User's Guide: the ESTCP-PFAS-LEACH Tier 2 Model (PFAS-LEACH-Numerical-1D)

Beta Version

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How to cite

The Tier 2 PFAS-LEACH-Numerical-1D model was developed based on the modeling framework and numerical approaches described in Guo et al. (2020) and Zeng et al. (2021). If you use the Tier 2 model, please cite the following respective references.

- Zeng, J., & Guo, B., 2026. *User's Guide for the 1D Numerical Solver for PFAS Fate and Transport in the Subsurface: the ESTCP PFAS-LEACH Tier 2 Model (PFAS-LEACH-Numerical-1D)*. University of Arizona, Tucson, Arizona, United States.
- Zeng, J., Brusseau, M.L., & Guo, B., 2021. *Model validation and analyses of parameter sensitivity and uncertainty for modeling long-term retention and leaching of PFAS in the vadose zone*. *Journal of Hydrology*, 603, 127172.
- Guo, B., Zeng, J. and Brusseau, M.L., 2020. *A mathematical model for the release, transport, and retention of per- and polyfluoroalkyl substances (PFAS) in the vadose zone*. *Water Resources Research*, 56(2), e2019WR026667.

How to download

Users can download the package here: https://github.com/GuoSFPLab/PFAS-LEACH-Numerical-1D

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1 Quick-start Guide

1.1 What is PFAS-LEACH-Numerical-1D?

1.1.1 Model overview and tier structure

PFAS-LEACH-Numerical-1D is the Tier 2 component of PFAS-LEACH, a decision-support framework for evaluating PFAS leaching from source zones. PFAS-LEACH includes four tiers with different levels of process complexity. Tier 2 is a one-dimensional numerical model for variably saturated flow and PFAS fate and transport in porous media, with emphasis on vadose-zone leaching and potential impacts on underlying groundwater. In addition to Tier 2, PFAS-LEACH includes an Excel tool for simplified Tier 3 and Tier 4 applications and a comprehensive Tier 1 three-dimensional model (PFAS-LEACH-COMP) (Guo et al., 2020; Zeng and Guo, 2021).

1.1.2 Governing processes and numerical formulation

In PFAS-LEACH-Numerical-1D, water flow is described by the Richards equation for transient variably saturated conditions under time-varying atmospheric forcing (e.g., precipitation, irrigation, evapotranspiration), with vertically heterogeneous hydraulic properties. PFAS transport is represented by coupled advection-dispersion and retention processes, including equilibrium and kinetic adsorption to solid surfaces and to air–water interfaces, with optional surfactant-induced flow effects. Optional first-order precursor decay and root-water uptake allow coupled hydrologic and vegetation-process simulations. The governing equations are solved with a mass-conservative, cell-centered finite-volume method using adaptive time stepping and convergence control.

1.1.3 Model applicability and scope

Although developed for PFAS applications, the numerical framework can also be applied to other dissolved contaminants that undergo advection-dispersion and retention in unsaturated soils (e.g., nutrients, pesticides, and selected organic contaminants). By adjusting transport, sorption, and reaction parameters, the model can be used to evaluate leaching and retention behavior in the vadose zone.

1.1.4 Ongoing development and future extensions

Ongoing development includes extensions for multi-component transport, dual-porosity/dual-permeability formulations, and explicit plant-uptake coupling. Planned additions include competitive sorption, time-varying degradation pathways, and dynamic soil-climate effects to improve applicability to complex field-scale problems.

1.2 What input data do I need?

Except when running the provided example cases, users must provide a complete set of case-specific input files. Required inputs are grouped as follows:

- **System control**: global simulation settings, including total simulation time, time-step control, numerical convergence criteria, activation of optional processes (e.g., root-water uptake, surfactant-induced flow, and groundwater contamination assessment options).
- **Soil properties**: vertical profiles of hydraulic and physical parameters, including saturated hydraulic conductivity, water-retention parameters, bulk density, dispersivity, and sorption-related properties. Spatial heterogeneity along the profile is supported.
- **PFAS properties**: chemical-specific parameters controlling PFAS transport and retention, such as molecular weight, solid-phase adsorption parameters, air–water interfacial adsorption properties, surface-tension-related coefficients, kinetic adsorption, and precursor decay rates.
- **Plant parameters**: vegetation characteristics required by the root-water uptake module, including plant growth stages, rooting depth development, leaf area index, and canopy-related parameters.
- **Initial conditions**: initial states of the soil profile, including water pressure head, aqueous-phase PFAS concentration, and initial PFAS concentration in kinetic solid-phase and air–water interfacial adsorption sites.
- **Boundary conditions**: time-dependent atmospheric and hydraulic boundary conditions, such as precipitation, irrigation, potential evapotranspiration, other surface fluxes, groundwater level or pressure head at the lower boundary, and free-drainage conditions.
- **Output control**: user-defined options for saving simulation results, including selection of observation depths, output times, and generation of time series and profile data for water flow and PFAS transport variables.

1.3 How to run the model

The model package uses a predefined directory structure. Edit input files only; do not modify executable or support files. The package contains:

- Folder `INPUT/`: contains all input files required for a simulation, including system control, soil properties, PFAS properties, boundary conditions, plant parameters, and output control. Users should edit these files according to the instructions provided in this User Guide.
- Folder `OUTPUT/`: stores all output files generated during model execution. Existing files in this folder may be overwritten when the model is re-run.
- Compiled executable of PFAS-LEACH-Numerical-1D, typically distributed under a `bin/` folder (e.g., `../bin/ESTCP_2025.exe` in the example package). Users should not modify, move, or rename this file or its parent directory.
- `Run.bat`: the batch file used to launch the model. *Double-click this file to start a simulation after all input files have been prepared.*

To run the model, prepare all required input files in `INPUT/`, then launch the executable from the case folder (or run `Run.bat` when provided). During execution, the model reads inputs, solves water flow and PFAS transport, and writes outputs to `OUTPUT/`.

1.4 Simulation outputs and data visualization

Model outputs are written in standard CSV format in `OUTPUT/` for maximum compatibility with common analysis tools (e.g., Excel, R, Python, MATLAB). A lightweight Python script is provided for quick visualization: `plot_outputs.py`.

To run it, ensure Python 3 with `pandas` and `matplotlib` installed (e.g., `python -m pip install –user pandas matplotlib`), open a terminal in your folder containing `plot_outputs.py`, and execute it.

For first-time Python users: install Python 3 from https://www.python.org/downloads/ (Windows users should check `Add Python to PATH`); open `Command Prompt` or `PowerShell`; use `cd` to enter the folder that contains `plot_outputs.py`; then run the installation command above and execute `plot_outputs.py`.

The script automatically scans all output files and generates three PDF reports in the folder `FIGURES/`: `FIGURES/Time series.pdf` (grouped time-series panels, including top/bottom head and concentrations, water and PFAS balances, and mass-balance errors), `FIGURES/Monitored cells.pdf` (one subplot per variable with all monitored cells overlaid), and `FIGURES/Profiles.pdf` (one subplot per variable with all profile times overlaid, depth increasing downward). These PDFs provide a rapid quality check; for publication-quality figures, users should load the CSV files directly into their preferred plotting environment.

2 Input data

2.1 Input Data

All model input files are provided in *Comma-Separated Values* (`.csv`) format. You may edit these files in Microsoft Excel or in any text editor that preserves plain-text CSV formatting. To ensure reliable parsing, keep comma delimiters unchanged and avoid spreadsheet-specific formatting (e.g., merged cells, hidden symbols, or non-ASCII characters).

When editing files in Microsoft Excel, click **Save** before running the model (`Run.bat`). You do not need to close the files before execution.

The default units used throughout the model are **mg** for mass, **cm** for length, and **day** for time. Water terms expressed in **cm** represent equivalent water depth per unit area (cm^3/cm^2). The time units **d** and **day** are interchangeable in all input and output files. For logical input fields, you may use either **T**/**F** or **.True.**/**.False.** formats; both are accepted by the model.

All input files are listed below:

- `INPUT/System_ctrl.csv`
- `INPUT/PFAS_properties.csv`
- `INPUT/Soil_profile.csv`
- `INPUT/Root_uptake.csv`[1]
- `INPUT/Boundary_conditions.csv`
- `INPUT/Groundwater_pollution.csv`[2]
- `INPUT/Output_ctrl.csv`

Notes:

[1] The input file `INPUT/Root_uptake.csv` is required only when `Root_uptake_on = T` is specified in `INPUT/System_ctrl.csv`.

[2] The input file `INPUT/Groundwater_pollution.csv` is required only when `GW_dilution_on = T` is specified in `INPUT/System_ctrl.csv`.

2.2 System control: `INPUT/System_ctrl.csv`

Table 1 summarizes the system-control parameters used to configure numerical solution settings in PFAS-LEACH-Numerical-1D. These parameters define simulation duration, adaptive time stepping, convergence criteria for both water flow and PFAS transport, and activation of optional modules such as root-water uptake and groundwater dilution analysis. Review the definitions, units, and usage notes in Table 1 before model execution.

Table 1: `INPUT/System_ctrl.csv`.

Parameters	Unit	Descriptions
tEnd	d	Total simulation duration. The simulation is assumed to start at time t = 0.
dt0	d	Initial time step size.
dtMin & dtMax	d	Minimum and maximum allowable time step sizes.

Surfactant_induced_flow	logical (T/F)	Logical flag controlling whether the surfactant-induced flow effects are included.
		Input handling:
		• **If** `Surfactant_induced_flow = T`:
		  • Flow behavior dependent on surface-tension gradients is activated.
		  • This option accounts for surfactant-induced modifications to unsaturated flow dynamics (e.g., (Zeng and Guo, 2021)).
		• **If** `Surfactant_induced_flow = F`:
		  • Surfactant-induced flow effects are neglected.

Root_uptake_on	logical (T/F)	Logical flag controlling whether the root-water uptake module is activated.
		Input handling:
		• **If** `Root_uptake_on = T`:
		  • The root-water uptake module is activated.
		  • Plant-specific parameters are used to compute water uptake distributed within the root zone.
		• **If** `Root_uptake_on = F`:
		  • Root-water uptake is disabled.
		  • Evapotranspiration is represented as an outward vapor flux imposed at the land surface.
		  • In this case, ET_0 in `INPUT/Boundary_conditions.csv` must be specified as the *potential evapotranspiration* (ETp), rather than a reference evapotranspiration estimated using methods such as FAO Penman–Monteith.

h_A	cm	h_A: threshold soil water pressure head at the land surface that limits further drying. **Model behavior:** • When the surface pressure head decreases to h_A, further drying due to evaporation or transpiration is suppressed. • A constant pressure head boundary condition, $h_{\text{top}} = h_A$, is imposed at the land surface until precipitation or irrigation resumes. **Physical interpretation:** h_A represents the onset of supply-limited evaporation and serves as an empirical parameter accounting for the loss of liquid-phase near the soil surface. **Typical values:** • Coarse-textured soils: $h_A \approx -10^3$ cm • Fine-textured soils: $h_A \approx -10^4$–10^5 cm **Note:** Because h_A implicitly represents unresolved near-surface processes (e.g., vapor diffusion and surface resistance), users are encouraged to select its value based on soil texture and to evaluate its influence through sensitivity analysis.
dt_Increase	–	Time-step scaling factor applied when nonlinear convergence within the current time step is achieved efficiently. **Input handling:** • Applied when the number of iterations in the current time step is less than `N_Iter_L`. • The subsequent time step is increased as $$\Delta t_{\text{new}} = \Delta t \times \text{dt\_Increase}.$$ **Constraint:** dt_Increase > 1.
dt_Reduce	–	Time-step scaling factor applied when nonlinear convergence in the current time step is slow or unstable. **Input handling:** • Applied when the number of iterations in the current time step exceeds `N_Iter_H`. • The subsequent time step is reduced as $$\Delta t_{\text{new}} = \Delta t \times \text{dt\_Reduce}.$$ **Constraint:** dt_Reduce < 1.
N_Iter_L	–	Lower iteration threshold defining efficient nonlinear convergence. **Input handling:** • If the number of iterations required for convergence is less than `N_Iter_L`, the time step for the subsequent step is increased using dt_Increase.
N_Iter_H	–	Upper iteration threshold defining inefficient or unstable nonlinear convergence. **Input handling:** • If the number of iterations required for convergence exceeds `N_Iter_H`, the time step for the subsequent step is reduced using dt_Reduce.

Max_N_Iter	–	Maximum number of nonlinear iterations permitted within a single time step for either the soil water flow or PFAS transport equations. **Input handling:** • If the number of iterations exceeds `Max_N_Iter`, the current time step is rejected. • The solver retries the same time step with a reduced time-step size until convergence is achieved.
Tol_th	cm^3/cm^3	ϵ_θ: convergence tolerance for volumetric soil water content used in the Richards equation. **Convergence criterion:** $\|\theta^{k+1} - \theta^k\| \leq \epsilon_\theta$, where k and $k+1$ denote successive nonlinear iteration levels.
Tol_h	cm	ϵ_h: convergence tolerance for soil water pressure head used in the Richards equation. **Convergence criterion:** $\|h^{k+1} - h^k\| \leq \epsilon_h$, where k and $k+1$ denote successive nonlinear iteration levels.
Tol_C	mg/cm^3	ϵ_C: convergence tolerance for aqueous-phase PFAS concentration in the transport equation. **Convergence criterion:** $\|C^{k+1} - C^k\| \leq \epsilon_C$, where k and $k+1$ denote successive nonlinear iteration levels.

GW_dilution_on	logical (T/F)	Logical flag controlling estimation of the groundwater dilution factor (DF, dimensionless).
		Input handling:
		• **If** `GW_dilution_on = T`:
		  • The model computes the groundwater dilution factor DF.
		  • See Section 2.7 for details on the formulation and assumptions.
		• **If** `GW_dilution_on = F`:
		  • Groundwater dilution is not evaluated.

2.3 PFAS properties: `INPUT/PFAS_properties.csv`

PFAS-specific properties are specified in `INPUT/PFAS_properties.csv`. These parameters control PFAS transport behavior, interfacial activity, and retention processes, including solid-phase sorption, air–water interfacial adsorption, surfactant-induced flow effects, and chemical decay. Table 2 summarizes the required PFAS properties and definitions.

Table 2: `INPUT/PFAS_properties.csv`.

Parameters	Unit	Descriptions
Molecular weight	g/mol	M_w: molecular weight of the modeled PFAS compound.
a, b	mg/L, –	a and b: empirical parameters used to describe PFAS-induced surface tension reduction based on the Szyszkowski equation (Guo et al., 2020).
Chi	–	χ: interfacial activity coefficient accounting for electrostatic effects at the air–water interface. **Recommended values:** • χ = 1.0 for nonionic PFAS, or for ionic PFAS in solutions with swamping background electrolytes. • χ = 2.0 for ionic surfactants in solutions without swamping electrolytes (e.g., deionized water).

sigma$_0$	dyn/cm	σ_0: reference surface tension of the aqueous phase in the absence of PFAS; a typical value is σ_0 = 72.0 dyn/cm. **Note:** 1 dyn = 1 g $\cdot$ cm/s^2 = 10^{-5} N.
Dm	cm^2/d	D_m: molecular diffusion coefficient of PFAS in the aqueous phase.
Fs	–	F_s: fraction of solid-phase sorption sites exhibiting instantaneous (equilibrium) adsorption. The remaining fraction, $1 - F_s$, is treated as kinetic solid-phase adsorption.
alpha_s	1/d	α_s: first-order rate constant for kinetic solid-phase adsorption.
Faw	–	F_{aw}: fraction of air–water interfacial adsorption sites assumed to be instantaneous. The remaining fraction, $1 - F_{aw}$, is treated as kinetic air–water interfacial adsorption.
alpha_aw	1/d	α_{aw}: first-order rate constant for kinetic air–water interfacial adsorption.
Aaw_SF	–	*SF*: empirical scaling factor accounting for additional air–water interfacial area not captured by the thermodynamic formulation (e.g., microscale surface roughness of soil grains or other site-specific effects). Users may set Aaw_SF (*SF*) = 1.0 as a default. The PFAS-LEACH Excel tool (Tiers 3 & 4) has provided several approaches for estimating *SF*.

Aaw_LookUpTable	logical (T/F)	Logical flag controlling the use of a pre-generated lookup table for air–water interfacial area (A_{aw}) as a function of water content (θ).
		Input handling:
		• **If** `Aaw_LookUpTable = T`:
		  • A_{aw} values are obtained by interpolation from a pre-generated lookup table during pre-processing.
		  • This option substantially reduces computational cost (by approximately 80%) compared to on-the-fly calculations.
		• **If** `Aaw_LookUpTable = F`:
		  • A_{aw} is computed dynamically during the simulation.

PFAS_release_depth	–	Number of numerical cells adjacent to the land surface over which applied PFAS mass is uniformly and instantaneously mixed during a contamination event.
		Input handling:
		• **If** `PFAS_release_depth = 1`:
		  • PFAS mass is applied exclusively to the top numerical cell.
		• **If** `PFAS_release_depth` $>$ 1:
		  • PFAS mass is uniformly distributed among the specified number of surface-adjacent cells.
		Constraints: 1 $\leq$ `PFAS_release_depth` $\leq$ *N*, where *N* is the total number of numerical cells in the model domain.

First_order_decay	1/d	λ: first-order decay-rate constant for degradable PFAS (e.g., precursor compounds). **Model representation:** • PFAS decay is represented as a first-order reaction term in the advection–dispersion equation. • The decay term is expressed as $R = \theta\lambda C$, where C is aqueous-phase PFAS concentration and θ is volumetric water content. **Note:** This formulation provides a lumped representation of PFAS transformation processes and is commonly applied to precursor degradation (e.g., Chen and Guo (2025)).

2.4 Soil profiles: `INPUT/Soil_profile.csv`

The file `INPUT/Soil_profile.csv` provides vertical profile information required by the model. It specifies soil hydraulic and physical parameters, PFAS adsorption parameters, and initial conditions for pressure head, aqueous PFAS concentration, kinetic solid-phase adsorption, and kinetic air–water interfacial adsorption. All parameters are assigned cell by cell according to vertical coordinate (z).

Table 3: `INPUT/Soil_profile.csv`.

Parameters	Unit	Descriptions
z	cm	z: vertical location of the numerical cell center, defined along the positive downward z-axis. By default, the top of the first numerical cell coincides with the land surface (where z = 0).
Ksat	cm/d	K_{sat}: saturated hydraulic conductivity.
ths & thr	cm^3/cm^3	θ_s and θ_r: saturated and residual volumetric water contents, respectively.
alpha & n	1/cm, $-$	α_{VG} and n_{VG}: shape parameters of the soil-water retention curve described by the van Genuchten model. The parameter m_{VG} is estimated internally as $m_{VG} = 1 - 1/n_{VG}$.
rhob	g/cm^3	ρ_b: soil bulk density.
alphaL	cm	α_L: longitudinal dispersivity in the vadose zone, representing vertical PFAS spreading caused by spatial variability in pore-water velocity. **Physical interpretation:** α_L is an empirical parameter accounting for mechanical dispersion associated with heterogeneity in flow pathways. Several methods have been proposed to estimate α_L as a function of spatial scale. A commonly used empirical relationship is $$\alpha_L = 82 \left[\log\left(\frac{L}{100}\right)\right]^{2.446},$$ where L (cm) denotes characteristic domain length (Xu and Eckstein, 1995). For PFAS leaching to groundwater, L is commonly taken as the depth to the groundwater table. **Note:** This relationship was developed under saturated flow conditions and does not explicitly account for the dependence of α_L on water saturation in the vadose zone.
Kf & Nf	See Notes.	K_f and N_f: Freundlich solid-phase adsorption parameters. Linear solid-phase adsorption can be simulated by setting N_f = 1, for which the Freundlich coefficient K_f reduces to the linear distribution coefficient K_d (cm^3/g). Notes: K_f has a unit of $(mg/g)/(mg/cm^3)^{N_f}$, and N_f is dimensionless. When compared with the commonly used unit of K_f $(\mu mol/g)/(\mu mol/cm^3)^{N_f}$, the Freundlich coefficient can be converted as $$K_f^{(mg)} = K_f^{(\mu mol)} (0.001 M_w)^{1-N_f},$$ where M_w is the molecular weight of the compound (g/mol or µg/µmol). Equivalently, $$\frac{mg/g}{(mg/cm^3)^{N_f}} = (0.001 M_w)^{1-N_f} \frac{\mu mol/g}{(\mu mol/cm^3)^{N_f}}.$$

θ_0	cm^3/cm^3	θ_0: initial volumetric soil water content.
		Input handling:
		• **If** $\theta_0 > 0$:
		  • θ_0 is accepted as the initial condition.
		  • The model enforces $\theta_r \leq \theta_0 \leq \theta_s$.
		• **If** $\theta_0 \leq 0$:
		  • The input value of θ_0 is ignored.
		  • The initial condition is specified using the input value of h_0.

h_0	cm	h_0: initial soil water pressure head.
		Input handling:
		• **If** $\theta_0 \leq 0$:
		  • h_0 is accepted as the initial condition.
		• **If** $\theta_0 > 0$:
		  • The input value of h_0 is ignored.
		  • The model enforces $\theta_r \leq \theta_0 \leq \theta_s$.

C_0	mg/L	C_0: initial aqueous-phase PFAS concentration.
		Input handling:
		• **If** $C_0 > 0$:
		  • C_0 is accepted as the initial aqueous-phase concentration.
		  • The input value of $C_{tot,0}$ is ignored.
		  • $C_{tot,0}$ is computed internally as
		  $C_{tot,0} = \theta C_0 + F_s \rho_b K_f C_0^{N_f} + \rho_b C_{s,2,0} + F_{aw} K_{aw} A_{aw} C_0 + C_{aw,2,0}$.
		• **If** $C_0 < 0$:
		  • A positive value of $C_{tot,0}$ must be specified.
		  • If $C_{tot,0} \leq 0$, all initial concentrations are set to zero (equivalent to $C_0 = 0$, $C_{s,2,0} = 0$, $C_{aw,2,0} = 0$, and $C_{tot,0} = 0$).
		• **If** $C_0 = 0$:
		  • If $C_{tot,0} \leq 0$, all initial concentrations are set to zero (equivalent to $C_0 = 0$, $C_{s,2,0} = 0$, $C_{aw,2,0} = 0$, and $C_{tot,0} = 0$).
		  • If $C_{tot,0} > 0$, the model accepts the input values for $C_{tot,0}$ and internally back-calculates C_0 following the rules defined in entry "$C_{tot,0}$" (at the end of this table).

$C_{s,2,0}$	mg/g	$C_{s,2,0}$: initial PFAS concentration in the kinetic solid-phase adsorption domain.
		Input handling:
		• **If** $C_{s,2,0} \geq 0$:
		  • The input value is accepted as the initial condition for the kinetic solid-phase domain.
		  • This combination ($C_0 \leq 0$ with $C_{s,2,0} \geq 0$) is allowed but generally not recommended.
		• **If** $C_{s,2,0} < 0$:
		  • The instantaneous and kinetic solid-phase adsorption domains are assumed to be initially at equilibrium.
		  • This assumption is representative of long-term PFAS retention.
		  • Accordingly, $C_{s,2,0} = (1 - F_s) K_f C_0^{N_f}$.

$C_{aw,2,0}$	mg/cm^3	$C_{aw,2,0}$: initial PFAS concentration in the kinetic air–water interfacial adsorption domain.
		Input handling:
		• **If** $C_{aw,2,0} \geq 0$:
		  • The input value is accepted as the initial condition for the kinetic air–water interfacial domain.
		  • This combination ($C_0 \leq 0$ with $C_{aw,2,0} \geq 0$) is allowed but generally not recommended.
		• **If** $C_{aw,2,0} < 0$:
		  • The instantaneous and kinetic air–water interfacial adsorption domains are assumed to be initially at equilibrium.
		  • Accordingly, $C_{aw,2,0} = (1 - F_{aw})\, K_{aw}\, A_{aw}\, C_0$.

$C_{tot,0}$	mg/cm^3	$C_{tot,0}$: initial total PFAS concentration.
		Input handling:
		• **If** $C_{tot,0} > 0$ **and** $C_0 < 0$:
		  • The input value of $C_{tot,0}$ is accepted.
		  • The initial aqueous-phase concentration C_0 is back-calculated using
		  $C_{tot} = \theta C + \rho_b \left(F_s K_f C^{N_f} + C_{s,2}\right) + F_{aw} K_{aw} A_{aw} C + C_{aw,2}.$
		  • The initial values of $C_{s,2,0}$ and $C_{aw,2,0}$ are obtained as follows:
		  • If the corresponding input values are > 0, they are accepted.
		  • Otherwise, equilibrium with the instantaneous domains is assumed, i.e., $C_{s,2,0} = (1 - F_s)\, K_f\, C_0^{N_f}$ and $C_{aw,2,0} = (1 - F_{aw})\, K_{aw}\, A_{aw}\, C_0$.
		• **If** $C_{tot,0} \leq 0$ **or** $C_0 \geq 0$:
		  • The input value of $C_{tot,0}$ is ignored.
		  • The model uses the input values for C_0, $C_{s,2,0}$, and $C_{aw,2,0}$.

2.5 Plant growth and root-water uptake: `INPUT/Root_uptake.csv`

The file `INPUT/Root_uptake.csv` defines plant-growth and root-water-uptake parameters used when the root-water uptake module is activated. These parameters describe plant phenological development, rooting-depth evolution, evapotranspiration partitioning, and the pressure-head-dependent response of root-water uptake. Users may refer to FAO 56 (Allen et al., 1998) for plant-specific parameter values across a wide range of plants and management systems. At present, this module is designed for single-year (annual) crops/plants and does not represent multi-year perennial growth cycles.

Note: The input file `INPUT/Root_uptake.csv` is required only when `Root_uptake_on = T` is specified in `INPUT/System_ctrl.csv`.

Table 4: `INPUT/Root_uptake.csv`.

Parameters	Unit	Descriptions
t_Seedling	d	t_{Seedling}: day of year when the plant is planted or emerges, marking the start of the growing season.

t1	d	t_1: plant age (measured from t_{Seedling}) before which plant evapotranspiration remains minimal.
t2	d	t_2: plant age at which plant evapotranspiration reaches its maximum value.
t3	d	t_3: plant age at the onset of senescence, typically corresponding to the harvest-ready stage.
t4	d	t_4: end of the plant life cycle, indicating final harvest time.
Kc_init, Kc_mid, Kc_end	–	$K_{c,\text{init}}$, $K_{c,\text{mid}}$, and $K_{c,\text{end}}$: crop coefficients representing the initial, mid-season, and late-season growth stages, respectively.
LRoot_0	cm	Initial rooting depth at seedling emergence.
LRoot_max	cm	Maximum rooting depth attained at full plant development.
LAI_max	–	LAI_{max}: maximum leaf area index achieved during the growing season.
K_canopy	–	K_{canopy}: canopy radiation extinction coefficient governing light attenuation within the plant canopy. Typical values range from 0.5 to 0.75, depending on solar angle, plant architecture, and leaf orientation. A default value of K_{canopy} = 0.6 is used in the model.
h1	cm	h_1: anaerobiosis pressure head, above which root-water uptake is suppressed due to oxygen stress.
h2	cm	h_2: pressure head threshold below which root-water uptake occurs at the maximum rate.
h3	cm	h_3: limiting pressure head below which root-water uptake begins to decrease linearly.
h4	cm	h_4: wilting-point pressure head, below which root-water uptake ceases.

2.6 Boundary conditions: `INPUT/Boundary_conditions.csv`

Time-varying boundary conditions are specified in `INPUT/Boundary_conditions.csv`. This file defines atmospheric and hydraulic boundary conditions, including precipitation, irrigation, evapotranspiration, groundwater boundary settings, and PFAS loading at the land surface. All boundary variables are provided as time series and aligned with the simulation times listed in the first column (`t`, in days).

Any temporal resolution is supported for boundary-condition inputs. For example, the boundary time spacing does not need to match the internal numerical time step or follow a daily interval. Boundary values are applied stepwise between specified time points.

A surface ponding condition is activated automatically when the pressure head at the top numerical cell reaches zero, allowing excess water to accumulate at the land surface.

Table 5: `INPUT/Boundary_conditions.csv`.

Parameters	Unit	Descriptions
t	d	Simulation time corresponding to each set of boundary-condition values.
Precipitation	cm/d	Precipitation flux applied at the land surface.

Irrigation	cm/d	Irrigation water flux applied at the land surface. This flux is assumed to be free of PFAS. This column may also be used to represent other water inputs, such as surface flow (e.g., flooding) or managed recharge, if applicable. If irrigation water contains PFAS, the corresponding flux should instead be specified using the column for `Contaminated_water_flux`.

ET_0	cm/d	ET_0: evapotranspiration input.
		Input handling:
		• **If** `Root_uptake_on = T` (in `INPUT/System_ctrl.csv`):
		  • ET_0 represents the *reference evapotranspiration*.
		  • Typical estimates include values from methods such as FAO Penman–Monteith.
		• **If** `Root_uptake_on = F` (in `INPUT/System_ctrl.csv`):
		  • ET_0 must represent the *potential evapotranspiration* (ETp).
		  • Crop coefficients are not applied in this mode.
		  • ET_0 is treated as an outward vapor flux boundary condition at the land surface.
		Note: ETp may be estimated from different methods (e.g., lysimeter measurements or modeling approaches) and should be distinguished from *reference evapotranspiration* (ET_0).

top_BC	cm	`top_BC`: indicator specifying the upper boundary condition type.
		Input handling:
		• **If** `top_BC` ≤ -999999:
		  • The upper boundary is treated as an open flux boundary.
		• **If** `top_BC` > -999999:
		  • A constant pressure head boundary is imposed at the upper boundary.
		  • The prescribed pressure head is equal to `top_BC` (unit: cm).
		  • This option is primarily intended for laboratory column experiments.
		Recommendation: For most field-scale applications, set `top_BC` ≤ -999999.

bot_BC	cm	`bot_BC`: indicator specifying the lower boundary condition type.
		Input handling:
		• **If** `bot_BC` ≤ -999999:
		  • The lower boundary is treated as a free–drainage boundary.
		• **If** `bot_BC` > 999999:
		  • A no-flux boundary is imposed at the lower boundary.
		• **If** $-999999 <$ `bot_BC` < 999999:
		  • A constant pressure head boundary is applied at the lower boundary.
		  • The prescribed pressure head is equal to `bot_BC` (unit: cm).

Contaminated_water_flux	cm/d	Flux of PFAS-contaminated water applied at the land surface (e.g., fire training applications involving AFFF solutions containing PFAS).

PFAS_mass_flux	mg/d/cm^2	Mass flux of the modeled PFAS applied at the land surface, normalized by unit area (1 cm^2). The model domain area is implicitly assumed to be 1 cm^2.
		Input interpretation:
		• **Aqueous PFAS inputs** (e.g., AFFF solutions):
		  • *PFAS_mass_flux* is computed as *PFAS_mass_flux* = *Contaminated_water_flux* $\times C_{\text{PFAS}}$, where C_{PFAS} is aqueous PFAS concentration.
		  • The associated water application must be specified in the *Contaminated_water_flux* column.
		• **Dry mass inputs** (e.g., biosolids):
		  • *PFAS_mass_flux* is computed as *PFAS_mass_flux* = (mass of biosolids) $\times$ (PFAS concentration by weight).
		  • Any accompanying water application may either be specified in the *Contaminated_water_flux* column or omitted if the biosolids are sufficiently dry.

2.7 Groundwater pollution: `INPUT/Groundwater_pollution.csv`

Following the dilution-factor approach in U.S. EPA guidance USEPA (1996), PFAS-LEACH-Numerical-1D estimates the groundwater dilution factor (DF), defined as the ratio between PFAS aqueous concentration in leachate exiting the vadose zone and the corresponding concentration at a downgradient receptor well located a distance L_{plume} from the source area.

The dilution factor is calculated as

$$DF = 1 + \frac{q_{gw}\,\delta_{gw}}{I_f\,L_{plume}},$$

where q_{gw} (cm/d) is the lateral Darcy flux of groundwater beneath the contaminated site, I_f (cm/d) is the average drainage or net-infiltration water flux, and L_{plume} (cm) is the distance between the vadose-zone source and the downgradient receptor well. The source area is assumed square. When deriving soil screening levels, this assumption may be conservative for sites with longer dimensions perpendicular to groundwater flow and nonconservative for sites with longer dimensions parallel to groundwater flow (USEPA, 1996). In such cases, the effective source length may be approximated as the square root of source area.

The parameter b_{sat} (cm) represents the saturated thickness of the downgradient aquifer. The vertical dispersivity of the saturated zone, α_v (cm), is estimated as

$$\alpha_v = 0.0056\,L_{plume}.$$

The groundwater mixing-zone thickness, δ_{gw} (cm), is constrained by $\delta_{gw} \leq b_{sat}$ and is calculated as

$$\delta_{gw} = \sqrt{2\,\alpha_v\,L_{plume}} + b_{sat}\left(1 - e^{\frac{-I_f\,L_{plume}}{q_{gw}\,b_{sat}}}\right),$$

where q_{gw} is the average groundwater flux.

The parameters required for estimating the groundwater dilution factor, including q_{gw}, L_{plume}, and b_{sat}, are provided by the user in the file `INPUT/Groundwater_pollution.csv`. A summary of these parameters is given in Table 6.

Note: The input file `INPUT/Groundwater_pollution.csv` is required only when `GW_dilution_on = T` is specified in `INPUT/System_ctrl.csv`.

Table 6: `INPUT/Groundwater_pollution.csv`.

Parameters	Unit	Descriptions
Groundwater_Darcy_flux	cm/d	q_{gw}: average lateral Darcy flux of groundwater in the downgradient saturated zone receiving leachate from the vadose zone source area.
Lateral_plume_length	cm	L_{plume}: horizontal distance between the downgradient receptor well and the original PFAS source zone. **Physical meaning:** L_{plume} defines the characteristic transport length scale used in evaluating PFAS plume migration and attenuation within the saturated zone.
Thickness_of_saturated_zone	cm	b_{sat}: thickness of the downgradient saturated zone. **Physical meaning:** b_{sat} represents the effective vertical thickness of the aquifer contributing to groundwater flow and PFAS transport.

2.8 Output control: `INPUT/Output_ctrl.csv`

The output-control file `INPUT/Output_ctrl.csv` specifies how and when simulation results are written. The model can generate (i) detailed one-dimensional profiles at user-defined times and (ii) time series of state variables and mass-balance components at selected numerical cells.

The first row of `INPUT/Output_ctrl.csv` defines vertical subzones used for mass-balance reporting. Subsequent rows control where and when detailed output is recorded.

Table 7: `INPUT/Output_ctrl.csv`.

Parameters	Unit	Descriptions
Observed_cells	cell IDs	IDs of numerical cells selected for time-series output. **Input handling:** • The number of monitored cells is user-defined. • Valid cell IDs satisfy $1 \leq \text{ID} \leq N$, where N is the total number of numerical cells in the one-dimensional domain. • Multiple cell IDs must be specified as a comma-separated list in a single line (e.g., `5, 10, 80` in row #2). **Output:** Detailed time-series results for the specified cells are written to `OUTPUT/3.Observations.csv`. **Note:** • All values must be provided on a single line. Line breaks within this entry are not permitted. • The model will append the last numerical cell (ID = N) to the observed cell IDs if is not specified by the user.

t_profile	d	Simulation times at which full one-dimensional profiles are saved. **Input handling:** • Users may specify an arbitrary number of output times. • All specified values must satisfy $t_{\text{profile}} \leq t_{\text{End}}$. • Multiple times must be provided as a comma-separated list in a single line (row #4). **Output:** At each specified time, a profile file named `OUTPUT/1.Profile-Time-XXX.csv` (XXX = 1, 2, ...) is generated. **Note:** • All values must be provided on a single line. Line breaks within this entry are not permitted. • The model will append the end of the simulation (*t* = *tEnd*) to t_profile if it is not specified by the user.

3 Output data

All simulation results generated by PFAS-LEACH-Numerical-1D are written to the folder `OUTPUT/`. Depending on the output-control settings, the following files may be generated:

- `OUTPUT/1.Profile-Time-1.csv`
- `OUTPUT/1.Profile-Time-2.csv`
- `OUTPUT/1.Profile-Time-3.csv`

  ...

- `OUTPUT/2.Time series.csv`
- `OUTPUT/3.Observations.csv`
- `OUTPUT/4.Summary.csv`

3.1 1D profiles: `OUTPUT/1.Profile-Time-XXX.csv`

The files `OUTPUT/1.Profile-Time-XXX.csv` store detailed one-dimensional profiles of the simulated domain at user-specified times. Each row corresponds to one numerical cell, and each column represents a state variable or PFAS-related quantity.

The suffix `XXX` is the profile identifier (`iPrint = 1, 2, ...`), corresponding to the output-time order in `INPUT/Output_ctrl.csv` (see Table 8).

Table 8: `OUTPUT/1.Profile-Time-XXX.csv`.

Parameters	Unit	Descriptions
iPrint	–	Identifier of the printed profile, following the order defined in `INPUT/Output_ctrl.csv`.
time	d	Simulation time at which the profile is printed.
z	cm	Vertical location of the numerical cell center along the positive downward *z*-axis.
h	cm	h: soil water pressure head.
th	cm^3/cm^3	θ: volumetric soil water content.

Sw	–	$S_w = \theta/\theta_s$: water saturation.
C	mg/L	C: aqueous-phase PFAS concentration.
Aaw	cm^2/cm^3	A_{aw}: air–water interfacial area.
Cs1	mg/g	$C_{s,1}$: PFAS concentration in instantaneous solid-phase adsorption sites. Note that $C_{s,1}$ must be multiplied by ρ_b to represent the concentration of instantaneous solid-phase adsorption.
Cs2	mg/g	$C_{s,2}$: PFAS concentration in kinetic solid-phase adsorption sites. Note that $C_{s,2}$ must be multiplied by ρ_b (g/cm^3) to represent the concentration of kinetic solid-phase adsorption.
Caw1	mg/cm^3	$C_{aw,1}$: PFAS concentration in the instantaneous air–water interfacial adsorption sites.
Caw2	mg/cm^3	$C_{aw,2}$: PFAS concentration in the kinetic air–water interfacial adsorption sites.
Ctot	mg/cm^3	C_{tot}: total soil PFAS concentration in the numerical cell, including mass in porewater and on instantaneous and kinetic adsorption sites at solid surfaces and air–water interfaces. $C_{tot} = \theta C + F_s \rho_b K_f C^{N_f} + \rho_b C_{s,2} + F_{aw} K_{aw} A_{aw} C + C_{aw,2}$

3.2 Time series: `OUTPUT/2.Time series.csv`

The file `OUTPUT/2.Time series.csv` reports domain-integrated and boundary-specific variables as time series over the simulation period.

Table 9: `OUTPUT/2.Time series.csv`.

Parameter	Unit	Description
time	d	Simulation time.
htop	cm	h_{top}: water pressure head at the top boundary of the domain.
hbot	cm	h_{bot}: water pressure head at the bottom boundary of the domain.
ctop	mg/L	C_{top}: aqueous PFAS concentration at the top boundary.
cbot	mg/L	C_{bot}: aqueous PFAS concentration at the bottom boundary.
water_input	cm	W_{in}: cumulative water input by precipitation, irrigation, and pollutant (contaminated water).
ET	cm	ET_{tot}: cumulative water loss due to evapotranspiration.
water_drainage	cm	$Drainage_{\text{tot}}$: cumulative water drainage from the bottom boundary.
water_tot	cm	W_{tot}: total water storage in the domain, $$W_{\text{tot}} = \sum_{\text{domain}} (\theta \, \Delta z).$$
water_MB_error	%	err_{water}: relative mass balance error for the water flow simulation. **Definition:** $$err_{\text{water}} = \frac{W_{\text{in}} + W_{\text{tot},0} - W_{\text{out}} - W_{\text{tot}}}{W_{\text{in}} + W_{\text{tot},0}} \times 100\%,$$ where $W_{\text{in}} = P_{\text{tot}} + I_{\text{tot}} + W_{\text{cont}}$ and $W_{\text{out}} = ET_{\text{tot}} + Drainage_{\text{tot}}$, with P_{tot}, I_{tot}, and W_{cont} as cumulative precipitation, irrigation, and contaminated-water input, respectively. **Description:** All water terms are expressed as equivalent water depth (cm) per unit area. $W_{\text{tot},0}$ and W_{tot} denote the total water storage in the domain at the initial and current times, respectively.
pfas_in	mg	$PFAS_{\text{in}}$: total PFAS mass input from the land surface.

pfas_decay	mg	$PFAS_{decay}$: total PFAS mass lost due to degradation.
pfas_discharge	mg	$PFAS_{dis}$: total PFAS mass discharged through the bottom boundary.
pfas_tot	mg	$PFAS_{tot}$: total PFAS mass within the domain, $$PFAS_{tot} = \sum_{domain} (C_{tot}\,\Delta z).$$
pfas_MB_error	%	err_{PFAS}: relative mass balance error for PFAS transport simulation. **Definition:** $$err_{PFAS} = \frac{PFAS_{in} + PFAS_{tot,0} - PFAS_{out} - PFAS_{tot}}{PFAS_{in} + PFAS_{tot,0}} \times 100\%.$$ where $PFAS_{out} = PFAS_{dis} + PFAS_{decay}$. **Description:** All PFAS mass terms are expressed in mg per unit area. $PFAS_{tot,0}$ and $PFAS_{tot}$ denote the total PFAS mass in the domain at the initial and current times, respectively.

3.3 Observations: `OUTPUT/3.Observations.csv`

The file `OUTPUT/3.Observations.csv` provides time series of the same variables reported in profile files, but only for user-selected numerical cells and at higher temporal resolution. Variables are identified by suffixed names; for example, `h-5` denotes water pressure head at numerical cell #5. Units are consistent with the rest of the input/output files.

3.4 Final summary: `OUTPUT/4.Summary.csv`

The file `OUTPUT/4.Summary.csv` summarizes overall simulation statistics and, when enabled, groundwater contamination metrics such as estimated dilution factor.

Table 10: `OUTPUT/4.Summary.csv`.

Parameter	Unit	Description
Total days	d	Total simulated time period.
Length of 1D domain	cm	Vertical length of the modeled one-dimensional domain.
Number of numerical cells	–	Total number of cells used in the spatial discretization.
CPU cost	s	Total CPU time consumed by the simulation.
Average drainage/net infiltration	cm/d	I_f: Average water drainage flux at the bottom boundary over the simulation period.
Lateral groundwater Darcy flux	cm/d	q_{gw}: User-specified average lateral groundwater Darcy flux in the downgradient saturated zone.
Lateral plume length	cm	L_{plume}: User-specified horizontal distance between the PFAS source zone and the downgradient receptor in groundwater.
Mixing zone thickness	cm	δ_{gw}: Estimated thickness of the downgradient groundwater mixing zone.
Groundwater dilution factor	–	DF: Estimated groundwater dilution factor.

4 Examples

Three example simulations are provided to demonstrate typical applications of PFAS-LEACH-Numerical-1D. In all examples, Vinton soil is used, either as a laboratory-scale column medium or as a representation of the full vadose zone. Perfluorooctanoic acid (PFOA) is selected as the target PFAS compound in all three simulations.

Table 11 summarizes the soil hydraulic parameters of the Vinton soil used in the examples, and Table 12 lists the chemical and adsorption parameters for PFOA.

Table 11: Parameters for Vinton soil used in the examples.

Parameters	unit	Vinton	Accusand
K_{sat}	cm/d	100.0	1,800
θ_s	cm^3/cm^3	0.359	0.294
θ_r	cm^3/cm^3	0.07	0.03
α_{VG}	1/cm	0.02	0.046
n_{VG}	–	4.0	4.5
ρ_b	g/cm^3	1.627	1.65
K_f	$(mg/g)/(mg/cm^3)^{N_f}$	0.2351	0.0407
N_f	–	0.87	0.87

Table 12: Parameters for PFOA used in the examples.

Parameters	unit	Values
M_w	g/mol	414.07
a	mg/L	62.11
b	–	0.19
χ	–	1.0
σ_0	dyn/cm	72
D_m	cm^2/d	0.423
F_s	–	0.4
α_s	1/d	0.0018
F_{aw}	–	0.9
α_{aw}	1/d	0.0015

4.1 Example 1: PFAS leaching in a soil column under steady-state flow

4.1.1 Parameter setup

Example 1 simulates a laboratory-scale PFOA leaching experiment in a one-dimensional soil column under steady-state water-flow conditions. The porous medium is Vinton soil (sandy loam) collected in Arizona, and downward flow is prescribed as a constant Darcy flux of q = 4 cm/d.

During an initial injection period of 2.4 hours (0.1 d), PFOA is applied at the column inlet with a constant aqueous concentration of C_{in} = 0.25 mg/L. This corresponds to a solute mass flux of

$$J_{in} = qC_{in} = 0.001 \text{ mg}/\text{d}/\text{cm}^2.$$

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	z (cm)	Ksat (cm/d)	ths (cm^3/cm^3)	thr (cm^3/cm^3)	alpha (1/cm)	n (-)	rhob (g/cm^3)	alphaL (cm)	Kf (mg/g)/(mg/cm^3)^Nf	Nf (-)	h0 (cm)	theta0(cm^3/cm^3)	C0 (mg/L)	Cs20 (mg/g)	Caw20 (mg/cm^3)	Ctot0(mg/cm^3)
2	0.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
3	0.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
4	1.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
5	1.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
6	2.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
7	2.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
8	3.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
9	3.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
10	4.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
11	4.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
12	5.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
13	5.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
14	6.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
15	6.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
16	7.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
17	7.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
18	8.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
19	8.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
20	9.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
21	9.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-60.622189	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00

Figure 1: Example 1: `Exp1/INPUT/Soil_profile.csv`

Following the injection period, the inlet concentration is set to zero to represent clean-water flushing, while the imposed water flux remains unchanged.

To eliminate transient flow effects and ensure a strictly steady hydraulic state, constant-pressure-head boundary conditions are imposed at both the top and bottom of the column, such that $h_{\text{top}} = h_{\text{bot}} = h_0$. The initial pressure head throughout the domain is also set uniformly to $h(z, 0) = h_0$.

Under gravity-driven flow with a unit hydraulic gradient, the Darcy flux satisfies $q = K(h_0)$. The value of h_0 is therefore determined by back-calculating from the van Genuchten–Mualem hydraulic functions using the soil parameters listed in Table 11. Solving $K(h_0) = 4$ cm/d yields $h_0 = -60.62$ cm.

This configuration initializes the soil column under the target steady-state flow condition before PFAS transport. Consequently, the simulated PFOA breakthrough behavior reflects advection, dispersion, and retention processes rather than transient variations in soil moisture or hydraulic gradients.

4.1.2 Input files

Figures 1–4 show screenshots of the input files used in Example 1.

Groundwater contamination and root-water uptake are not considered in this example. Therefore, the files `INPUT/Groundwater_pollution.csv` and `INPUT/Root_uptake.csv` are not required. In `INPUT/System_ctrl.csv`, the parameters `GW_dilution_on` and `Root_uptake_on` are set to `F`.

All spatially distributed parameters are specified in `Exp1/INPUT/Soil_profile.csv` (Figure 1). This file defines the spatial discretization, soil hydraulic parameters, transport parameters (e.g., dispersivity and solid-phase adsorption), and initial conditions (initial water pressure head, initial aqueous concentration, and initial PFAS concentrations in the kinetic

solid-phase and kinetic air–water interfacial sites). Note that the first column specifies the cell-center location, not the location of the upper or lower cell boundaries.

	A	B	C
1	Parameters	Values	Unit
2	tEnd	5	d
3	dt0	1.00E-08	d
4	dtMin	1.00E-15	d
5	dtMax	1.00E-01	d
6	Surfactant_induced_flow	F	True/False
7	Root_uptake_on	F	T/F
8	hA	-5.00E+02	cm
9	dt_Increase	1.5	-
10	dt_Reduce	0.5	-
11	N_Iter_L	12	-
12	N_Iter_H	20	-
13	Max_N_Iter	50	-
14	Tol_th	1.00E-07	cm^3/cm^3
15	Tol_h	1.00E-07	cm
16	Tol_C	1.00E-10	mg/cm^3
17	GW_dilution_on	F	T/F

(a) `Exp1/INPUT/System_ctrl.csv`

	A	B	C
1	Parameter	Value	Unit
2	Molecular_weight	414.07	g/mol
3	a	62.1105	mg/L
4	b	0.19	-
5	Chi	1	-
6	sigma0	72	dyn/cm
7	Dm	0.42336	cm2/d
8	Fs	0.4	-
9	alpha_s	0.001805556	1/d
10	Faw	0.9	-
11	alpha_aw	0.0015	1/d
12	Aaw_SF	1	-
13	Aaw_LookUpTable	T	True/False
14	PFAS_release_depth	1	-
15	First_order_decay	0	1/d

(b) `Exp1/INPUT/PFAS_properties.csv`

Figure 2: Example 1: Input configuration files

The file `Exp1/INPUT/System_ctrl.csv` (Figure 2a) controls global simulation settings and numerical solver behavior, including time stepping, iteration limits, and convergence criteria. It also enables or disables optional modules such as root-water uptake (`Root_uptake_on`) and groundwater risk analysis (`GW_dilution_on`).

PFAS properties (except the solid-phase adsorption parameters K_f and N_f, which are specified in `Soil_profile.csv`) are provided in `Exp1/INPUT/PFAS_properties.csv` (Figure 2b). This file includes parameters for interfacial activity, kinetic adsorption, air–water interfacial area, first-order decay, and boundary mixing.

Boundary conditions are specified in `Exp1/INPUT/Boundary_conditions.csv` (Figure 3).

	A	B	C	D	E	F	G	H
1	t (d)	Precipitation (cm/d)	Irrigation (cm/d)	ET0 (cm/d)	top_BC (cm)	bot_BC (cm)	Contaminated_water_flux (cm/d)	PFAS_mass_flux (mg/d/cm^2)
2	0.1	0	0	0	-60.6222	-60.6222	0	0.001
3	2	0	0	0	-60.6222	-60.6222	0	0
4	3	0	0	0	-60.6222	-60.6222	0	0
5	4	0	0	0	-60.6222	-60.6222	0	0
6	5	0	0	0	-60.6222	-60.6222	0	0

Figure 3: Example 1: `Exp1/INPUT/Boundary_conditions.csv`

	A	B	C	D	E	F	G	H	I	J
1	Observed_cells									
2	5	10	15	50						
3	t_profile(d)									
4	0.5	1	1.5	2	2.5	3	3.5	4	4.5	5

Figure 4: Example 1: `Exp1/INPUT/Output_ctrl.csv`

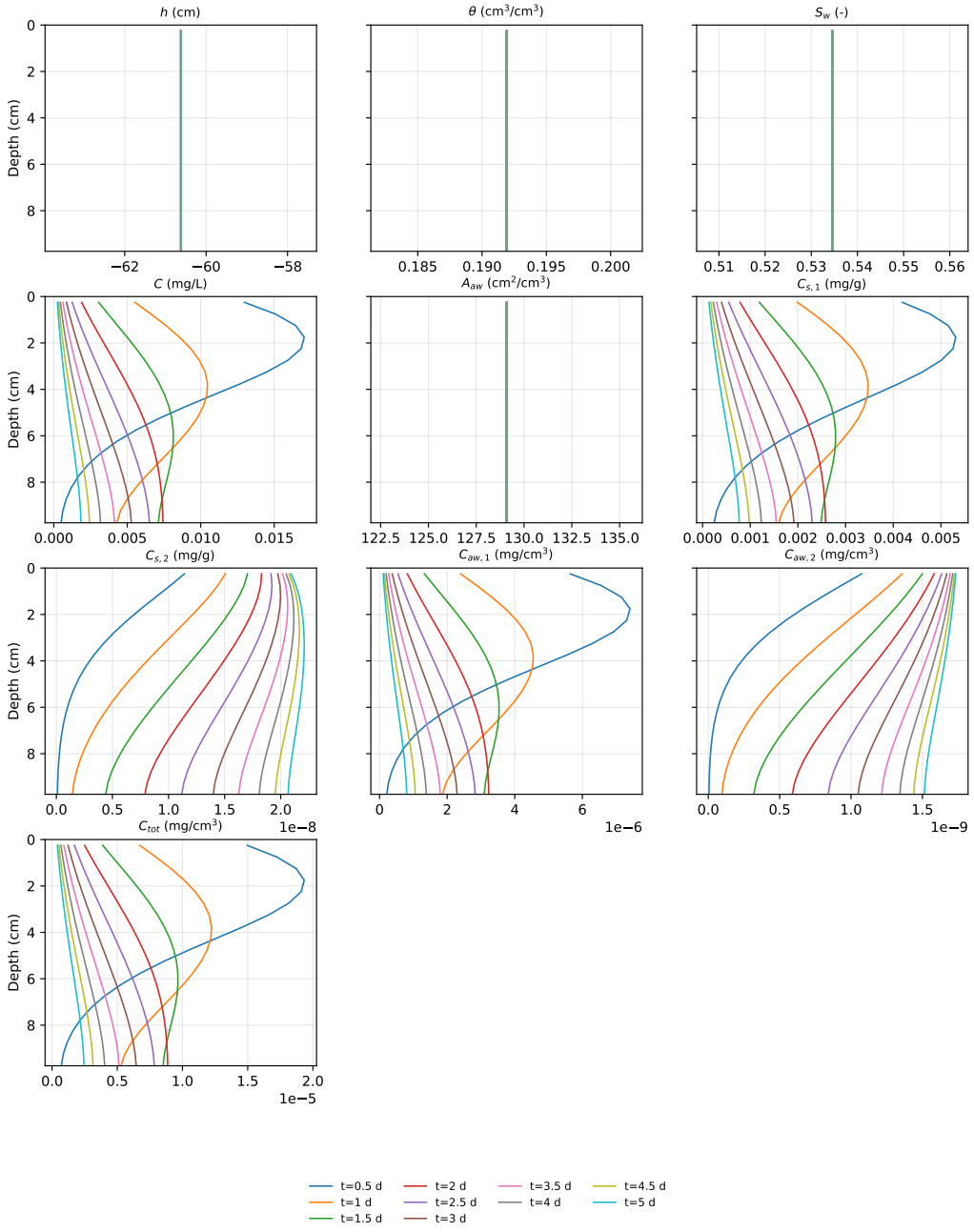

Figure 5: Example 1: Simulated profiles.

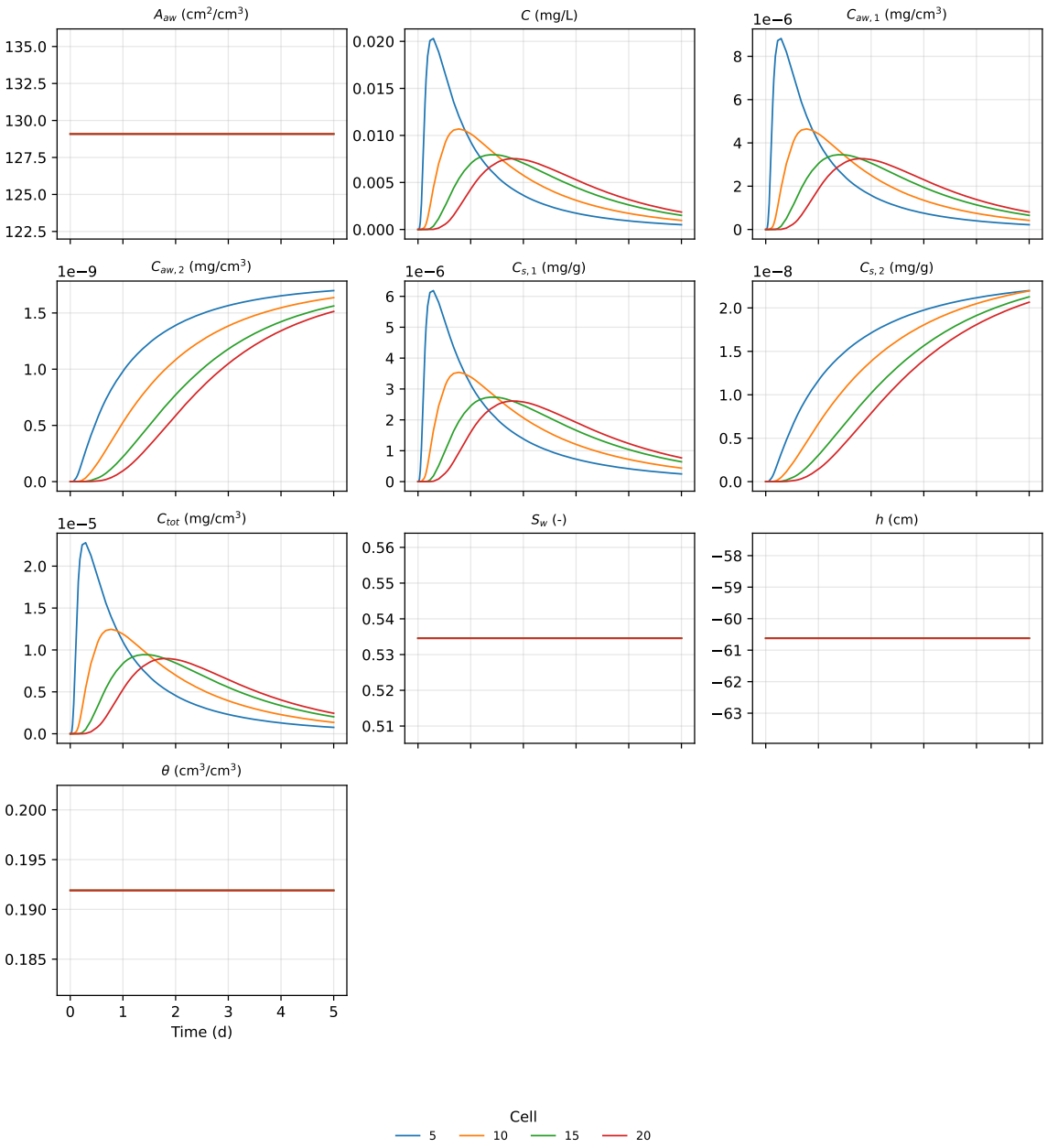

Figure 6: Example 1: Monitored cells. The monitored cell IDs are 5, 10, 15, and 20; the corresponding cell centers are located at z = 2.25, 4.75, 7.25, and 9.75 cm, respectively.

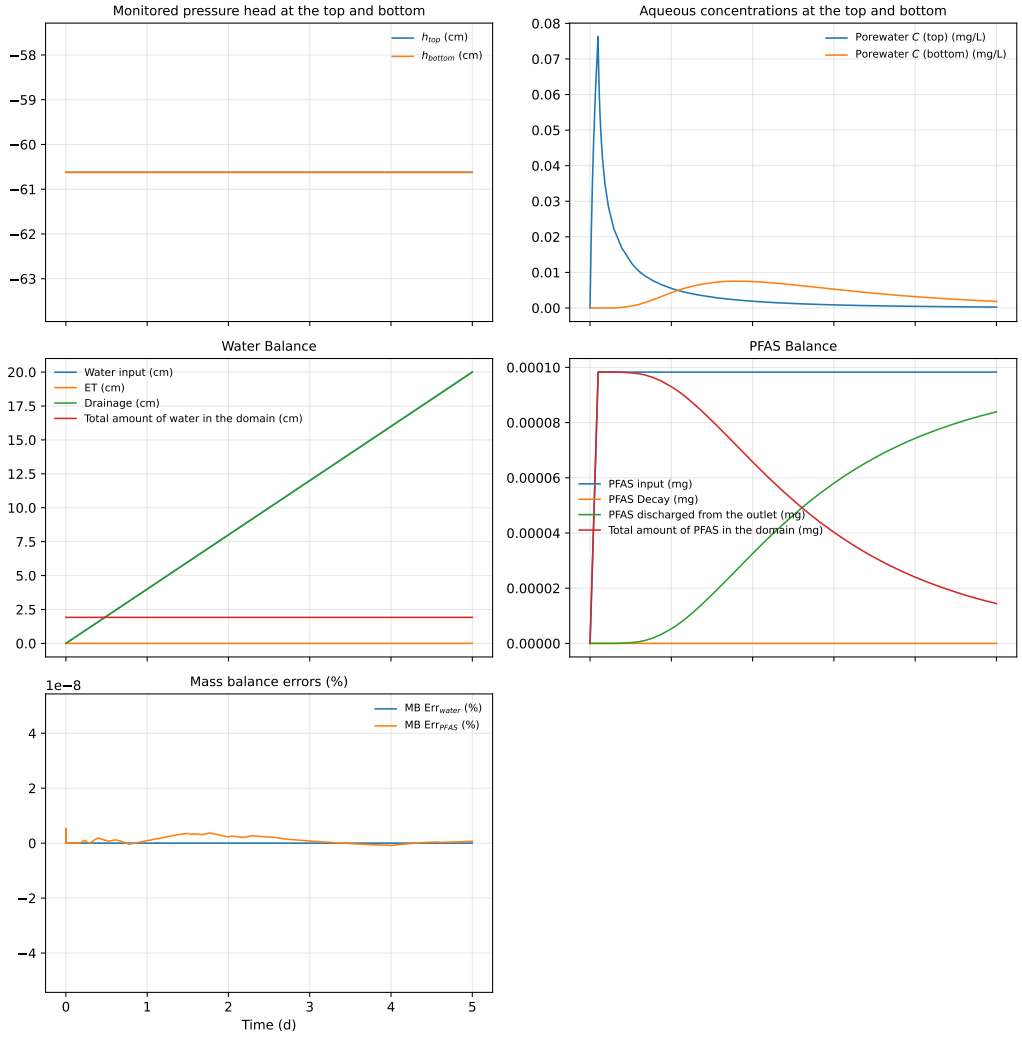

Figure 7: Example 1: Time series.

The file `Exp1/INPUT/Output_ctrl.csv` (Figure 4) defines two user-specified output settings: (1) IDs of numerical cells to monitor and (2) times for exporting full-domain profiles. Profile outputs are saved as `Exp1/OUTPUT/1.Profile-Time-XXX.csv`, where `XXX` = 1, 2, 3, ... corresponds to the sequence of profile times listed in `Exp1/INPUT/Output_ctrl.csv`.

4.1.3 Output files and modeling results

Guidance on interpreting output files is provided in Section 3. Figures 5–7 display the simulation results for Example 1, including time-varying one-dimensional profiles, time series for monitored variables at user-specified cells, and comprehensive time series for all variables across the entire domain.

Note: Example 1 does not include groundwater contamination analysis. Consequently, the file `OUTPUT/4.Summary.csv` contains only basic information related to the simulation.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	z (cm)	Ksat (cm/d)	ths (cm^3/cm^3)	thr (cm^3/cm^3)	alpha (1/cm)	n (-)	rhob (g/cm^3)	alphaL (cm)	Kf (mg/g)/(mg /cm^3)^Nf	Nf (-)	h0 (cm)	theta0(c m^3/cm^ 3)	C0 (mg/L)	Cs20 (mg/g)	Caw20 (mg/cm^ 3)	Ctot0(mg /cm^3)
2	0.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
3	0.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
4	1.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
5	1.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
6	2.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
7	2.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
8	3.25	1800	0.294	0.03	0.046	4.5	1.65	2	0.04074185	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
9	3.75	1800	0.294	0.03	0.046	4.5	1.65	2	0.04074185	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
10	4.25	1800	0.294	0.03	0.046	4.5	1.65	2	0.04074185	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
11	4.75	1800	0.294	0.03	0.046	4.5	1.65	2	0.04074185	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
12	5.25	1800	0.294	0.03	0.046	4.5	1.65	2	0.04074185	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
13	5.75	1800	0.294	0.03	0.046	4.5	1.65	2	0.04074185	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
14	6.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
15	6.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
16	7.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
17	7.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
18	8.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
19	8.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
20	9.25	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00
21	9.75	100	0.359	0.07	0.02	4	1.627	2	0.2351	0.87	-300	-1	0.00E+00	0.00E+00	0.00E+00	-1.00E+00

Figure 8: Example 2: `Exp2/INPUT/Soil_profile.csv`

4.2 Example 2: Modeling PFAS leaching in a heterogeneous soil column with transient water flow

4.2.1 Parameter setup

Example 2 simulates PFAS breakthrough behavior in a one-dimensional soil column under transient water-flow conditions. The primary objective is to demonstrate model capability for coupled non-steady-state water flow and PFAS transport, and to illustrate how transient hydrologic conditions influence PFAS leaching dynamics.

The model configuration is identical to Example 1 in PFAS properties, spatial discretization, and output settings. However, a coarse-sand layer (thickness = 3 cm, Accusand parameters in Table 11) is added over $z \in [3, 6]$ cm. The only differences between the two examples are initial hydraulic conditions and boundary conditions for water flow and solute input. Consequently, differences in simulated PFAS breakthrough behavior can be directly attributed to transient water-flow effects rather than changes in material properties or chemical parameters.

The same input files for system control, PFAS properties, and output control used in Example 1 are adopted here and are therefore not repeated in this section.

4.2.2 Input files

In `Exp2/INPUT/Soil_profile.csv` (Figure 8), the initial soil water pressure head is specified as spatially uniform throughout the column, with a value of $h_0 = -300$ cm. This initial condition represents a relatively dry soil state compared to Example 1, in which the soil column was initialized under steady-state flow conditions. As a result, significant transient redistribution of soil moisture occurs following the onset of infiltration.

	A	B	C	D	E	F	G	H
1	t (d)	Precipitation (cm/d)	Irrigation (cm/d)	ET0 (cm/d)	top_BC (cm)	bot_BC (cm)	Contaminated_water_flux (cm/d)	PFAS_mass_flux (mg/d/cm^2)
2	0.1	0	0	0	-999999.99	-999999.99	1	0.001
3	2	1	0	0	-999999.99	-999999.99	0	0
4	3	0	0	0	-999999.99	-999999.99	0	0
5	4	0	0	0	-999999.99	-999999.99	0	0
6	5	2	0	0	-999999.99	-999999.99	0	0

Figure 9: Example 2: `Exp2/INPUT/Boundary_conditions.csv`

Boundary conditions are specified in `Exp2/INPUT/Boundary_conditions.csv` (Figure 9). The upper boundary is set as an open flux boundary by specifying `top_BC < -999999` (e.g., `top_BC = -999999.99`), which allows infiltration to be prescribed directly through surface water flux. The lower boundary is set to free drainage (unit-gradient boundary) by specifying `bot_BC < -999999` (e.g., `bot_BC = -999999.99`).

During the initial injection period of 0.1 d (2.4 hours), a constant PFOA mass flux of 0.001 mg/d/cm^2 is applied at the land surface. Simultaneously, a short-term downward water flux of q_{top} = 1 cm/d is imposed. After the injection period (t = 0.1 d), PFAS mass flux is set to zero; PFAS-free water is then applied at the top boundary with q_{top} = 1 cm/d from t = 0.1 d to t = 2 d. From t = 2 d to t = 4 d, no water or PFAS is applied. From t = 4 d to t = 5 d, water application resumes at q_{top} = 2 cm/d and remains until the end of the simulation. This boundary setup produces advective PFAS flushing under transient moisture conditions. The free-drainage lower boundary remains unchanged.

4.2.3 Modeling results

Figures 10–12 display the simulation results for Example 2, including time-varying one-dimensional profiles, time series for monitored variables at user-specified cells, and comprehensive time series for all variables across the entire domain.

Compared to Example 1, the PFAS breakthrough curves and concentration profiles exhibit pronounced transient behavior associated with the evolving soil moisture distribution. As infiltration proceeds, changes in water content alter pore-water velocities, air–water interfacial area, and retention capacity, leading to time-dependent variations in PFAS transport and retardation.

The results demonstrate the ability of PFAS-LEACH-Numerical-1D to capture coupled transient flow and transport processes, including delayed PFAS arrival at the column outlet, nonuniform concentration profiles during wetting fronts, and dynamic mass-balance responses. This example highlights the importance of accounting for transient hydrologic conditions when interpreting PFAS leaching behavior in heterogeneous unsaturated soils.

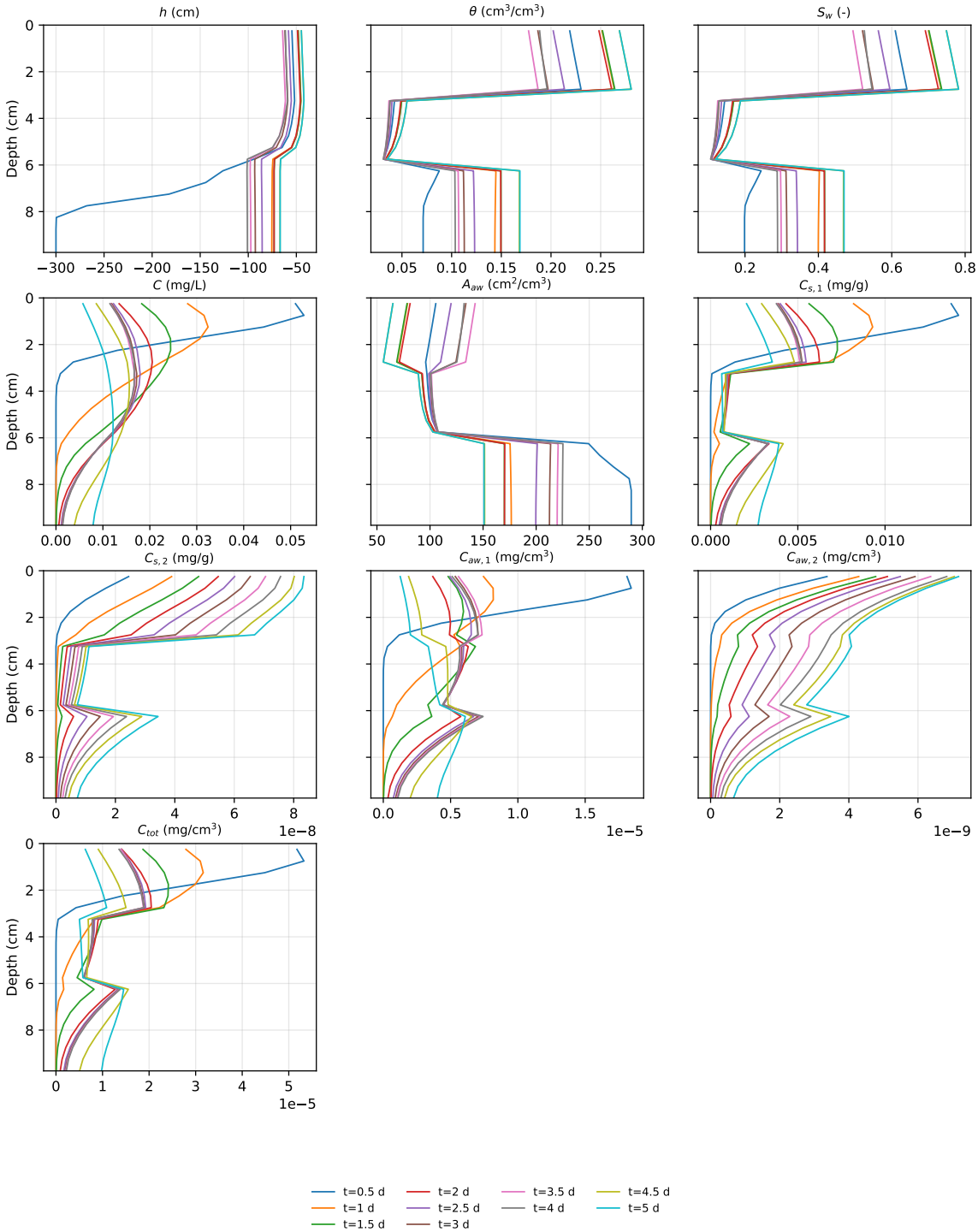

Figure 10: Example 2: Simulated profiles.

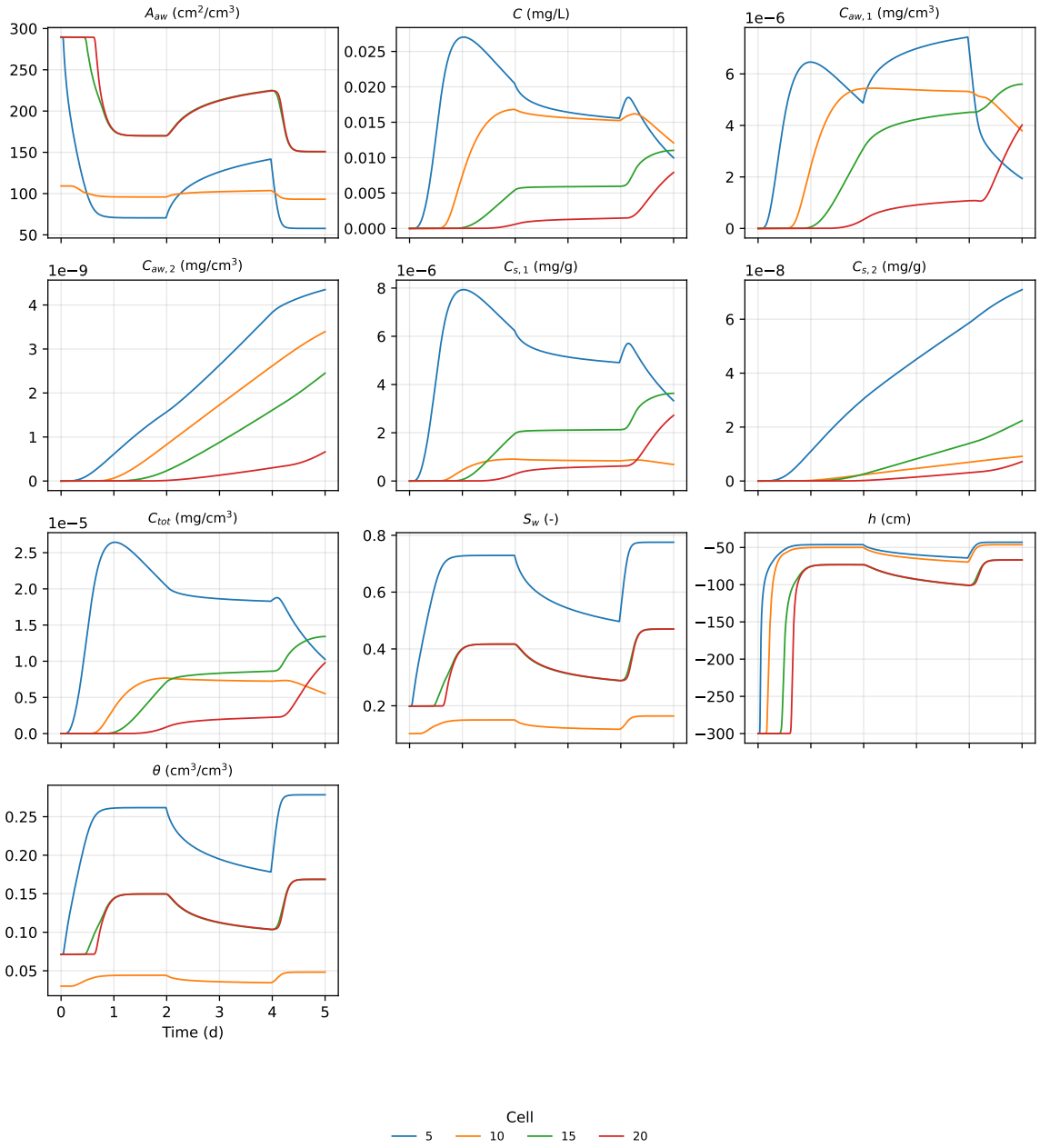

Figure 11: Example 2: Monitored cells. The monitored cell IDs are 5, 10, 15, and 20; the corresponding cell centers are located at z = 2.25, 4.75, 7.25, and 9.75 cm, respectively.

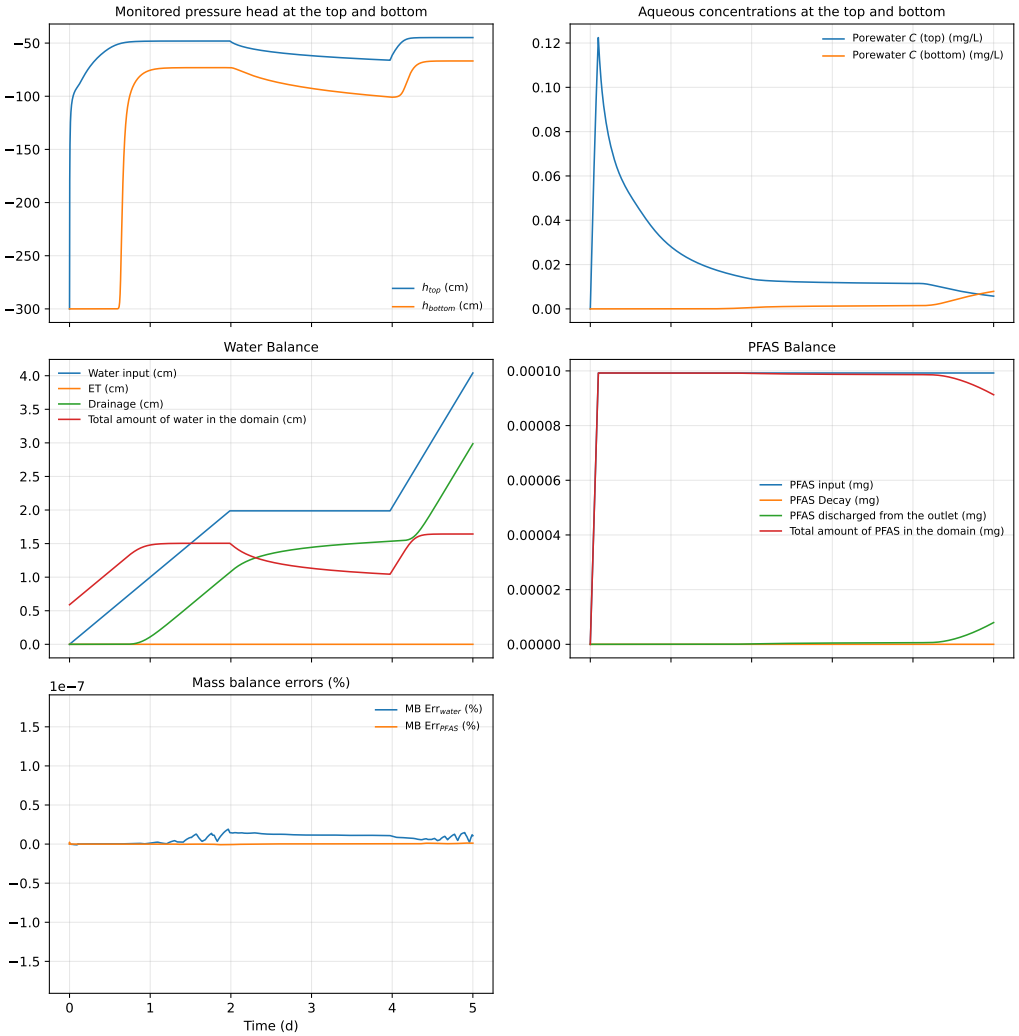

Figure 12: Example 2: Time series.

4.3 Example 3: Modeling PFAS discharge to groundwater

4.3.1 Parameter setup

Example 3 simulates long-term leaching of PFOA from a contaminated vadose zone at a synthetic fire-training-area site and evaluates potential PFAS discharge to downgradient groundwater. The site is assumed to have experienced approximately 30 years of fire-training activities involving PFAS-containing aqueous film-forming foam (AFFF). At simulation start, AFFF application has ceased.

The vadose zone is assumed to be 4 m thick, with the groundwater table located more than 6 m below the ground surface. The initial hydraulic condition of the vadose zone corresponds to field capacity, with an approximately uniform water pressure head of $h \approx -100$ cm. Initial distributions of water pressure head and PFOA concentration in the vadose zone were generated using synthetic numerical simulations reported by Zeng et al. (2021).

The vertical domain is discretized into 40 uniform numerical cells, each with a thickness of 10 cm. The simulation spans a period of 20 years (7,300 days) and is driven by realistic semi-arid climate conditions representative of Arizona, including time-varying precipitation and reference evapotranspiration. The climate forcing data were adopted from previous studies (Guo et al., 2020).

4.3.2 Input files

In Example 3, soil hydraulic properties, PFAS properties, and spatial discretization follow the same setup as in Examples 1 and 2. Output control settings are also similar, but monitoring locations and output times are adjusted to reflect the longer simulation period and the focus on groundwater discharge. These input files are not reproduced here and can be found in the corresponding example folders.

Unlike Examples 1 and 2, Example 3 activates both the root-water uptake module and the groundwater contamination risk evaluation. In `Exp3/INPUT/System_ctrl.csv` (Figure 13a), the parameters `Root_uptake_on` and `GW_dilution_on` are both set to `T`.

Vegetation at the site is assumed to be turf grass typical of arid regions such as Arizona, where seasonal variation in growth is limited due to persistent water stress. As a result, crop coefficients are assumed to be constant and relatively low, with $K_{c,init} = K_{c,mid} = K_{c,end} = 0.1$. The five growth-stage timing parameters ($t_{Seedling}$, t_1, t_2, t_3, and t_4) are therefore prescribed in a simplified manner, with $t_{Seedling} = 0$ and $t_4 = 365$ d, while $t_1 = 60$ d, $t_2 = 150$ d, $t_3 = 300$ d.

The initial rooting depth is assumed to be equal to the maximum rooting depth, such that $L_{Root,0} = L_{Root,max} = 20$ cm. The maximum leaf area index is set to $LAI_{max} = 2.2$, representative of turf grass. Because the crop coefficient is constant, the specific value of LAI_{max} has a negligible impact on simulated evapotranspiration. The corresponding input file is shown in Figure 13b.

Boundary condition settings for Example 3 are similar to those used in Example 2 (Figure 14), with an open flux boundary at the land surface and a free-drainage boundary at the bottom of the domain. No irrigation is applied at the site, and no additional PFAS mass input is specified at the surface (i.e., PFAS-related columns are set to zero).

	A	B	C
1	Parameters	Values	Unit
2	tEnd	7300	day
3	dt0	1.00E-08	day
4	dtMin	1.00E-15	day
5	dtMax	1.00E+00	day
6	Surfactant_induced_flow	T	True/False
7	Root_uptake_on	T	T/F
8	hA	-1.00E+03	cm
9	dt_Increase	1.5	-
10	dt_Reduce	0.5	-
11	N_Iter_L	20	-
12	N_Iter_H	35	-
13	Max_N_Iter	50	-
14	Tol_th	1.00E-08	cm^3/cm^3
15	Tol_h	1.00E-08	cm
16	Tol_C	1.00E-10	mg/cm^3
17	GW_dilution_on	T	T/F

(a) `Exp3/INPUT/System_ctrl.csv`

	A	B	C
1	Parameters	Values	Unit
2	t_Seedling	0	day
3	t1	60	day
4	t2	150	day
5	t3	300	day
6	t4	365	day
7	Kc_ini	0.1	-
8	Kc_mid	0.1	-
9	Kc_end	0.1	-
10	LRoot_0	20	cm
11	LRoot_max	20	cm
12	LAI_max	2.2	-
13	K_canopy	0.6	-
14	h1	-10	cm
15	h2	-25	cm
16	h3	-650	cm
17	h4	-80000	cm

(b) `Exp3/INPUT/Root_uptake.csv`

Figure 13: Example 3: Input configuration files

Because root-water uptake is activated, the evapotranspiration input (column `ET_0`) represents reference evapotranspiration estimated from meteorological data using the FAO 56 Penman–Monteith method.

Parameters required for groundwater contamination risk evaluation are provided in `Exp3/INPUT/Groundwater_pollution.csv` (Figure 15). These parameters are used to estimate the dilution factor and assess potential PFAS impacts at downgradient groundwater receptors.

4.3.3 Output files and modeling results

In addition to basic system information, the output summary for Example 3 includes additional entries related to groundwater contamination assessment, such as the estimated mixing zone thickness and dilution factor (Figure 16).

Figures 17–19 display the simulation results for Example 3, including time-varying one-dimensional profiles, time series for monitored variables at user-specified cells, and comprehensive time series for all variables across the entire domain.

	A	B	C	D	E	F	G	H
1	t (d)	Precipitation (cm/d)	Irrigation (cm/d)	ET0 (cm/d)	top_BC (cm)	bot_BC (cm)	Contaminated_ water_flux (cm/d)	PFAS_mass_flux (mg/d/cm^2)
2	1	0	0	0.049707	-999999.99	-999999.99	0	0
3	2	0	0	0.066144	-999999.99	-999999.99	0	0
4	3	0	0	0.07269	-999999.99	-999999.99	0	0
5	4	0	0	0.126074	-999999.99	-999999.99	0	0
6	5	0	0	0.052537	-999999.99	-999999.99	0	0
7	6	0	0	0.053445	-999999.99	-999999.99	0	0
8	7	0	0	0.051122	-999999.99	-999999.99	0	0
9	8	0	0	0.04834	-999999.99	-999999.99	0	0
10	9	0	0	0.035102	-999999.99	-999999.99	0	0
11	10	0	0	0.038451	-999999.99	-999999.99	0	0
12	11	0	0	0.034775	-999999.99	-999999.99	0	0
13	12	0	0	0.048151	-999999.99	-999999.99	0	0
14	13	0	0	0.029991	-999999.99	-999999.99	0	0
15	14	0	0	0.025386	-999999.99	-999999.99	0	0
16	15	0	0	0.029967	-999999.99	-999999.99	0	0
17	16	0	0	0.026735	-999999.99	-999999.99	0	0
18	17	0	0	0.02596	-999999.99	-999999.99	0	0
19	18	0	0	0.024974	-999999.99	-999999.99	0	0
20	19	0	0	0.021797	-999999.99	-999999.99	0	0
21	20	0	0	0.016073	-999999.99	-999999.99	0	0
22	21	0.292	0	0.041071	-999999.99	-999999.99	0	0
23	22	0	0	0.082922	-999999.99	-999999.99	0	0
24	23	0	0	0.046187	-999999.99	-999999.99	0	0

Figure 14: Example 3: `Exp3/INPUT/Boundary_conditions.csv`

	A	B	C
1	Parameters	Values	Unit
2	Groundwater_Darcy_flux	50	cm/day
3	Lateral_plume_length	10000	cm
4	Thickness_of_saturated_zone	500	cm

Figure 15: Example 3: `Exp3/INPUT/Groundwater_pollution.csv`

	A	B	C
1	Total days	7300	day
2	Length of 1D domain	400	cm
3	Number of numerical cells	40	-
4	CPU COST	6.27	seconds
5	Average recharge	0.04	cm/day
6	Lateral groundwater flux	50	cm/day
7	Lateral plume length	10000	cm
8	Mixing zone thickness	1065.69	cm
9	Groundwater dilution factor (DF)	144.1	-

Figure 16: Example 3: Summary of the simulation results.

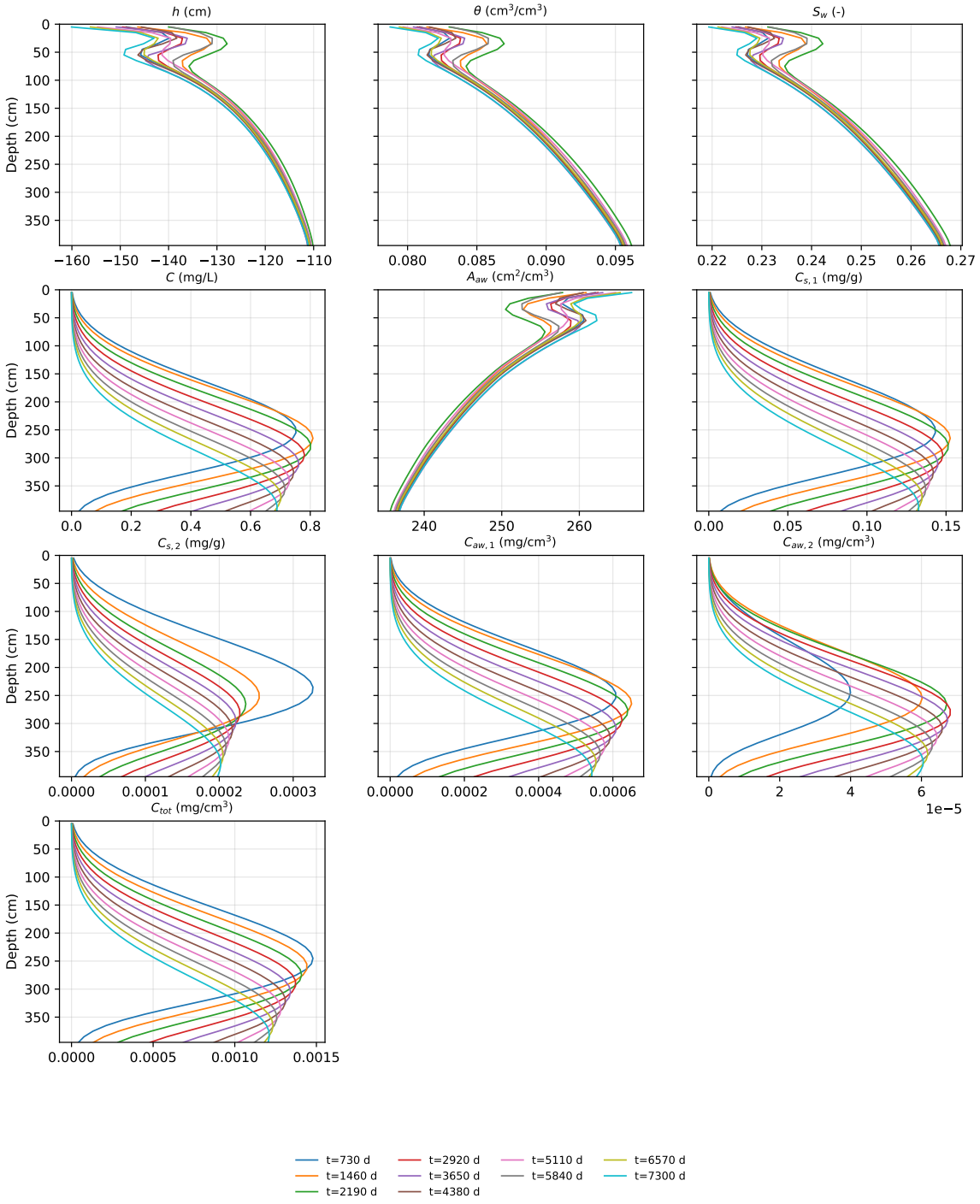

Figure 17: Example 3: Simulated profiles.

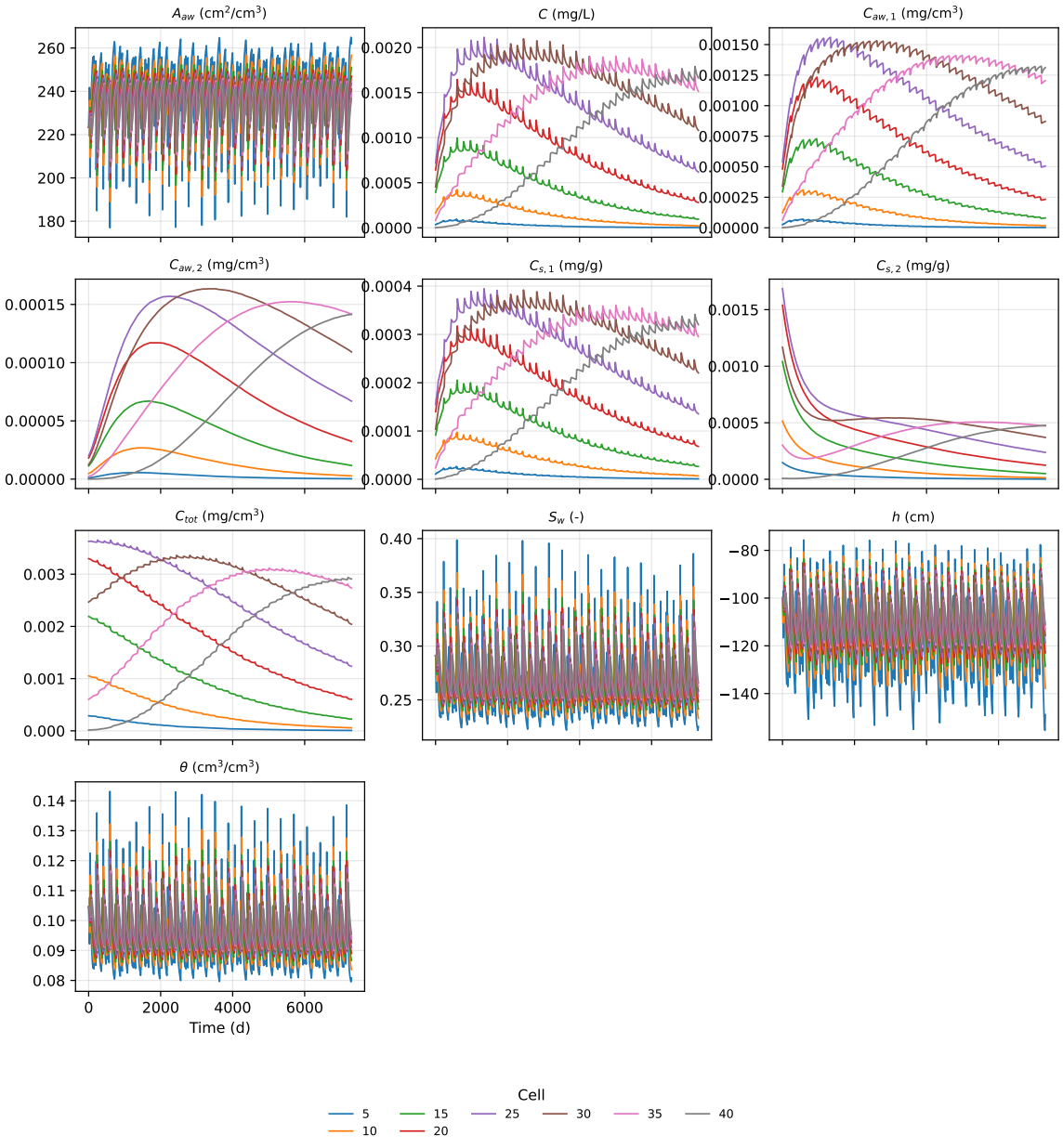

Figure 18: Example 3: Monitored cells. The monitored cell IDs are 5, 10, 15, 20, 25, 30, 35, and 40; the corresponding cell centers are located at z = 45, 95, 145, 195, 245, 295, 345, and 395 cm, respectively.

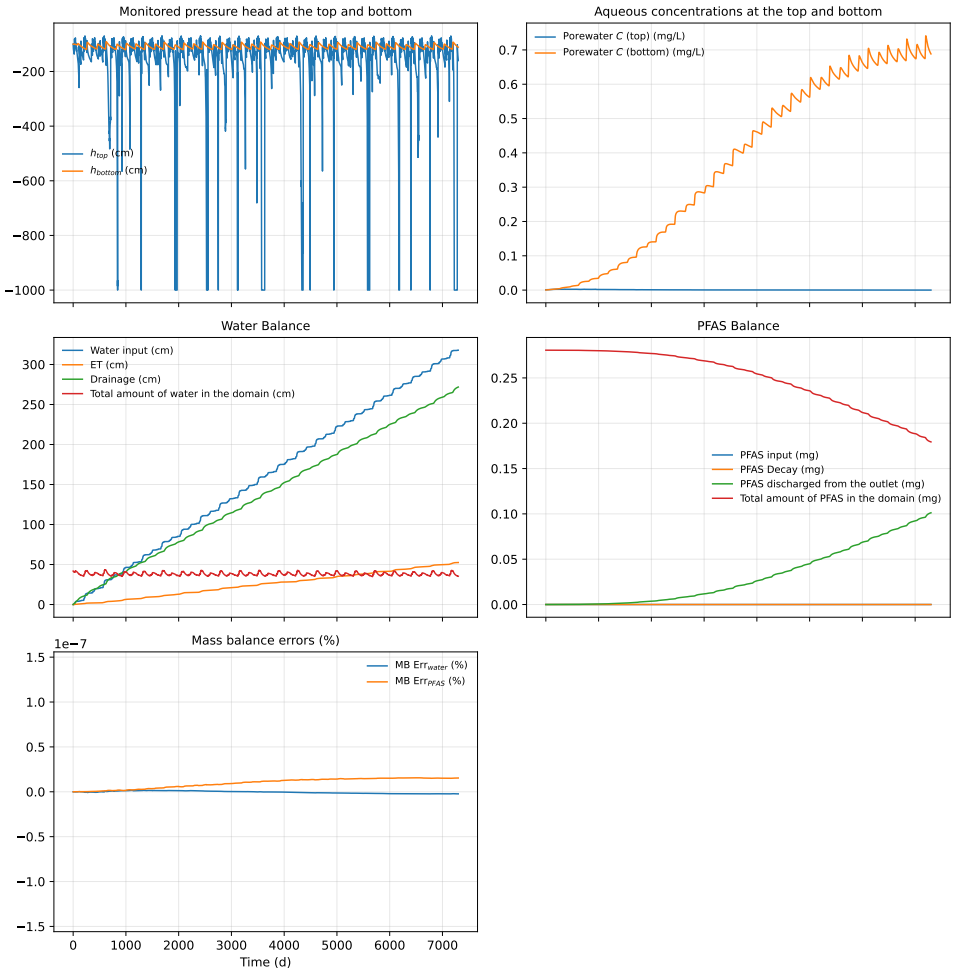

Figure 19: Example 3: Time series.

References

Allen, R.G., Pereira, L.S., Raes, D., Smith, M., et al., 1998. Fao irrigation and drainage paper no. 56. Rome: food and agriculture organization of the United Nations 56, e156.

Chen, S., Guo, B., 2025. Semi-analytical solutions for nonequilibrium transport and transformation of pfas and other solutes in heterogeneous vadose zones with structured porous media. Advances in Water Resources , 105099.

Guo, B., Zeng, J., Brusseau, M.L., 2020. A mathematical model for the release, transport, and retention of per-and polyfluoroalkyl substances (pfas) in the vadose zone. Water Resources Research 56, e2019WR026667.

USEPA, 1996. Soil screening guidance: Technical background document, second edition. Office of Solid Waste and Emergency Response .

Xu, M., Eckstein, Y., 1995. Use of weighted least-squares method in evaluation of the relationship between dispersivity and field scale. Groundwater 33, 905–908.

Zeng, J., Brusseau, M.L., Guo, B., 2021. Model validation and analyses of parameter sensitivity and uncertainty for modeling long-term retention and leaching of pfas in the vadose zone. Journal of Hydrology 603, 127172.

Zeng, J., Guo, B., 2021. Multidimensional simulation of pfas transport and leaching in the vadose zone: Impact of surfactant-induced flow and subsurface heterogeneities. Advances in Water Resources 155, 104015.