distribution	Mean Values	Coefficient of Variation	
Surface tension parameter	a	mg/L	N	62.1	0.10	
Surface tension parameter	b	(-)	N	0.19	0.10	PFAS Type
Surface tension parameter	σ_0	dyn/cm		71.0		PFOA
Molar mass	M	g/mol		414.07		
Molecular diffusion coefficient	D_0	cm^2/s	N	4.90E-06	0.10	
Molar volume	V_m	cm^3/mol		237.20		
Organic carbon-water partition coefficient	K_{oc}	cm^3/g	Log$_{10}$ N	136.2	0.20	
Solid–phase adsorption coefficient	K_d	cm^3/g	Log$_{10}$ N	0.56		Estimate K_d
Air–water interfacial adsorption coefficient	K_{aw}	cm^3/cm^2	Log$_{10}$ N	3.69E-03		Estimate K_{aw}

Figure 19: Module 2 input. Parameters for PFAS properties with mean values and coefficient of variations.

For groundwater dilution (Figure 20), CV values are assigned to U_{gw}, L, and b_{sat}, but left blank for α_v, δ_{gw}, and DF. Their variability will be internally computed from the variability of the other groundwater dilution parameters (dark-orange cells) based on the estimation function. The computed coefficient of variation value (CV) for α_v, δ_{gw}, and DF will be returned after running the simulation.

③ Groundwater Dilution			Probability Distribution	Mean Values	Coefficient of Variation	
Groundwater darcy flux	U_{gw}	m/yr	Log$_{10}$ N	365.00	0.20	
Lateral site width	L	m	N	3.00	0.20	
Saturated zone thickness	b_{sat}	m	N	0.35	0.20	
Vertical dispersivity	α_v	m	Log$_{10}$ N	0.02		
Mixing zone thickness	δ_{gw}	m	N	0.32		Estimate α_v, δ_{gw}, DF
Dilution Factor	DF	(-)	Log$_{10}$ N	151.00		

Figure 20: Module 2 input. Parameters for groundwater dilution with mean values and coefficient of variations.

The simulation information is summarized in Figure 21. The total simulation time is 100 yr, and the time step for the time series output is 1 yr. The output time point for soil concentration profiles accepts a single value for one model run, which is set to t_p = 10 yr in this example. The acceptable groundwater concentration $C_{gw,a}$ is set to 0.004 μg/L for PFOA. The number of Monte Carlo realizations is set to 100, which determines the sample size for uncertainty analysis.

⑤ Simulation Information			Parameter Values		# of Monte Carlo simulations	100
Simulation time (time series)	t	yr	100			
Output time interval (time series)	dt	yr	1		Basic Solver	
Output time point (single profile)	t_p	yr	10		(Equilibrium solid-phase sorption)	
Acceptable groundwater concentration	$C_{gw,a}$	ug/L	0.004			

Figure 21: Module 2 input. Parameters for simulation information.

3.3.2 Results

Example results for the Monte Carlo simulations are presented in Figures 22 and 23.

Figure 22 shows the vadose-zone mass discharge rate for the entire contaminated site (μg/year) or, if the site area is set to 1 m^2, the discharge rate per unit area. It presents the vadose-zone mass discharge rate as a function of time. The gray lines represent individual Monte Carlo realizations, while the colored curves denote the representative percentiles. The percentiles are determined based on the ranking of leaching risk, such that the 5th percentile (blue line) corresponds to relatively low leaching risk, the median (orange line) represents the central tendency, and the 95th percentile (green line) reflects relatively high leaching risk. These results highlight the variability of PFAS leaching behavior, demonstrating how parameter uncertainty influences both the timing and magnitude of mass discharge from the vadose zone. Figure 23 shows the corresponding soil concentration profiles in the vadose zone after 10 years. The black line denotes the initial profile ($t = 0$), while the blue, orange, and green lines represent the 5th percentile, median, and 95th percentile profiles, respectively. These results illustrate the depth-dependent distribution of PFAS concentrations and how they evolve over time under parameter uncertainty.
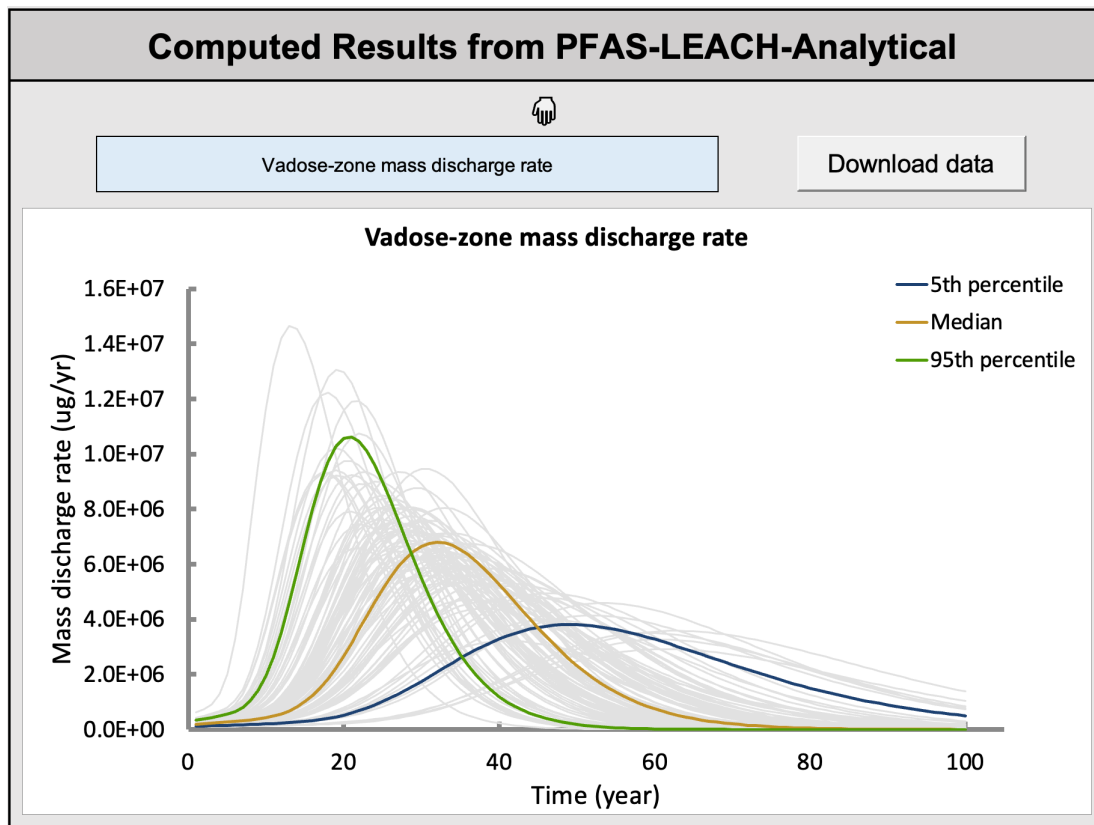

Figure 22: Module 2 output. Vadose-zone mass discharge rate computed with PFAS-LEACH-Analytical (basic solver). The gray lines represent individual Monte Carlo realizations, while the colored curves indicate the 5th percentile, median, and 95th percentile based on leaching risk ranking.
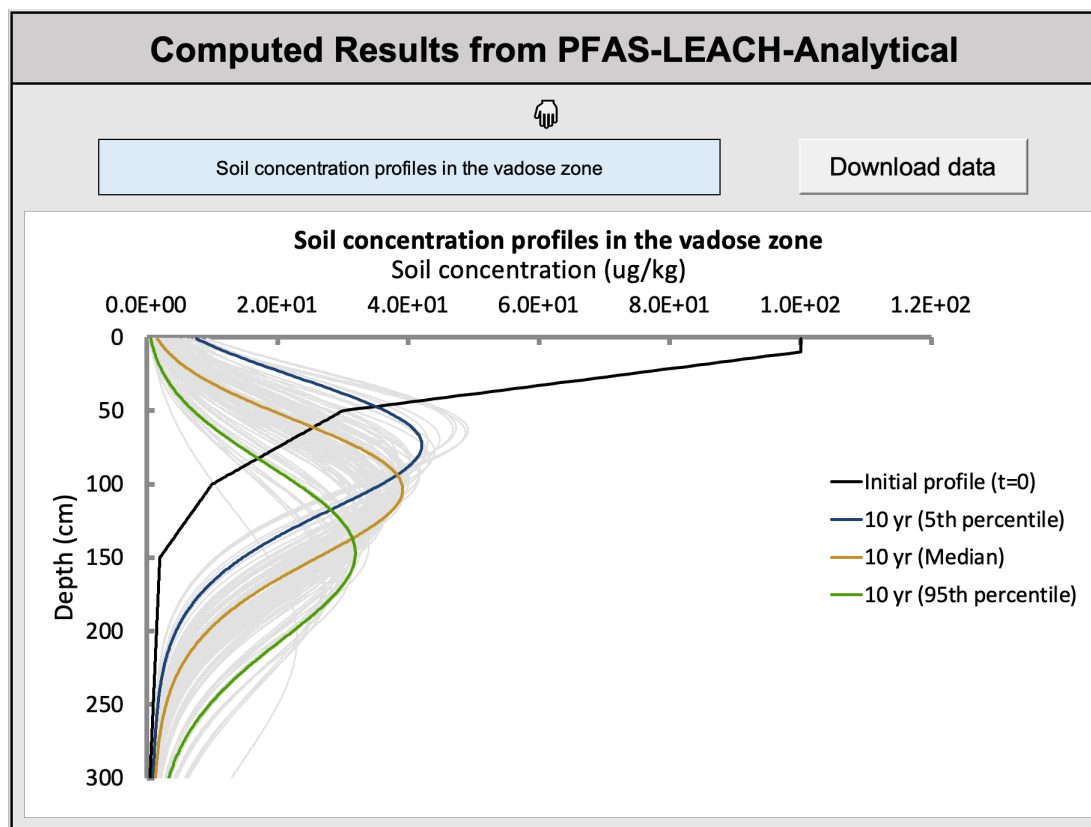
Figure 23: Module 2 output. Soil concentration profiles in the vadose zone computed with PFAS-LEACH-Analytical (basic solver). The black line indicates the initial profile (t = 0). Gray lines represent individual Monte Carlo realizations after 10 years, while the blue, orange, and green lines show the 5th percentile, median, and 95th percentile profiles based on leaching risk ranking.

Figure 24 summarizes the soil screening levels (SSLs) and the retardation, attenuation, and dilution factors computed from the Monte Carlo simulations by PFAS-LEACH-Analytical. The SSLs are reported as the 5th percentile, median, and 95th percentile values for all three approaches: PFAS-LEACH-Analytical (SSL_{Tier3}), PFAS-LEACH-DAF (SSL_{Tier4}), and the USEPA Standard DAF ($SSL_{EPA\ standard}$). The results show that SSL values decrease from the 5th to the 95th percentile, reflecting increasing leaching risk scenarios.

The lower panel displays additional variables computed with PFAS-LEACH-Analytical, including the air–water interfacial retardation (R_{AW}), solid–water retardation (R_S), total retardation factor (R), vadose-zone attenuation factor (AF_{VZ}), dilution factor (DF), PFAS residence time (T_R), and the duration exceeding the acceptable groundwater concentration ($t_{gw,e}$). Each parameter is reported as the 5th percentile, median, and 95th percentile, illustrating the uncertainty in SSL derivation arising from parameter variability. The spreads among percentiles vary across parameters: for instance, R_{AW} and DF show relatively wide ranges, highlighting the strong influence of interfacial retention and dilution on SSL variability, whereas AF_{VZ} appears less variable across the different percentiles. The estimated PFAS residence time (T_R) reflects leaching risk: longer T_R indicates prolonged persistence in the vadose zone and sustained potential for groundwater contamination, whereas shorter T_R suggests quicker migration but over a shorter exposure window. The duration exceeding the acceptable groundwater concentration indicates the duration of exposure under unacceptable risks.

Soil Screening Levels			5th Percentile	Median	95th Percentile
Soil screening level (PFAS-LEACH-Analytical)	SSL_{Tier3}	ug/kg	9.68	5.07	2.32
Soil screening level (PFAS-LEACH-DAF)	SSL_{Tier4}	ug/kg	2.16	1.15	0.56
Soil screening level (USEPA Standard DAF)	$SSL_{EPA\ standard}$	ug/kg	0.80	0.36	0.20
Retardation, attenuation, and dilution factors (PFAS-LEACH-Analytical)					
Air–water interfacial retardation	R_{AW}	(-)	14.3	9.2	5.5
Solid–water interfacial retardation	R_S	(-)	5.8	3.5	1.9
Total retardation factor	R	(-)	19.5	13.9	10.2
Vadose-zone attenuation factor	AF_{VZ}	(-)	4.8	4.4	4.1
Dilution factor	DF	(-)	230.2	135.9	74.1
Estimated PFAS residence time	T_R	yr	67.2	38.1	24.3
Duration exceeding the acceptable groundwater concentration	$t_{gw,e}$	yr	82.0	61.0	43.0

Figure 24: Module 2 output. SSLs computed from PFAS-LEACH-Analytical (basic solver), PFAS-LEACH-DAF, and USEPA Standard DAF, and other important parameters computed from PFAS-LEACH-Analytical (basic solver).

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