



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

Version 1.0-beta

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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.

Acknowledgement

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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 this user guide and 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.

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NOTE: This is a *preliminary* and *abbreviated* user guide to aid the beta testing of the Excel tool for the PFAS-LEACH Tier 3 and Tier 4 models. It focuses on providing the users with the operational steps for how to use the Excel tool. A full comprehensive version of the user guide that includes the underlying theories and technical details, more examples, and additional elaborations will be released in version 1.0.

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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.

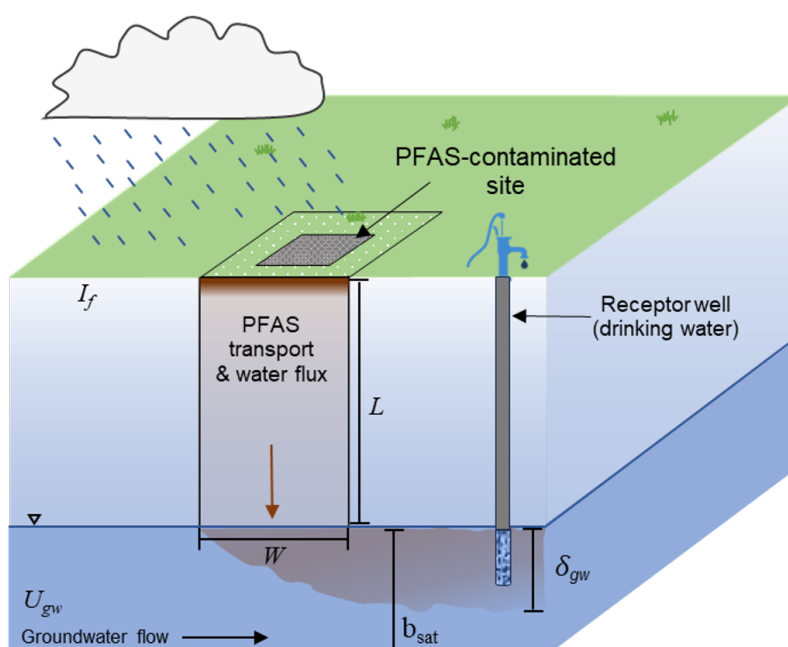


Figure 1: Conceptual diagram of the PFAS-LEACH-Analytical model presentation of PFAS leaching in the vadose zone and dilution in groundwater (Smith et al., 2024).

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), 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.

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.

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 soil bulk density. Descriptions for more generally how the input parameters can be estimated are presented in [Section 2](#).

What are Module0 and Module1 of the Excel tool?

The Excel tool includes two modules: *Module0* and *Module1*. *Module0* is the base model for quantifying PFAS leaching and deriving SSLs. *Module1* adds an additional capability of parameter sensitivity analysis. Each module includes an Input tab and an Output tab as user interfaces. We have also developed a *Module2* that adds the additional capacity for conducting Monte-Carlo-type uncertainty analysis (currently under internal testing), which will be included in the next release.

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.
- Homogenous, 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 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 ([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 in porewater concentrations as input parameters to estimate or constrain

air–water interfacial area, 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 to leverage 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

Module0 and *Module1* share the same structure of the user interface, with the only difference being that *Module1* includes an additional capability of parameter sensitivity analysis.

2.1.1 Overall structure of the user interface

Both *Module0* and *Module1* have a tab for input (e.g., “Module0_input”) and a tab for output (e.g., “Module0_output”). The *Input Screen* tab includes five sections to specify the input parameters for soil properties and site conditions, PFAS properties, groundwater dilution, initial PFAS soil concentration profile, and simulation information. Users should work through these five sections *sequentially* as entries in the later sections may depend on those in the earlier sections. We briefly introduce the five sections below.

- *Section 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).
- *Section 2 (PFAS Properties)* seeks input for the physicochemical parameters of the PFAS to determine their partitioning to air–water interfaces and solid–water interfaces.
- *Section 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 DAF approach for computing a site-specific dilution factor.
- *Section 4 (Initial PFAS Soil Concentration Profile)* specifies the initial concentration distribution of the PFAS in the soil profile. The initial soil concentration data can be arbitrary and with any spatial resolution.
- *Section 5 (Simulation Information)* inputs information to set up the simulation (e.g., simulation time, output time step, 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 the users.
- *Blue Cells*
These cells can be manually entered by the user. If the values are not available, these cells can be populated with default 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.

- *Yellow Cells*

These cells are only present in *Module1* and are for the user to input or adjust uncertainty bounds for the sensitivity analysis.

NOTE: 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.

2.2 Description of input parameters

Below we elaborate on the input parameters in each of the five sections to 4) in 'Module0_input' and 'Module1_input'. After that, we comment on the input parameters for the sensitivity analysis of Module1.

2.2.1 Soil properties and site conditions

Table 1: Input parameters for soil properties and site conditions

Parameter	Description
Depth to groundwater L (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.
Contaminated site area A (m ²)	PFAS-LEACH-Analytical is a 1D model, thus the computed mass discharge rate needs to multiply the lateral area of the contaminated site. Alternatively, the user can also set a unit area (i.e., 1 m ²) if desired, for example, when the mass discharge rates computed from PFAS-LEACH-Analytical are used as input for a groundwater flow and transport model (e.g., MODFLOW/MT3D-USGS).
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}).

Parameter	Description
Net infiltration rate I_f (cm/yr)	<p>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).</p> <p>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.</p> <p>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).</p>
Soil bulk density ρ_b (g/cm ³)	<p>The mass of oven-dry soil per unit volume of bulk soil, including both soil particles and pore spaces.</p> <p>If no measured values are available, ρ_b can be estimated by selecting a soil from the list of the eleven reference soil types.</p>
Saturated hydraulic conductivity K_{sat} (cm/day)	<p>If no measured values are available, K_{sat}, θ_r, θ_s, α, 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 bulk density.</p> <p>Various versions of the Rosetta model can be found here: https://soil-modeling.org/resources-links/model-portal/rosetta</p> <p>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.</p>
Residual water content θ_r (—)	See notes in the entry for “ K_{sat} ” for how to estimate if no measured values are available.
Saturated water content θ_s (—)	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 to estimate the A_{aw} scaling factor.
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.

Parameter	Description
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 the empirical model of Xu and Eckstein (1995) , i.e., $\alpha_L = 0.83[\log(L/100)]^{2.414}$ where L is the depth to groundwater. Note that the empirical model of Xu and Eckstein (1995) does not consider the dependence of α_L on water saturation.
Water content θ (—)	<p>Representative θ in the vadose zone, which may be measured by moisture probes such as time-domain reflectometer (TDR) probes or estimated from soil samples collected at the site.</p> <p>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 Module1 or Monte-Carlo analysis using the to-be-released Module2).</p>

Parameter	Description
Air–water interfacial area scaling factor $SF (-)$	<p>An empirical parameter to account for the additional air–water interfacial area not represented by the thermodynamic approach, e.g., due to the impact of microscale surface roughness of soil grains or other field-specific factors.</p> <p>The Excel tool provides an option to estimate the scaling factor caused by microscale surface roughness using an empirical equation reported by Brusseau (2023),</p> $SF = (-0.65S_w + 1.33)(-0.45d_{50} + 5),$ <p>where $S_w = \theta/\theta_s$ is water saturation and d_{50} is the soil median grain diameter (cm). 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 or silt fractions).</p> <p>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., $C_{soil} = \theta C_{aq} + \rho_b K_d C_{aq} + K_{aw} C_{aq} A_{aw}$. As such, A_{aw} can be estimated as</p> $A_{aw} = \frac{C_{soil} - \theta C_{aq} - \rho_b K_d C_{aq}}{K_{aw} C_{aq}},$ <p>where C_{soil} is soil PFAS concentration, θ is volumetric water content, C_{aq} is porewater PFAS concentration, ρ_b is soil bulk density, K_d is solid-phase adsorption coefficient, and K_{aw} is air–water interfacial adsorption coefficient. This approach assumes all of the parameters in the equation are available or can be estimated, and A_{aw} is the only unknown parameter.</p> <p>The air–water interfacial area A_{aw} estimated above corresponds to a specific water content (i.e., water saturation). We then estimate the scaling factor by taking the ratio between the porewater-estimated A_{aw} and that estimated by the thermodynamic approach. Because the scaling factor estimated above leverages in situ data in the field, it provides a means to potentially accounts 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).</p> <p>We note that for a conservative assessment of risks (i.e., overestimating PFAS leaching) at the contaminated site, users can simply assume that SF equals to 1.</p>

Parameter	Description
Air-water interfacial Area A_{aw} (cm ² /cm ³)	<p>The total area of the air–water interfaces per bulk unit volume of the soil.</p> <p>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) as</p> $A_{aw} = SF \frac{\phi}{\sigma_0} \int_{S_w}^1 p_c dS_w,$ <p>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 is capillary pressure, which is a function of water saturation via the van Genuchten model. Note that the standard thermodynamic-based approach (Leverett, 1941; Morrow, 1970) does not account for the impact of microscale surface roughness (i.e., $SF = 1$).</p>

2.2.2 PFAS properties

Table 2: Parameters for PFAS properties

Parameter	Description
Surface tension parameter a (mg/L)	<p>A fitting parameter of the Szyszkowski equation that describes the surface tension as a function of PFAS concentration in the aqueous solution.</p> <p>a, b, and σ_0 are used to determine the air–water interfacial adsorption coefficient K_{aw}.</p> <p>The Excel tool provides reference values for the three surface tension parameters for a list of 10 PFAS, which can be selected using the drop-down menu “PFAS type”. The list of PFAS with reference surface tension parameters may be expanded to cover a wider range of PFAS in the next release of the Excel tool.</p>
Surface tension parameter b (–)	<p>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.</p>
Surface tension parameter σ_0 (dyn/cm)	<p>Surface tension of the porewater when no PFAS is present. See notes in the entry for a for how this parameter is used.</p>

Parameter	Description
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.
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.
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.
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)	<p>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. For most contaminated sites and PFAS, it is usually a good approximation to use $C_{rep} = 0$ when estimating K_{aw}.</p> <p>The Excel tool provides reference values for the surface tension parameters for a list of 10 PFAS. When no surface tension parameters are available, the Excel tool has the option to estimate K_{aw} with the QSPR method.</p>
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

Parameter	Description
Groundwater darcy flux U_{gw} (m/yr)	Darcy velocity of the groundwater beneath the contaminated site.
Lateral site width W (m)	The lateral width of the contamination site parallel to the groundwater flow.
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 $\alpha_v = 0.0056W$.
Mixing zone thickness δ_{gw} (m)	<p>Computed estimate for the thickness of the groundwater mixing zone (m), which is calculated using the following equation</p> $\delta_{gw} = \sqrt{2\alpha_v W} + b_{sat} \left[1 - \exp \left(\frac{-I_f W}{U_{gw} b_{sat}} \right) \right].$ <p>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.</p>
Dilution Factor DF (—)	<p>It's used to estimate the extent to which contaminants leached from soil are diluted after entering groundwater, which is calculated by the following equation</p> $DF = 1 + \frac{U_{gw} \delta_{gw}}{I_f W}.$

2.2.4 Initial PFAS soil concentration profile

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 as a function of the depth).

Often, soil samples are only collected at a limited number of depth locations. In the Excel tool, users can provide soil PFAS concentrations at an arbitrary number of depth locations. The depth is rounded to 1 cm. The discrete soil concentrations are then interpolated in space to obtain an approximate soil concentration profile at the resolution of 1 cm. Two methods are provided for the spatial interpolation (piecewise constant and piecewise linear) of which users can select via the drop-down menu of "Interpolation methods".

Please note the following when entering the soil concentration data:

- Depth below land surface should not exceed the total depth to groundwater (L).
- Users are recommended to input soil PFAS concentrations at $z = 0$ and $z = L$. If they are not available, users can provide estimates. If no values are provided by the user, soil PFAS concentrations at $z=0$ and $z=L$, 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 30 depth-discrete PFAS soil concentration data points.

2.2.5 Simulation information

Table 4: Parameters for simulation information

Parameter	Description
Simulation time t (yr)	Total simulation time.
Output time interval dt (yr)	The temporal resolution of the output time series (e.g., groundwater mass discharge rate).
Acceptable groundwater concentration $C_{gw,a}$ (ng/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 Module1 sensitivity analysis

Most of the input parameters for soil properties and site conditions, PFAS properties, and groundwater dilution can be perturbed 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 mean, depending on whether the parameter positively or negatively correlate with leaching. For example, the 'left' bound for A_{aw} is greater than the mean while the right bound is smaller than the mean. In this case, the relative deviations for both the left and right bounds are negative.

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, 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.

Table 5: Functional Buttons

Functional Button	Required Parameters	Description
Estimate α_L Estimate α_L	L	α_L is approximated using the empirical model of Xu and Eckstein (1995) , i.e., $\alpha_L = 0.82[\log(L/100)]^{2.446}$ where L is the depth to groundwater. The empirical model of Xu and Eckstein (1995) does not consider the dependence of α_L on water saturation.
Estimate θ Estimate θ	$\theta_r, \theta_s, I_f, K_{sat}, n$	<p>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.</p> <p>Users should note that 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 (Module1) or Monte-Carlo analysis (Module2).</p>

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} , θ , ρ_b , K_d , C_{aq} , K_{aw} , C_{aq}	<p>The A_{aw} scaling factor approximates the impact of microscale grain surface roughness on air–water interfacial area. Approach 1: It is estimated using an empirical equation reported by Brusseau (2023),</p> $SF = (-0.65S_w + 1.33)(-0.45d_{50} + 5),$ <p>where d_{50} is the soil median grain diameter (cm). Approach 2: This method allows users to input up to 10 sets of lysimeter-measured porewater concentrations and corresponding water contents at different depths. Note: All three values (depth, concentration, and water content) must be provided for each row; otherwise, that row will be ignored. An SF value is calculated for each valid row using,</p> $A_{aw} = \frac{C_{soil} - \theta C_{aq} - \rho_b K_d C_{aq}}{K_{aw} C_{aq}},$ <p>and the final output shown in the interface is the average of all calculated SF values.</p>
Estimate A_{aw} Estimate A_{aw}	θ_r , θ_s , n , θ , α , σ_0 , SF	<p>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</p> $A_{aw} = SF \frac{\phi}{\sigma_0} \int_{S_w}^1 p_c dS_w,$ <p>where $S_w = \theta/\theta_s$ is water saturation. $\phi = \theta_s$ is soil porosity. σ_0 is the surface tension. p_c 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., $SF = 1$).</p>

Name	Required Parameters	Description
Estimate K_d Estimate K_d	f_{oc}, K_{oc}	Linear solid-phase sorption coefficient. K_d is estimated as $K_d = f_{oc}K_{oc}$ assuming that hydrophobic interaction is the primary mechanism for solid-phase sorption.
Estimate K_{aw} Estimate K_{aw}	$T, M, V_m, a, b, \sigma_0, C_r$ a representative porewater 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. 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 : $K_{aw} = 0.0253V_m - 8.3777$
Estimate $\alpha_v, \delta_{gw}, DF$ Estimate $\alpha_v, \delta_{gw}, DF$	I_f, U_{gw}, W, b_{sat}	<p>The dilution factor (USEPA, 1996) can be computed as</p> $DF = 1 + \frac{U_{gw}\delta_{gw}}{I_f W},$ <p>where U_{gw} is the groundwater Darcy velocity (m/yr). I_f represents annual net infiltration (m/yr). W is the lateral width of the contamination site (m). δ_{gw} represents a computed estimate for the thickness of the groundwater mixing zone (m), which is calculated using the following equation</p> $\delta_{gw} = \sqrt{2\alpha_v W} + b_{sat} \left[1 - \exp\left(\frac{-I_f W}{U_{gw} b_{sat}}\right) \right],$ <p>where the vertical groundwater dispersivity α_v is estimated as $0.0056W$, and b_{sat} represents the saturated thickness of the water-bearing unit (m). 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. By definition, δ_{gw} cannot exceed b_{sat}.</p>

Name	Required Parameters	Description
Basic solver 	Parameters with an asterisk (and optionally other parameters)	<p>The basic solver assumes equilibrium solid-phase sorption.</p> <p>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'.</p>
Advanced solver 	Parameters with an asterisk (and optionally other parameters)	<p>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 $1/\alpha_s$ 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.</p> <p>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 ($t_{\text{residence}} \sim \min(RL\theta/I_f, RL^2\theta/I_f/\alpha_L)$) and compare with α_s to assess if it is necessary to use the advanced solver.</p> <p>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'.</p>

2.4 Navigating the Outputs

The Output tab for Module0 and Module1 ('Module0_Output' and 'Module1_Output') both includes two parts.

The first part consists of time series of three computed variables:

- Vadose-zone mass discharge rate of the entire contaminated site ($\mu\text{g}/\text{year}$) or the mass discharge rate of a unit area if the contaminated site area is set to 1 m^2 . 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 m^2). 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 ($\mu\text{g}/\text{L}$) at the edge of the contaminated site.

These time series 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. For example, the mass discharge rates data can be used as input in a groundwater flow and transport

model (e.g., MODFLOW/MT3D-USGS) to further assess PFAS transport in the saturated zone. **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.

In this Excel tool, 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 resulting concentration time series can be used as a source type—specifically, an arbitrary inflow concentration defined by a set of points—to establish time-varying boundary conditions in the ATRANS software. ATRANS then provides exact 3D analytical solutions for solute transport from a patch boundary condition within a semi-infinite saturated aquifer.

The second part presents the SSLs derived via three methods:

- SSL (PFAS-LEACH-Analytical) is the SSL derived from PFAS-LEACH-Analytical. It accounts for the attenuation of PFAS in the vadose zone and dilution in groundwater. The SSL can be written as

$$SSL_{\text{PFAS-LEACH-Analytical}} = C_{gw,a} \times AF_{vz} \times DF \times [K_d + (K_{aw}A_{aw} + \theta_w) \frac{1}{\rho_b}], \quad (1)$$

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, which represents the PFAS-specific attenuation processes in the vadose zone. $C_{gw,a}$ is an acceptable concentration in a groundwater receptor well, DF (-) is the dilution factor in groundwater, K_d is the solid-phase sorption coefficient, K_{aw} is the air–water interfacial adsorption coefficient, A_{aw} is the specific air–water interfacial area, θ_w is volumetric water content (-), and ρ_b 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 (PFAS-LEACH-DAF) is derived using the model 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

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

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

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

Additionally, the second part presents the retardation, attenuation, and dilution factors computed from 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 pore-water 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, $AF_{vz} = C_{pore,max}/C_{leach,max}$. Here, $C_{pore,max}$ is the highest measured initial porewater concentration of PFAS within the unsaturated zone, and $C_{leach,max}$ represents the peak PFAS concentration in the aqueous phase at the bottom boundary of the vadose zone (i.e., the leachate that would enter the groundwater), derived from the simulation results.
- 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 $t_{residence} \sim \min(RL\theta/I_f, RL^2\theta/I_f/\alpha_L)$.
- Duration exceeding the acceptable groundwater concentration, which is the time period during which the groundwater concentration in the receptor well exceeds $C_{gw,a}$.

Compared to Module0, Module1 has the additional capability to conduct sensitivity analysis. Its Output tab ("Module1_Output") also presents the results computed using the left and right bounds of the input parameters. **NOTE:** 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 mean, while the right bound is smaller than their mean.

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 two examples (one example for each module) to illustrate how to use the Module0 and Module1. The same case will be used for the two examples with the only difference being that the example for Module1 conducts an additional sensitivity analysis.

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 Module0

3.1.1 Inputs


① Soil Properties and Site Conditions			Parameter Values	Set Default Values
Depth to groundwater*	L	cm	300	<div>Soil Type </div> <div>User defined</div>
Contaminated site area (or unit area)	A	m ²	2500	
Temperature	T	°C	20.0	
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	(-)	0.064	
Saturated water content	θ_s	(-)	0.370	
Median grain size	d_{50}	cm	0.0460	
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	13.91	Estimate α_L
Water content*	θ	(-)	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	751.2	Estimate A_{aw}

Figure 2: Module0 input. Parameters for soil properties and site conditions.

For soil properties and site conditions, we have directly available values for the following parameters: L , 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 $\rho_b = 1.53$, we use [Rosetta 3](#) to estimate $K_s = 44.87$ cm/day, $\theta_r = 0.064$, $\theta_s = 0.37$, $\alpha = 0.018$, $n = 1.509$.
- α_L , θ , SF , and A_{aw} can be estimated using the functional buttons on the right (details of the functions are available in Table 5). **NOTE:** 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	Set Default Values
Surface tension parameter	a	mg/L	62.1	PFAS Type  PFOA
Surface tension parameter	b	(-)	0.19	
Surface tension parameter	σ_0	dyn/cm	71.0	
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: F_s 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: Module0 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 $\alpha_s = 1/10,000 \text{ hour}^{-1}$. 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	Estimate α_v , δ_{gw} , DF
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	
Dilution Factor*	DF	(-)	151.0	

Figure 4: Module0 input. Parameters for groundwater dilution.

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

at the site. Following the approach described in Table 5, α_v , δ_{gw} , and DF are estimated using the functional button on the right.

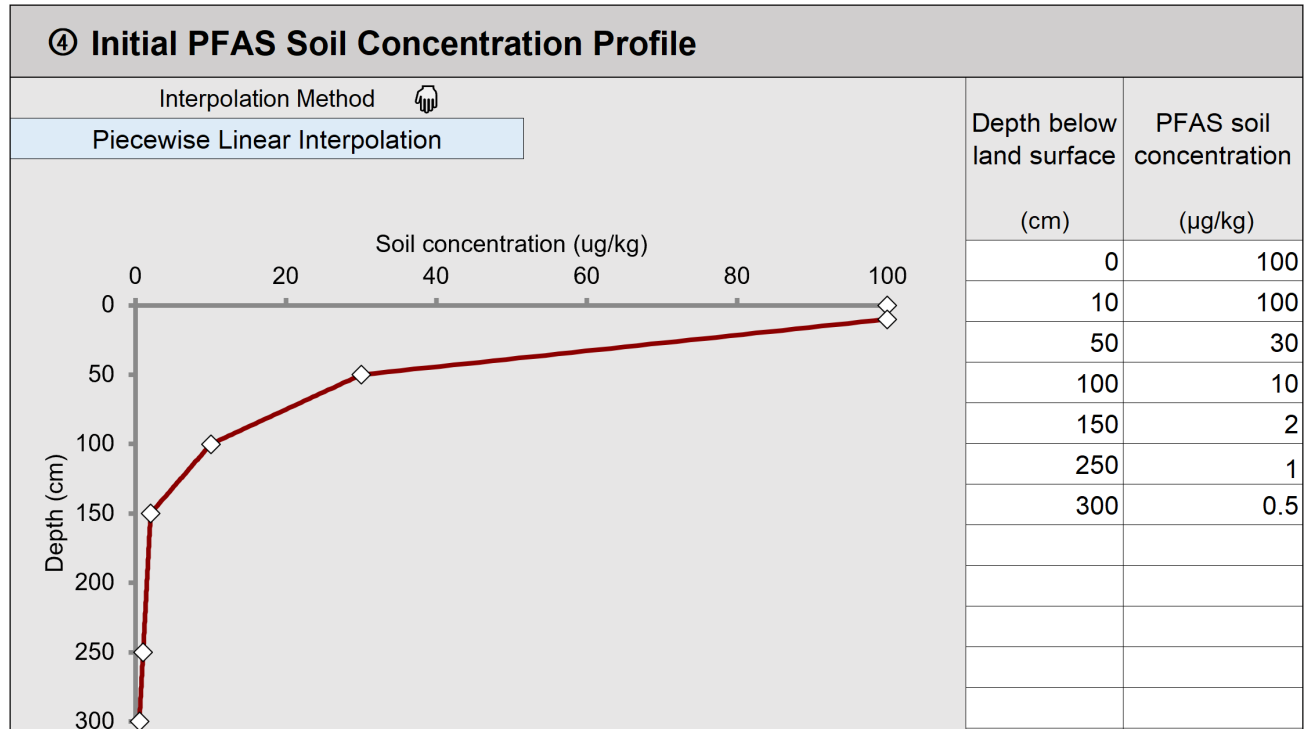


Figure 5: Module0 input. Parameters for initial PFAS soil concentration profile.

We have PFOA soil concentrations measured at 7 depth locations ($z = 10, 50, 100, 150, 250$ cm). The PFOA concentration at $z = 0$ cm is approximated as $100 \mu\text{g/kg}$ by assuming that it is the same as the concentration at $z = 10$ cm. We obtain the PFOA concentration at $z = 300$ cm ($0.5 \mu\text{g/kg}$) 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., $1 \mu\text{g/kg}$. 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.

We simulate 100 years of PFOA leaching and output the time series annually (see Figure 6). 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 transport dynamics throughout the vadose zone. The acceptable groundwater concentration is set as $C_{gw,a} = 4 \text{ ng/L}$. 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.

3.1.2 Results

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

⑤ Simulation Information			Parameter Values	Basic Solver (Equilibrium solid-phase sorption)
Simulation time (time series)*	t	yr	100	Advanced Solver (Kinetic solid-phase sorption)
Output time interval (time series)*	dt	yr	1	
Output time points (profiles)*	t_p	yr	5,10,30,50	
Acceptable groundwater concentration*	$C_{gw,a}$	ng/L	4	

Figure 6: Simulation information.

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 ($\mu\text{g}/\text{year}$) 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 ($\mu\text{g}/\text{L}$) at the edge of the contaminated site. 4) Aqueous concentration profiles in the vadose zone, showing vertical distributions of PFAS porewater concentration at selected time points, 5) Soil concentration profiles in the vadose zone, showing vertical distributions of PFAS total soil 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.

Additionally, the Output tab presents the PFOA SSLs computed from three approaches (PFAS-LEACH-Analytical, PFAS-LEACH-DAF (revised USEPA), and USEPA standard DAF). The Excel tool also presents other important variables computed from 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 ($t_{\text{residence}} \sim \min(RL\theta/I_f, RL^2\theta/I_f/\alpha_L) = 44.5$ years) is much greater than $1/\alpha_s = 10,000$ 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 user interface, which should display ‘Simulation progress: x% completed’.

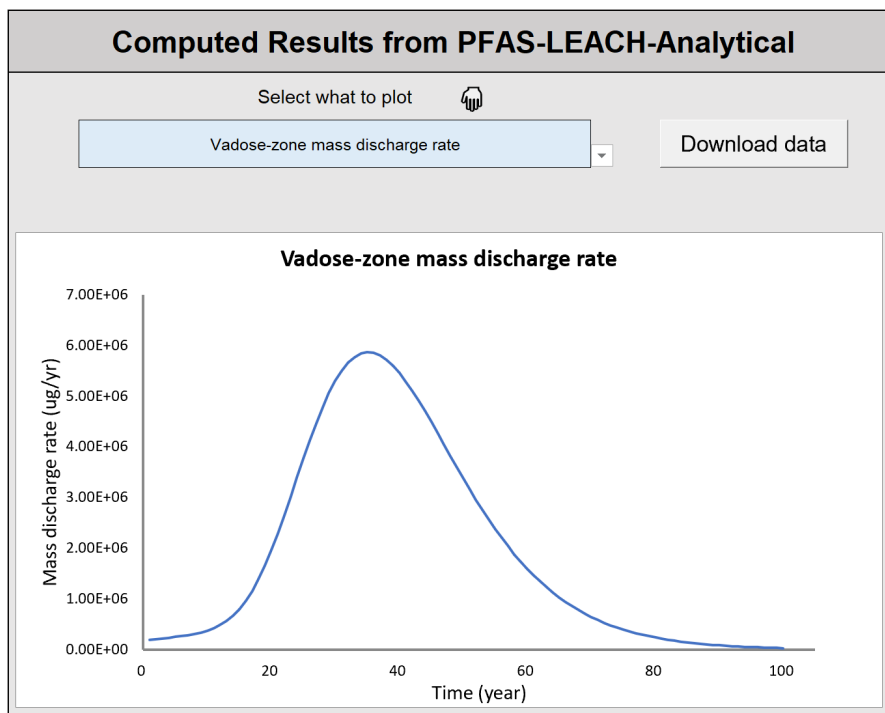


Figure 7: Module0 output. Mass discharge rate computed from PFAS-LEACH-Analytical (basic solver). Users can use the drop-down menu to also display mass remaining in the vadose zone and PFAS concentration in a receptor well.

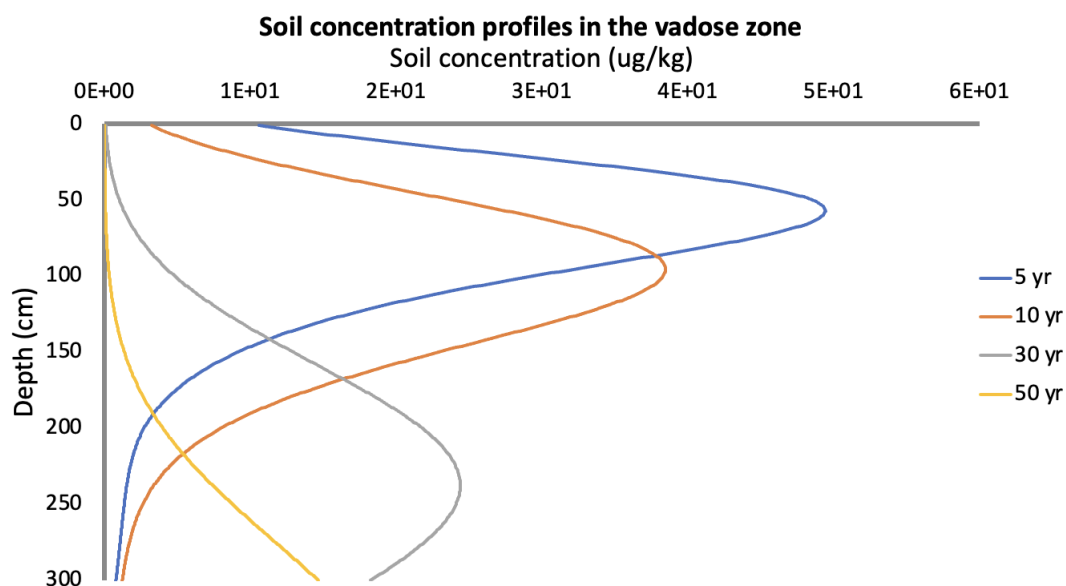


Figure 8: Module0 output. PFAS soil concentration profiles at selected time points from PFAS-LEACH-Analytical (basic solver). Users can use the drop-down menu to also display PFAS aqueous concentration profiles in the vadose zone.

Soil Screening Levels			Values
Soil screening level (PFAS-LEACH-Analytical)	SSL	ug/kg	6.9
Soil screening level (PFAS-LEACH-DAF)	$SSL_{EPA\ revised}$	ug/kg	1.5
Soil screening level (USEPA Standard DAF)	$SSL_{EPA\ standard}$	ug/kg	0.4
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}	(-)	4.6
Dilution factor	DF	(-)	151.0
Estimated PFAS residence time	T_R	yr	44.5
Duration exceeding the acceptable groundwater concentration	$t_{gw,e}$	yr	66.0

Figure 9: Module0 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).

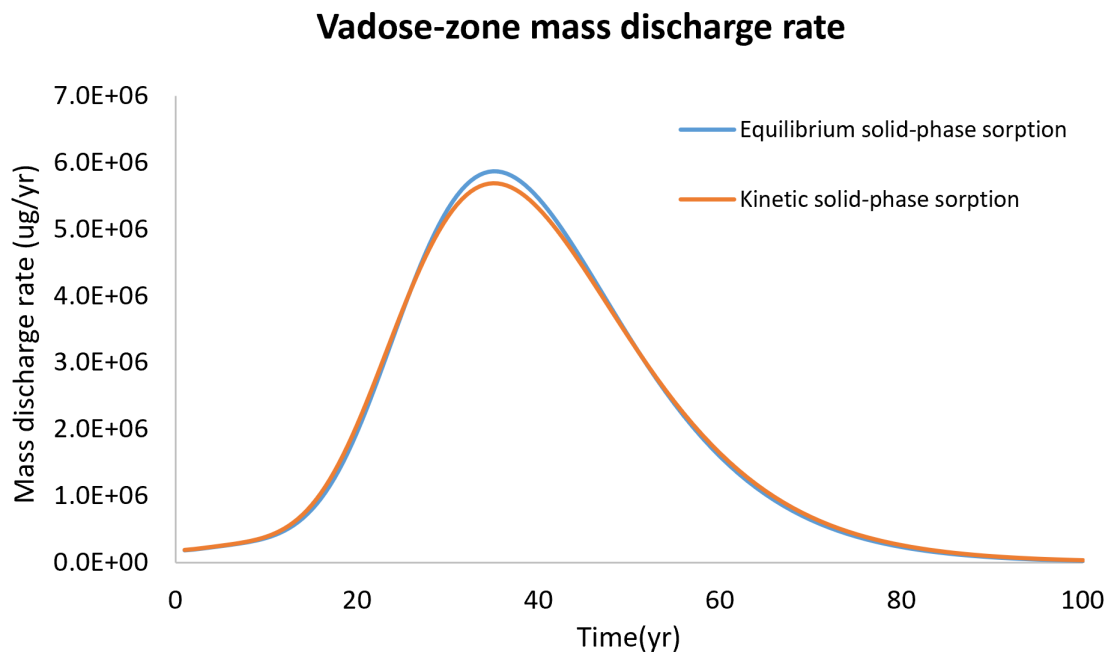


Figure 10: Module0 output. Simulated mass discharge rate by PFAS-LEACH-Analytical (equilibrium vs. kinetic solid-phase sorption).

3.2 Example for Module1

3.2.1 Inputs

Because we consider the same case for Module1, all the input parameters are the same as those presented in Section 3.1 for Module0. The only additional input information needed for Module1 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 $K_{aw} = 4.8 \times 10^{-3}$ cm (i.e., smaller leaching) and the right bound to $K_{aw} = 2.58 \times 10^{-3}$ cm (i.e., greater leaching). In this case, the relative deviation is -30% for both bounds. Alternatively, users can set deviations to 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 are the same as those in the example in Module0. Because the Module0 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		Mean value	Right bound		Set Default Values
			% deviation from mean	value	mean	value	% deviation from mean	
Depth to groundwater*	L	cm			300			Soil Type User defined Set default deviation: 0% Estimate α_L Estimate θ Estimate SF Estimate A_{aw}
Contaminated site area (or unit area)	A	cm ²			2500			
Temperature	T	°C			20.0			
Net infiltration*	I_f	cm/yr	30	18.14	25.92	33.70	30	
Soil bulk density*	ρ_b	g/cm ³	0	1.53	1.53	1.53	0	
Saturated hydraulic conductivity	K_s	cm/day	0	44.87	44.87	44.87	0	
Residual water content	θ_r	(-)	0	0.064	0.064	0.064	0	
Saturated water content	θ_s	(-)	0	0.370	0.370	0.370	0	
Median grain size	d_{50}	cm	0	0.0460	0.0460	0.0460	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	13.91	13.91	13.91	0	
Water content*	θ	(-)	19	0.178	0.219	0.280	28	
Air–water interfacial area scaling factor	SF	(-)	-8	5.07	4.71	4.18	-11	
Air–water interfacial area*	A_{aw}	cm ² /cm ³	-41	1057.0	751.2	341.2	-55	

Figure 11: Module1 input. Parameters for soil properties and site conditions.

3.2.2 Results

Figure 12 shows a screenshot of the computed vadose-zone mass discharge rate of the entire contaminated site, including the results computed from the left bound, mean, and right bound of the parameter sets.

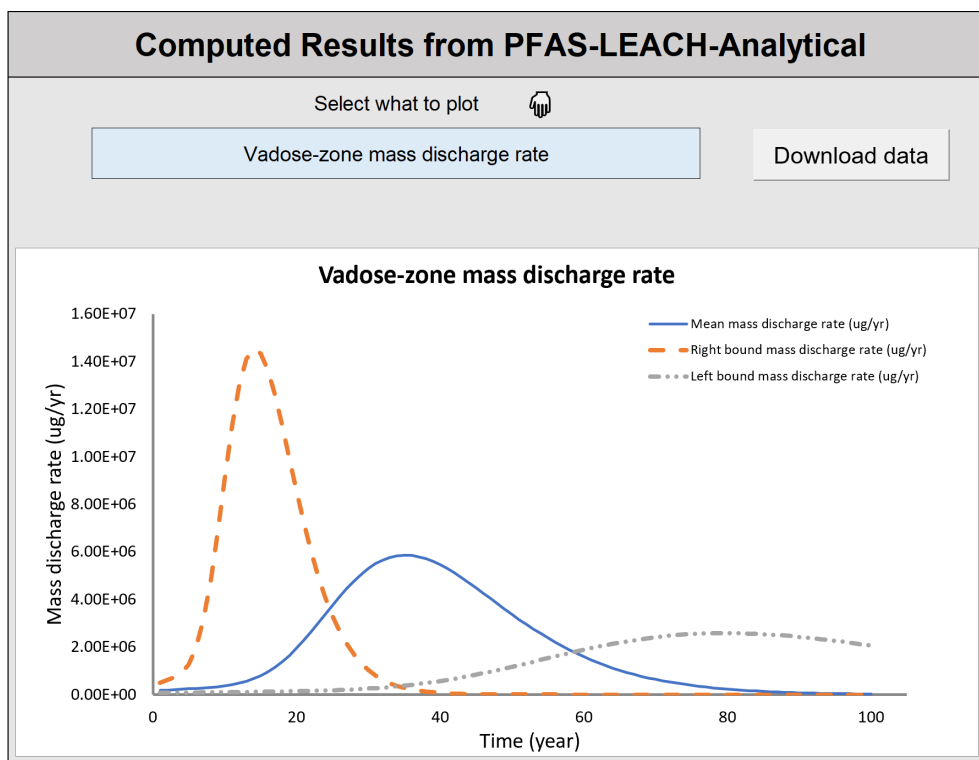


Figure 12: Module1 output. Mass discharge rate computed from PFAS-LEACH-Analytical (basic solver).

Figure 13 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 'mean', while the 'right bound' is smaller than their 'mean'.

Soil Screening Levels			Left bound	Mean	Right bound
Soil screening level (PFAS-LEACH-Analytical)	SSL	ug/kg	15.6	6.9	2.8
Soil screening level (PFAS-LEACH-DAF)	$SSL_{EPA\ revised}$	ug/kg	3.4	1.5	0.6
Soil screening level (USEPA Standard DAF)	$SSL_{EPA\ standard}$	ug/kg	0.6	0.4	0.3
Retardation, attenuation, and dilution factors (PFAS-LEACH-Analytical)					
Air–water interfacial retardation	R_{AW}	(-)	28.5	12.7	3.2
Solid–water interfacial retardation	R_S	(-)	4.8	3.9	3.1
Total retardation factor	R	(-)	34.3	17.6	7.2
Vadose-zone attenuation factor	AF_{VZ}	(-)	4.6	4.6	4.6
Dilution factor	DF	(-)	214.9	151.0	116.6
Estimated PFAS residence time	T_R	yr	100.9	44.5	17.9
Duration exceeding the acceptable groundwater concentration	$t_{gw,e}$	yr	62.0	66.0	33.0

Figure 13: Module1 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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