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# 2D Finite-difference Simulation of Transport of Post-wildfire PFAS Contamination

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**Abstract:** The frequency and size of wildfire events have increased significantly. Every year, approximately 650 million acres of forests are burned by wildfires. These events not only directly affect the physical, chemical, and biogeochemical properties of the soil and surface materials through the heating and combustion process but also indirectly through changes in vegetation and soil erosion. Moreover, the way humans respond to wildfires can also have an impact on the environment. For instance, the use of aqueous film-forming foams (AFFFs) is an effective method to suppress fires, but they contain per- and polyfluoroalkyl substances (PFAS) that are toxic and persistent in the soil environment. Hence, there is a growing need to understand the behaviour of PFAS in the environment, as they are becoming increasingly prevalent due to their use in fire-fighting foams. In addition to adsorption to soil particles, PFAS have a tendency to adhere to the interface between air and water in the soil, which complicates their presence and transport in unsaturated soils. The air-water interface can significantly increase the retention of PFAS during its transport. In this paper, a two-dimensional (2D) numerical model was developed to simulate the transport of PFAS by incorporating advection-dispersion and taking into account the impact of adsorption on the air-water interface and soil solid phase. This study shows that though advection is generally the dominant factor in PFAS transport in saturated systems, the presence of adsorption onto air-water interfaces in the soil can significantly affect transport rates and become dominant in unsaturated cases.

*Keywords: Wildfire, PFAS, contamination, finite-difference scheme, numerical model*

## 1 INTRODUCTION

The impact of wildfires and post-fire contamination of soil and groundwater has become more pronounced due to the increase in the frequency and intensity of wildfires worldwide. Not only do these fires pose direct hazards, but they can also lead to secondary contamination issues that pose a threat to human and environmental health. For example, the use of aqueous film-forming foams (AFFFs) during fire suppression can release per- and polyfluoroalkyl substances (PFAS) into the soil, which are mobile, toxic, and persist for long periods of time (Ahrens, 2011; Krafft & Riess, 2015; Rayne & Forest, 2009) leading to soil and groundwater contamination. This contamination has mainly affected drinking water and has been linked to a range of human health issues, including complications in fetuses and placentas (Blake & Fenton, 2020; Nian et al., 2020), alterations in baby growth (Liew et al., 2018), and cancer (Vieira et al., 2013), among others (Steenland et al., 2018; Xu et al., 2020).

Despite a significant amount of research in recent years, there is still much that is not known about PFAS, particularly in terms of their behaviour in soil and water environments (U.S. EPA, 2021). There is also a limited understanding of how PFAS move and spread in the environment and how they are transported and transformed in different environmental media. This has made it challenging for researchers and regulators to fully assess the risks posed by PFAS and develop effective strategies for managing this family of chemicals.

Recently, Gu et al. (2020) introduced a mathematical model for the transport of PFAS under transient, variably saturated flow in the vadose zone for the first time and implemented this model to a model source zone impacted by AFFF. Later, relying on the mathematical model and experimental data by Gu et al. (2020), Iradukunda and Farid (2022) developed a one-dimensional (1D) multiphysics numerical model to study the fate and transport of PFAS, incorporating transient seepage and advection-

dispersion, also accounting for the adsorption to the air-water interface and solid phase. Both the above-mentioned mathematical and numerical models are limited to analysing 1D problems and applicable to laboratory scale experiments, whereas a higher-dimensional model is required to investigate more complex and real-world problems.

In this study, a 2D numerical model is developed to improve the understanding of PFAS transport in soil environments. Additionally, utilizing the experimental data found in the literature (Guo et al., 2020) various scenarios have been simulated, taking into consideration the impacts of advection-dispersion and adsorption to air-water interface and solid-phase on the transport of PFAS.

## 2 MATHEMATICAL MODEL AND NUMERICAL FRAMEWORK

### 2.1 Mathematical model

The transport of PFAS is governed by the interaction of advection, hydrodynamic diffusion, and adsorption at solid (i.e., soil particles) and air-water interfaces, derived from conservation of mass, described as (Iradukunda & Farid, 2022; Zeng & Guo, 2021):

$$\rho_b \frac{\partial}{\partial t} K_f C^N + \frac{\partial}{\partial t}(A_{aw} K_{aw} C) + \nabla(\theta \boldsymbol{v} C) - \nabla \cdot (\theta \boldsymbol{D} \nabla C) = -\frac{\partial(\theta C)}{\partial t}, \quad (1)$$

where $\rho_b$ is the bulk density of the porous medium (g/cm$^3$); $K_f$ and $N$ are fitting parameters to Freundlich solid adsorption isotherm, found based on experimental data; $C$ is the aqueous concentration of PFAS (µmol/cm$^3$); $A_{aw}$ is the air-water interfacial area (cm$^2$/cm$^3$); $K_{aw}$ is the air-water interfacial adsorption coefficient (cm$^3$/cm$^2$); $\theta$ is the volumetric water content (cm$^3$/cm$^3$); $\boldsymbol{v} = q/\theta$ is the interstitial pore-water velocity (cm/s); $q$ is the Darcy flux (cm/s); and $\boldsymbol{D}$ is the dispersion/diffusion coefficient (cm$^2$/s). The air-water interfacial area, $A_{aw}$, depends on capillary pressure head, water saturation, and the imbibition and drainage history, which can be approximated as a function of water saturation, $S_w$, as follows (Guo et al., 2020).

$$A_{aw} = x_2 {S_w}^2 + x_1 S_w + x_0, \quad (2)$$

where $x_2$, $x_1$, and $x_0$ are fitting parameters for the soil and sand used in the experiment. Furthermore, the air-water interfacial adsorption coefficient can be described by the following equation (Brusseau, 2018; Kim et al., 1997).

$$K_{aw} = \frac{-1}{RTC}\left(\frac{\partial \sigma}{\sigma \ln C}\right)_T, \quad (3)$$

where the universal gas constant, $R = 8.1314$ JK$^{-1}$ mol$^{-1}$, $T$ is the temperature (K), and $\sigma$ is surface tension (dyne/cm), expressed by the Szyszkowski equation, in terms of aqueous concentration $C$ (Chang & Franses, 1995).

$$\sigma = \sigma_0 \left[1 - b \ln\left(1 + \frac{C}{a}\right)\right], \quad (4)$$

where $a$ (µmol/cm$^3$) and $b$ (-) are fitting parameters to the experimental data. Hence, inserting Equation (4) into Equation (3) yields:

$$K_{aw} = \frac{1}{RT} \frac{\sigma_0 b}{a + C}, \quad (5)$$

which shows that $K_{aw}$ monotonically increases as $C$ decreases and asymptotically approaches a maximum value.

For a 2D problem, Equation (1) can be written as:

$$F + \frac{\partial}{\partial t}(A_{aw} K_{aw} C) + \frac{\partial}{\partial x}(\theta v_x C) + \frac{\partial}{\partial z}(\theta v_z C) - \frac{\partial}{\partial x}\left(\theta D_x \frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial z}\left(\theta D_z \frac{\partial C}{\partial z}\right) = -\frac{\partial(\theta C)}{\partial t}, \quad (6)$$

where $F = \rho_b \frac{\partial}{\partial t} K_f C^N$, and $v_x$ and $v_z$, and $D_x$ and $D_z$ are components of $\boldsymbol{v}$ and $\boldsymbol{D}$, respectively.

### 2.2 Numerical framework

A 2D numerical framework was developed using MATLAB to solve the mathematical governing equation (Equation (6)) to outline the conservation of mass. The framework utilized in this paper is a finite-difference method using forward differences for first-order time derivatives and first-order space derivatives and central differences for higher-order space derivatives to discretise both the time and space domains. Two types of boundary conditions were considered in the simulation. Most of the boundaries were treated as impermeable boundaries modelled using Neumann boundary conditions, while the inlets and outlets were given constant aqueous concentration values ($C_1$ and $C_2$, respectively) using Dirichlet boundary conditions. In order to reduce the computational cost and provide numerical stability of the model, the horizontal grid size (∆x) and the vertical grid size (∆z) at a given time step (∆t) need to follow the mathematical relation below.

$$\Delta x = -D_x \frac{C_2 - C_1}{L} \Delta t, \text{ and } \frac{\Delta x}{\Delta z} = \sqrt{\frac{D_x}{D_z}}, \tag{7}$$

where $L$ is the vertical length of the soil domain. Moreover, relying on the Crank-Nicolson scheme (Chávez-Negrete et al., 2018), concentration $C$ on the right-hand side of Equation (6) for each node is written as the weighted average of the values ${C_{i,j}}^{t+1}$ and ${C_{i,j}}^{t}$ where ${C_{i,j}}^{t}$ is the concentration of PFAS at Node $(i,j)$. The finite-difference method was used to linearize the governing partial differential equation (PDE) described above (Equation 6) into Equation (8).

$$-C_{i,j+1}^{t+1}\left(-\frac{\theta_{i,j}v_{x_{i,j}}}{\Delta x}+\frac{\theta_{i,j}{D_{x_{i,j+1}}}-\theta_{i,j}{D_{x_{i,j}}}}{\Delta x^2}+\frac{\theta_{i,j+1}{D_{x_{i,j}}}}{\Delta x^2}\right)+C_{i,j}^{t+1}\left(\frac{F_{i,j}}{\Delta t}+\frac{Aaw_{i,j}Kaw_{i,j}}{\Delta t}+\frac{\theta_{i,j}v_{x_{i,j+1}}}{\Delta x}+\frac{v_{x_{i,j}}\theta_{i,j+1}}{\Delta x}-\right.$$

$$3\frac{v_{x_{i,j}}\theta_{i,j}}{\Delta x}+\frac{\theta_{i,j}v_{z_{i+1,j}}}{\Delta z}+\frac{v_{z_{i,j}}\theta_{i+1,j}}{\Delta z}-3\frac{v_{z_{i,j}}\theta_{i,j}}{\Delta z}+\frac{\theta_{i,j}{D_{x_{i,j+1}}}+\theta_{i,j+1}{D_{x_{i,j}}}}{\Delta x^2}+\frac{\theta_{i,j}{D_{z_{i+1,j}}}+\theta_{i+1,j}{D_{z_{i,j}}}}{\Delta z^2}+\frac{\theta_{i,j}}{\Delta t}+$$

$$\left.\frac{\theta_{i,j}^{t+1}-\theta_{i,j}^{t}}{2\Delta t}+\right)-C_{i+1,j}^{t+1}\left(-\frac{\theta_{i,j}v_{z_{i,j}}}{\Delta z}+\frac{\theta_{i+1,j}{D_{z_{i,j}}}}{\Delta z^2}+\frac{\theta_{i,j}{D_{z_{i+1,j}}}-\theta_{i,j}{D_{z_{i,j}}}}{\Delta z^2}\right)-C_{i,j-1}^{t+1}\left(\frac{\theta_{i,j}{D_{x_{i,j}}}}{\Delta x^2}\right)-C_{i-1,j}^{t+1}\left(\frac{\theta_{i,j}{D_{z_{i,j}}}}{\Delta z^2}\right)=$$

$$C_{i,j}^{t}\left(\frac{F_{i,j}}{\Delta t}+\frac{Aaw_{i,j}Kaw_{i,j}}{\Delta t}+\frac{\theta_{i,j}}{\Delta t}-\frac{\theta_{i,j}^{t+1}-\theta_{i,j}^{t}}{2\Delta t}\right), \tag{8}$$

where the Crank-Nicolson schema was used over each time step, i.e., $\theta_{i,j}=\frac{\theta_{i,j}^{t+1}+\theta_{i,j}^{t}}{2}$, $D_{i,j}=\frac{D_{i,j}^{t+1}+D_{i,j}^{t}}{2}$, and $A_{aw_{i,j}}=\frac{{A_{aw}}_{i,j}^{t+1}+{A_{aw}}_{i,j}^{t}}{2}$.

However, coefficients $F$ and $K_{aw}$ are nonlinear functions of $C$. To maintain the linearity of the discretised equation (Equation (8)), $F$ and $K_{aw}$ are updated using a successive iteration scheme. Basically, starting with an initial value of ${C_{i,j}}^{t}$ and ${S_w}_{i,j}^{t}$, $F_{i,j}^{t}$ and ${K_{aw}}_{i,j}^{t}$ are computed using Equations (2) and (5) to initiate a time step to determine ${C_{i,j}}^{t+1}$, and prior to proceeding to the next time step, a successive iteration scheme is employed to update the values of $F_{i,j}^{t}$ and ${K_{aw}}_{i,j}^{t}$, until convergence to the optimal $F_i^{t+1}$ and ${K_{aw}}_i^{t+1}$. This guarantee maintaining the linearity of Equation (8). This allows for solving the system of linear equations presented by Equation (6). At the subsequent time step, ${C_i}^{t+2}$ is calculated based on the average values of $F$ and $K_{aw}$ at time $t+1$ and $t$, and another successive iteration continues until converges to the best $F_i^{t+2}$, and ${K_{aw}}_i^{t+2}$. This process will repeat until the final time.

## 3 DATA AND PROBLEM FORMULATION

### 3.1 Experimental data and parameters

The model is designed in such a manner that it allows for the investigation of PFAS transport through diverse soil types and various scenarios. In this study, the transport of PFAS is simulated through

Accusand soil, and for this simulation, the necessary data and parameters were obtained from a study conducted by Guo et al. (2020).

***Table 1.*** *A summary of the parameters that are used in the simulations for Accusand soil.*

| Parameter | Value | Unit |
|---|---|---|
| $\boldsymbol{\rho_b}$ | 1.65 | g/cm$^3$ |
| $\boldsymbol{K_f}$ | 0.055 | (µmol/g)/(µmol/cm$^3$)$^N$ |
| $\boldsymbol{N}$ | 0.85 | - |
| $\boldsymbol{\sigma}$ | 71 | dyne/cm |
| $\boldsymbol{R}$ | 8.314 | J/K/mol |
| $\boldsymbol{T}$ | 293.15 | K |
| $\boldsymbol{a}$ | 0.004 | µmol/cm$^3$ |
| $\boldsymbol{b}$ | 0.017 | - |
| $\boldsymbol{x_2}$ | 548.54 | - |
| $\boldsymbol{x_1}$ | -1182.5 | - |
| $\boldsymbol{x_0}$ | 633.96 | - |

### 3.2 Problem formulation

The overall Transport Equation (6) was simulated based on two types of boundary conditions. Neumann boundary conditions are considered at all boundaries except for the inlet and outlets. Dirichlet boundary conditions were considered at the inlet and outlets. A constant supply of PFAS concentration is simulated at the inlet on the mid-point on the left vertical boundary. Outlets are considered exposed to an abundance of freshwater; hence, no accumulation of PFAS occurs at three outlets (end corners and mid- point) on the right vertical boundary. It was assumed that there is no initial PFAS contaminant in soil. Therefore, at all the nodes on the mesh grid the concentration of PFAS is 0. Then, for the first time step, PFAS was introduced at the inlet with a concentration of 12 mg/L. Neumann boundary conditions allowed us to simulate the transport of PFAS assuming there is a constant supply of PFAS at the inlet and an accumulation of PFAS concentration at outlets allowing breakthrough concentration.

The following is considered for all of the cases of simulations: (i) initially, the concentration of PFAS in the soil is $C = 0$ µmol/cm$^2$; (ii) except for the inlet and outlets, all other boundaries of soil are impermeable; (iii) the concentration of PFAS at the inlet $C_1 = 12$ mg/L and at outlets $C_2 = 0$ mg/L, for all time steps; (iv) time step size $\Delta t = 5$ seconds; (v) the soil sample size horizontal length $L = 2.1$ m and vertical length (thickness) $H = 2$ m; (vi) the components of the diffusion coefficient $\boldsymbol{D}$ have values $D_x = 5.5 \times 10^{-3}$ m$^2$/s and $D_z = 1.5 \times 10^{-3}$ m$^2$/s ($D_{xz}$ = 0 m$^2$/s); (vii) soil porosity $n = 0.00294$.

## 4 RESULTS AND DISCUSSION

### 4.1 Simulation results

Based on the data presented in the previous section, several scenarios have been numerically simulated for a soil sample with domain discretised into a $26 \times 14$ grid, to analyse the impact on PFAS transport due to diffusion, advection, and adsorption onto the air-water and solid-phase interfaces.

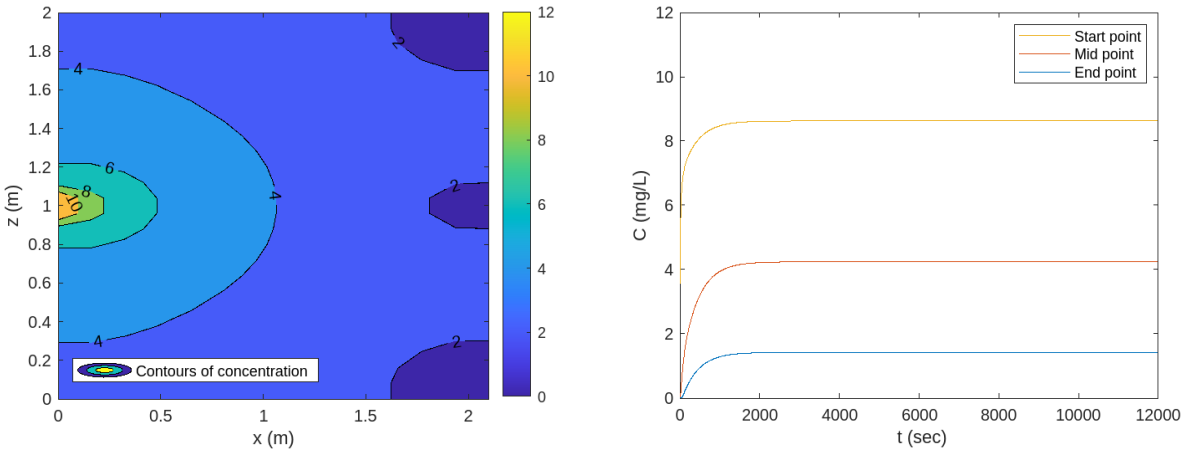
The results are demonstrated as snapshots in time of the spatial distribution of PFAS concentration and the time history at specific locations (i.e., node numbers). Time histories are shown for three nodes, one immediately after (to the right) of the inlet, referred to as the “Start point,” a node just before the outlet at the mid-vertical level, referred to as the “Endpoint,” and a node at the centre of the grid referred to as “Midpoint.”

### 4.1.1 Effect of diffusion coefficients on the transport of PFAS

To investigate the individual effect of diffusion coefficients on the transport of PFAS through fully saturated soil, other terms (e.g. advection, and adsorption onto the air-water and solid-phase interfaces) in Equation (8), were disregarded, and the governing equation would be as follows. This case is analysed for a water-saturated case ($S_w = 1$).

$$-\left(\theta D_x \frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial z}\left(\theta D_z \frac{\partial C}{\partial z}\right) = -\frac{\partial(\theta C)}{\partial t}. \quad (9)$$

The following figures show a snapshot of the spatial distribution after 12000 sec (3 hours and 20 min), and the time history of PFAS transportation.




(a) (b)

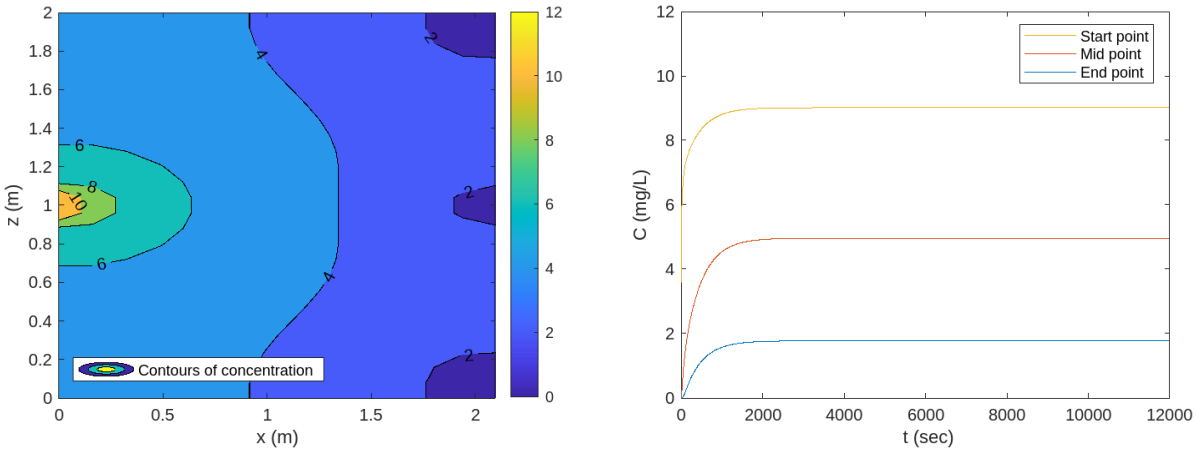
***Figure 1.*** *Diffusion due to a constant supply of PFAS at inlet on the left boundary and three outlets on the right boundary exposed to an abundance of freshwater considering: (a) spatial distribution at time t =12000 seconds; (b) time history of PFAS transportation at three nodes over time.*

### 4.1.2 Effect of advection-diffusion coefficients on the transport of PFAS

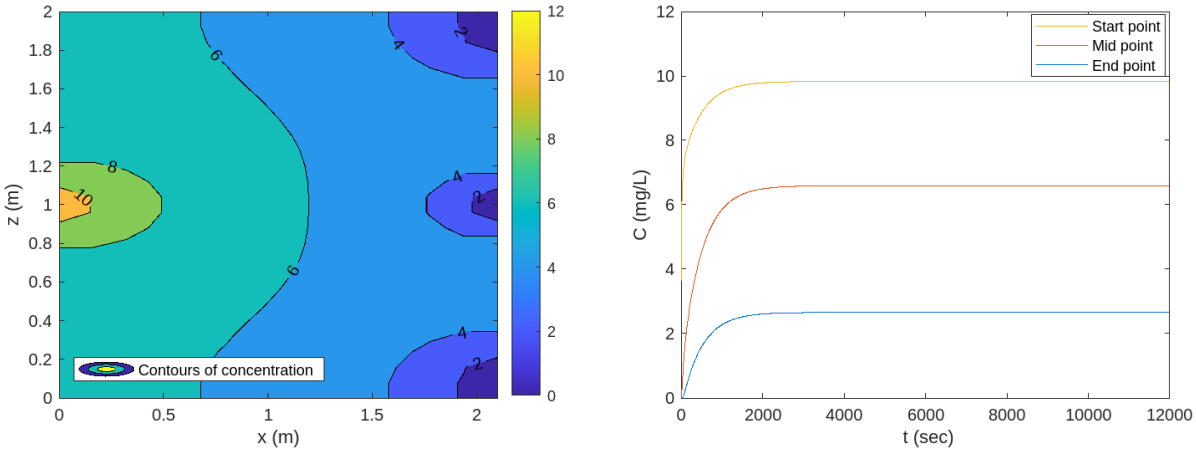
In this scenario, the advection term is introduced in addition to the diffusion coefficients, and the governing equation takes the following form.

$$\frac{\partial}{\partial x}(\theta v_x C) + \frac{\partial}{\partial z}(\theta v_z C) - \left(\theta D_x \frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial z}\left(\theta D_z \frac{\partial C}{\partial z}\right) = -\frac{\partial(\theta C)}{\partial t}. \quad (10)$$

To analyse advection and visualize its effect on PFAS transportation, two values of flow velocity, $\boldsymbol{v}$ are used:(i) $v_x = 1 \times 10^{-3}$ cm/s and $v_z = 0$ cm/s and (ii) $v_x = 3 \times 10^{-3}$ cm/s and $v_z = 0$ cm/s. This case is analysed for a water-saturated case ($S_w = 1$) .



(a) (b)




(c) (d)

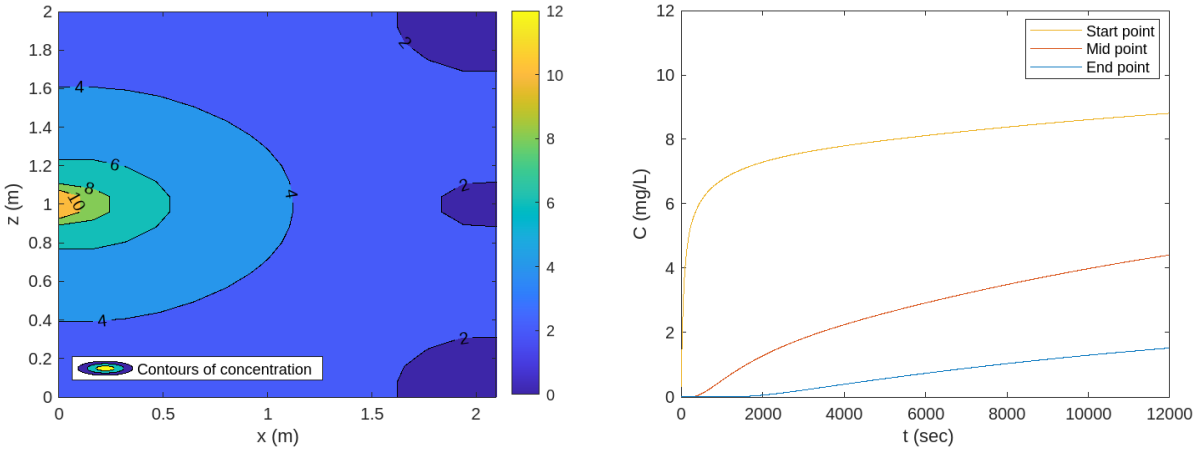
***Figure 2.*** *Diffusion and advection due to a constant supply of PFAS at inlet on the left boundary and three outlets on the right boundary exposed to an abundance of freshwater considering: (a) spatial distribution at time t =12000 seconds for* ***Scenario 1 ($v_x = 1 \times 10^{-3}$ cm/s)****; (b) time history of PFAS transportation at three nodes over time for* ***Scenario 1 ($v_x = 1 \times 10^{-3}$ cm/s)****; (c) spatial distribution at time t =12000 seconds for* ***Scenario 2 ($v_x = 3 \times 10^{-3}$ cm/s)****; (d) time history of PFAS transportation at three nodes over time for* ***Scenario 2 ($v_x = 3 \times 10^{-3}$ cm/s)****.*

### 4.1.3 Effect of adsorption onto solid-phase interfaces on the transport of PFAS

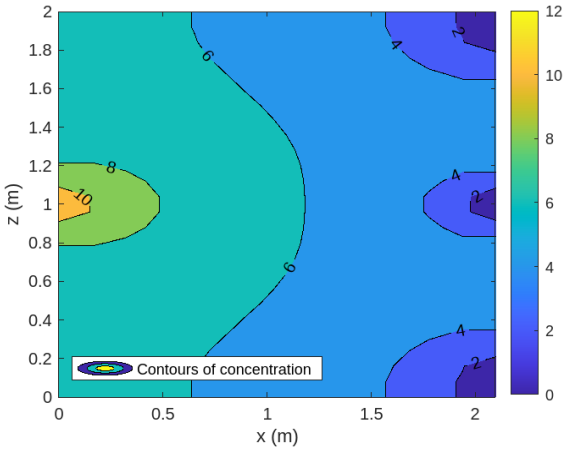
Adding the terms $F = \rho_b \frac{\partial}{\partial t} K_f C^N$ will introduce the adsorption onto solid-phase interfaces into Equation (9):

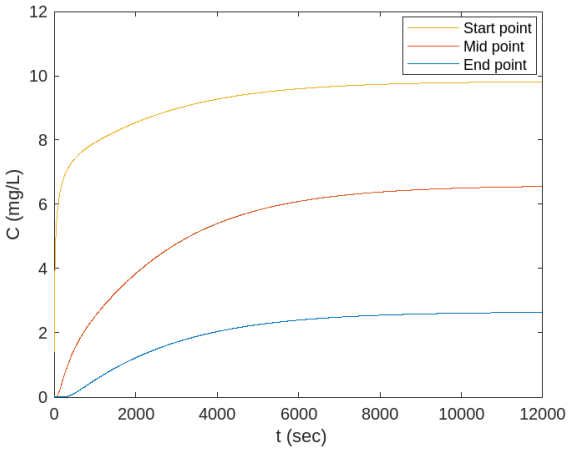
$$F + \frac{\partial}{\partial x}(\theta v_x C) + \frac{\partial}{\partial z}(\theta v_z C) - \frac{\partial}{\partial x}\left(\theta D_x \frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial z}\left(\theta D_z \frac{\partial C}{\partial z}\right) = -\frac{\partial(\theta C)}{\partial t}. \quad (11)$$

In this case, flow velocity v with components $v_x = 3 \times 10^{-3}$ cm/s and $v_z = 0$ cm/s was taken into consideration. The resulting two cases demonstrate the impact of solid-phase adsorption on PFAS diffusion (no advection). Two values were selected $K_f$: $K_f = 0.055$ µmol/g from the experimental data and a choice with less adsorptive nature, $K_f = 0.01$ µmol/g. This case is analysed for a water-saturated condition ($S_w = 1$).




(a) (b)




(c) (d)

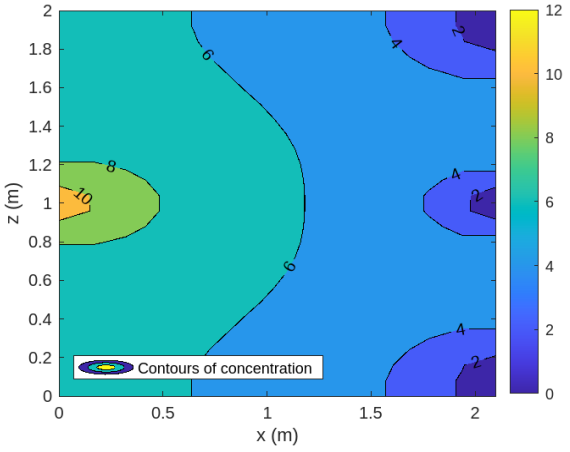
***Figure 3.*** *Diffusion and adsorption to soil, a constant supply of PFAS at inlet on the left boundary and three outlets on the right boundary exposed to an abundance of freshwater considering: (a) spatial distribution at time t =12000 seconds for* ***Scenario 1 ($K_f = 0.055$ μmol/g)****; (b) time history of PFAS transportation at three nodes over time for* ***Scenario 1 ($K_f = 0.055$ μmol/g)****; (c) spatial distribution at time t =12000 seconds for* ***Scenario 2 ($K_f = 0.01$ μmol/g)****; (d) time history of PFAS transportation at three nodes over time for* ***Scenario 2 ($K_f = 0.01$ μmol/g)****.*

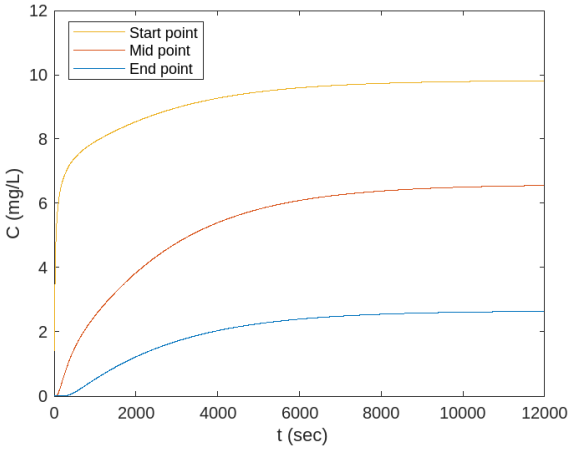
### 4.1.4 Effect of adsorption onto air-water interfaces on the transport of PFAS

Finally, considering the adsorption on air-water interfaces, Equation (11) turns into the following equation which represent the overall PFAS transport.

$$F + \frac{\partial}{\partial t}(A_{aw}K_{a\omega}C) + \frac{\partial}{\partial x}(\theta v_x C) + \frac{\partial}{\partial z}(\theta v_z C) - \frac{\partial}{\partial x}\left(\theta D_x \frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial z}\left(\theta D_z \frac{\partial C}{\partial z}\right) = -\frac{\partial(\theta C)}{\partial t}, \quad (6)$$

Results are shown for diffusion and adsorption to air-water interface for air content of 0%, 45%, and 90%, flow velocity components $v_x = 3 \times 10^{-3}$ cm/s, $v_z = 0$ cm/s and for $K_f = 0.01$ μmol/g.




(a) (b)

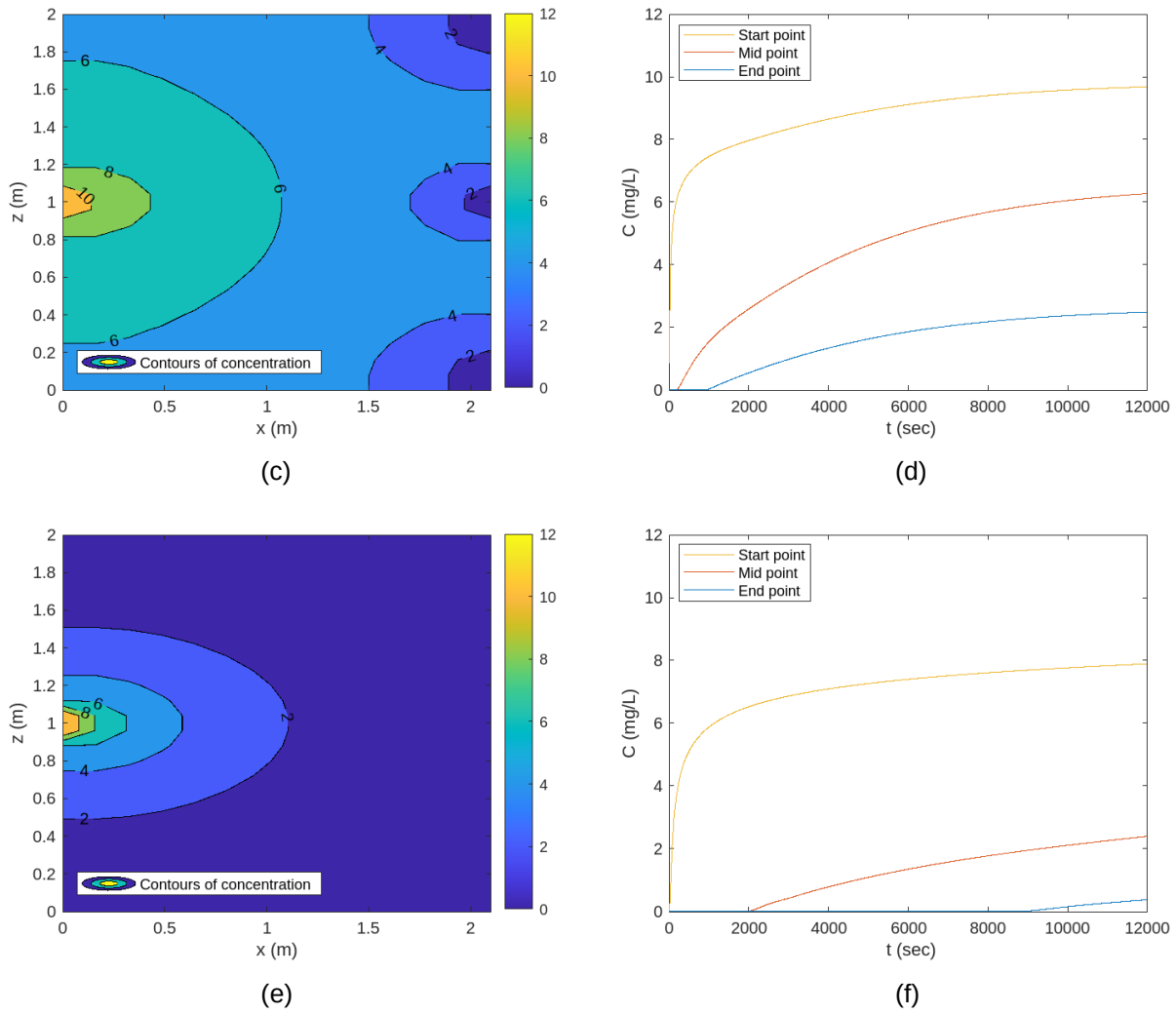



***Figure 4.*** *Diffusion due to a constant supply of PFAS at inlet on the left boundary and three outlets on the right boundary exposed to an abundance of freshwater considering: (a) spatial distribution at time t=12000 seconds for* ***Scenario 1 ($A_{air} = 0$, $S_{water} = 1$)****; (b) time history of PFAS transportation at three nodes over time for* ***Scenario 1 ($A_{air} = 0$, $S_{water} = 1$)****; (c) spatial distribution at time t =12000 seconds for* ***Scenario 2 ($A_{air} = 0.45$, $S_{water} = 0.55$)****; (d) time history of PFAS transportation at three nodes over time for* ***Scenario 2 ($A_{air} = 0.45$, $S_{water} = 0.55$)*** *(e) spatial distribution at time t =12000 seconds for* ***Scenario 3 ($A_{air} = 0.9$, $S_{water} = 0.1$)****; (f) time history of PFAS transportation at three nodes over time for* ***Scenario 3 ($A_{air} = 0.9$, $S_{water} = 0.1$).***

## 4.2 Discussion

Above simulation results demonstrate the relative importance of different transport mechanisms on PFAS movement. The impact of diffusion on the PFAS transport process and the temporal evolution at specified points are depicted in Figure 1. As expected, the transport of PFAS speeds up as soon as advection is introduced, as shown in Figure 2. As seen this faster transport is more pronounced for higher water flow flux. Figure 3 demonstrates that the transport process is retarded when adsorption onto the solid phase is introduced. The transport is more retarded for more adsorptive cases (higher $K_f$). Finally, Figure 4 shows that with the introduction of more air into the saturated soil, PFAS transport is retarded more.

Nevertheless, the dominant controlling factor for the movement of PFAS in saturated systems depends on the specific conditions of the system. In general, advection tends to be the dominant factor for PFAS transport in saturated systems. However, the presence of adsorption or air in the soil can significantly

impact PFAS transport rates and can become the dominant factor in unsaturated systems. Therefore, it is important to consider all of the relevant factors when analysing PFAS transport in a specific system. However, this study improves our knowledge of PFAS transport processes by delving deeper into how different factors, such as diffusion, advection, and adsorption, influence the movement of PFAS in the soil environment. The numerical model employed in this study offers a quantitative approach to analysing these factors and their relative contributions to PFAS transport, enabling researchers to more fully comprehend and forecast PFAS behaviour in the soil environment.

## 5 CONCLUSIONS

A two-dimensional (2D) numerical model is presented in this paper to simulate the transport of PFAS. The model's details were covered, and a range of results for various scenarios was exhibited to demonstrate the effects of diffusion, advection, and adsorption onto solid-phase and air-water interfaces at various air contents. The transport of PFAS is observed to accelerate significantly upon the introduction of advection, a mechanism that tends to exert dominant control over the transport process. Conversely, the transport process experiences retardation upon the addition of air, which leads to increased adsorption of PFAS onto the soil.

While the presented numerical model for PFAS transport provides valuable insights into the complex mechanisms governing the movement of PFAS in the environment, further improvements are necessary to address more complex situations. Ongoing efforts include the development and testing of a 2D model that incorporates transient seepage, and the design of a 3D version of the model to enhance its applicability in a wider range of scenarios. Furthermore, the validation of the model through experimentation is an essential step towards its wider adoption as a tool for understanding and managing PFAS contamination.

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