SANBORN HEAD

Development of Leaching-Based Soil Values for Select Per- and Poly-fluoroalkyl Substances (PFAS)

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1.0 INTRODUCTION

The New Hampshire Department of Environmental Services (NHDES) is in the process of developing Soil Remediation Standards (SRS)[1] for four (4) per- and polyfluoroalkyl substances (PFAS) including: perfluorooctane sulfonic acid (PFOS, CASRN #1763-23-1), perfluorohexane sulfonic acid (PFHxS, CASRN #355-46-4), perfluorononanoic acid (PFNA, CASRN #375-95-1), and perfluorooctanoic acid (PFOA, CASRN #335-67-1)[2]. Development of the SRS includes the consideration of leaching-based soil values that are intended to be protective of groundwater quality.

The goal of calculating leaching-based soil values is to determine the allowable concentration of contaminants in soil such that soil contaminated at, or remediated to, these concentrations should not leach a sufficient mass of contaminant to result in a violation of a NHDES Ambient Groundwater Quality Standard (AGQS)[3] (NHDES, 1998). Concentrations in soil greater than the leaching-based soil values have the potential to contaminate groundwater at levels greater than the AGQS in some soils. To accomplish this, the following were completed:

- As described in Section 2 of this report, review of available analytical or numerical models that have been identified for use in calculating leaching-based soil values for the four PFAS, including an evaluation of the applicability, benefits, and challenges of applying the identified models, and selection of a primary model to be used to calculate leaching-based soil values.
- As described in Section 3 of this report, review of the chemical-specific properties of the four PFAS that are applicable to their fate and transport in the environment and selection of properties used as input parameters in the selected model. PFOS, PFHxS, PFNA, and PFOA have environmental fate and transport properties that are different from properties of other substances for which leaching-based soil values have been established.
- As described in Section 4 of this report, review of the existing conceptual site model (CSM) used in the 2018 revision of the RCMP (NHDES, 1998)[4] and development of an alternative, updated CSM based on a review of recent environmental data and PFAS-specific release scenarios for calculation of leaching-based soil values. A description of non-chemical specific input parameters for each of the CSMs used in the modeling approach is also provided in Section 4.
- As described in Section 5 of this report, calculation of leaching-based soil values using the selected primary model and input parameters with completion of a sensitivity analysis on variables used, and calculation of leaching-based soil values using a secondary model to compare to the primary model results.

1.1 NHDES Approach to Calculate Existing Leaching-Based Soil Values for other Contaminants of Concern

NHDES began using computer models employing a risk-based approach for calculating leaching-based soil values with the adoption of the Risk Characterization and Management Policy

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[1] Soil Remediation Standards (SRS) for constituents are promulgated in Env-Or 600 at Section 606.19.

[2] CASRN refers to CAS Registry Number Verified Partner Program.

[3] Ambient Groundwater Quality Standards (AGQS) for constituents are promulgated in Env-Or 600 at Section 603.03.

[4] Note that the NHDES Risk Characterization and Management Policy has been subsequently revised in 2013 and 2018.

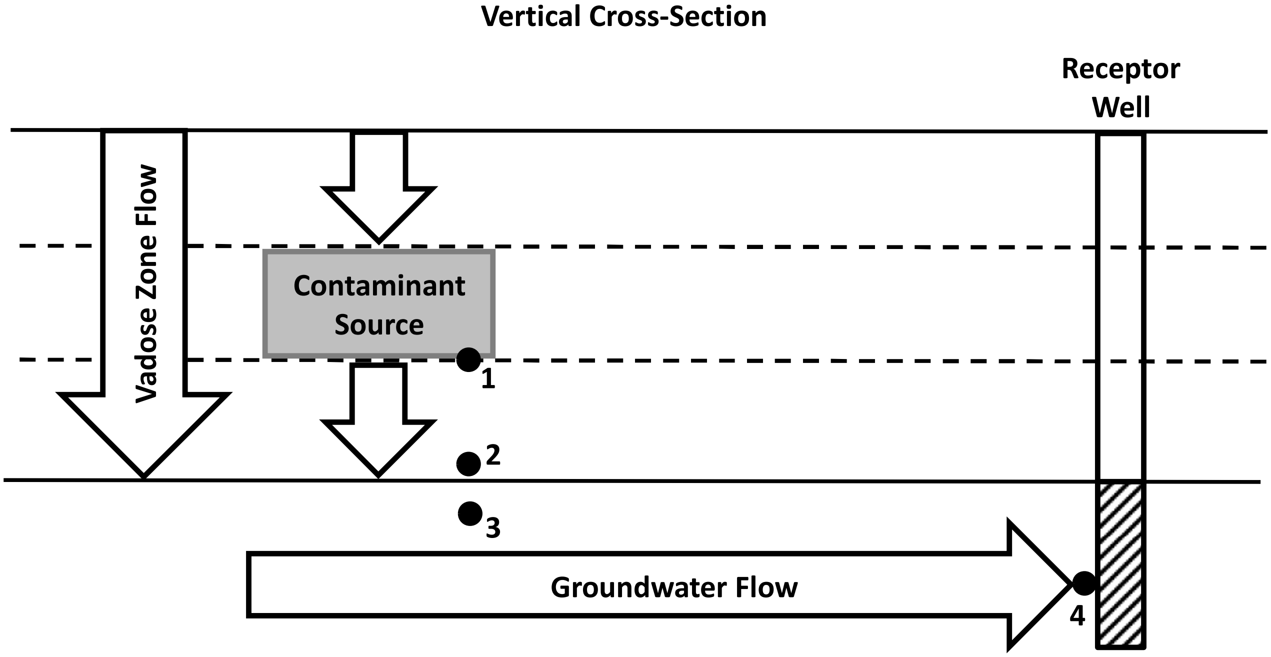
(RCMP) (NHDES, 1998). The computer-based methodology and input parameters used to establish the threshold levels of soil contamination that are not expected to adversely affect groundwater quality is described in Appendix B of the RCMP (1998), with subsequent revisions (e.g., to account for changing AGQS) described in later RCMP revisions (2013, 2018). The methodology uses the Seasonal Soil Compartment Model (SESOIL) and Analytical Model of Transport 1-, 2-, and 3-Dimensional Waste Transport (AT123D) model. SESOIL is used to model chemical-specific flow in the vadose zone to groundwater, and AT123D is used to model contaminant transport through the aquifer once the contaminant reaches the groundwater (commonly referred to as the water table). These models were originally developed for the United States Environmental Protection Agency (USEPA) as separate computer programs and are currently implemented by NHDES using a software program called SEVIEW, which is a single interface with enhanced versions of the SESOIL and AT123D models. Further description of the SEVIEW modeling approach is provided in Section 2.

1.2 General Approach to Calculate Leaching-Based Soil Values in New Hampshire

Calculation of leaching-based soil values is usually performed using a contaminant transport model that is applied to a representative CSM. As shown in Exhibit 1-1, the CSM typically includes leaching of a contaminant from a source in vadose zone soil, and transport of the contaminant through the vadose zone (i.e., unsaturated soil underlying the source area soil above the water table or groundwater) to a measurement point in groundwater (e.g., the groundwater table or a downgradient well). If a downgradient well is used as a measurement point, then the conceptual site model also includes transport of the contaminant in the groundwater.

- **Vadose Zone** (also referred to as the unsaturated zone) is the zone between the ground surface and the groundwater table, where soil is variably saturated as a result of wetting and drying of the soil.

Exhibit 1-1: Vertical cross-section for hypothetical CSM that corresponds with the varying approaches to model leaching-based soil values summarized in Exhibit 1-2.



1 – Soil Moisture Next to Contaminant Source
2 – Soil Moisture at Bottom of Vadose Zone
3 – Groundwater Beneath Contaminant Source
4 – Groundwater at Receptor Well

To calculate leaching-based soil values in this manner, assumptions about contaminant fate and transport are made to estimate concentrations in soil that may result in groundwater concentrations greater than (i.e., exceeding) groundwater criteria (e.g., the AGQS). Using this approach to calculate leaching-based soil values allows some level of a contaminant to remain while still being protective of groundwater.

A relatively simple approach for calculating leaching-based soil values is described in the USEPA guidance for Soil Screening Level (SSL) development (USEPA, 1996a; USEPA, 1996b). The SSL equation for migration to groundwater calculates screening levels using the following equations by (i) assuming linear partitioning to relate soil concentrations and soil leachate concentrations, (ii) if the contaminant is an organic contaminant, then calculating a soil-water partition coefficient based on organic partitioning, and (iii) assuming a dilution-attenuation factor (DAF) to relate soil leachate and groundwater concentrations.

(i) $$C_t = C_W\left(K_d + \frac{\theta_W + \theta_a H'}{\rho_b}\right)$$

(ii) $$K_d = K_{oc} \times f_{oc}$$

(iii) $$C_W = C_{GW} \times DAF_{USEPA}$$

Where:

C_t is screening level in soil;
C_W is target leachate concentration;
K_d is soil-water partition coefficient (used for inorganic contaminants);
θ_W is water-filled soil porosity;
θ_a is air-filled soil porosity;
n is total soil porosity;
ρ_b is dry soil bulk density;
H' is Henry's law constant (dimensionless);
K_{oc} is soil organic carbon-water partition coefficient (used for organic contaminants); and
f_{oc} is organic carbon content of soil;
C_{GW} is drinking water screening level; and
DAF_{USEPA} is the USEPA default dilution-attenuation factor of 20 for dilution and attenuation in groundwater (not including vadose zone dilution and attenuation).

The USEPA has published leaching-based Regional Screening Levels (RSLs) for PFOA, PFNA, PFHxS, and PFOS based on these SSL equations. The SSL equations include some aspects of soil leaching that are included in many other leaching models, such as partitioning to solids and volatilization to air. The representation of transport, dilution, and attenuation in the vadose zone and in groundwater is much simpler in the SSL equations than in many models. With the relatively simple approach, there is limited opportunity to use the SSL equations for development of leaching-based soil values that are more representative for New Hampshire. As noted in Exhibit 1-2 below, different approaches to estimating leaching-based soil values vary on their level of protectiveness for the scale of conditions being modeled (i.e., site-specific compared to larger areas such as state-wide). Part of developing leaching-based soil values is evaluating available data and input variables that are applied in a risk-based approach that allows some contamination to remain in the vadose zone soil while also being protective for most site conditions.

Use of the most conservative approaches, such as Point of Compliance 1 in Exhibit 1-2, or use of less conservative approaches but with numerous conservative assumptions, may result in concentrations that are not representative of field conditions and that could be below analytical laboratory practical quantitation limits. Typically, input parameter values are selected based on empirical data from the region of interest (e.g., the state of New Hampshire) to reduce conservatism, increase representativeness, and remain protective for a wide range of site conditions.

Models such as SESOIL and AT123D are designed to simulate the physical and chemical processes that control contaminant migration in the subsurface (ESCI, 2023). These models include dilution and attenuation processes to calculate the maximum groundwater concentration at a given point, by which a DAF and corresponding leaching-based soil value can be calculated. To model those processes, either specific representative model parameters are used, when available, or generally protective assumptions are made based on available information.

Exhibit 1-2: Variations in approaches for modeling of leaching-based soil values relative to location of the point of compliance (as shown in Exhibit 1-1).

Point of Compliance	Soil	Groundwater
1 **Vadose zone beneath contaminant release area**	Soil-water partitioning equation with contamination at the water table	No DAF
2 **Bottom of vadose zone beneath contaminant release area**	Vadose zone transport (e.g., SESOIL)	No DAF
3 **Groundwater directly beneath contaminant release area**	Vadose zone transport (e.g., SESOIL)	DAF calculated with no fate and transport in groundwater (i.e., receptor directly beneath the contaminant source)
4 **Groundwater downgradient of contaminant release area**	Vadose zone transport (e.g., SESOIL)	DAF calculated with groundwater fate and transport (e.g., AT123D).

Note: NHDES has used the Point of Compliance 4 approach to develop leaching-based soil values for other contaminants previously (NHDES, 1998). The approaches reviewed as part of this effort are also classified as Point of Compliance 4.

Modeled concentrations in water leaching from the vadose zone to groundwater can vary over many orders of magnitude depending on the values of input parameters (e.g., climate, soil type, contaminant release depth (depth to groundwater)) and the contaminant chemical properties. To evaluate how variations in the input values influence the calculated results, sensitivity analyses can be performed on input values used with the model equations.

1.3 Transport and Fate Background Information

This section describes the following processes that may affect the transport and fate of PFOA, PFNA, PFHxS, and PFOS in soil and groundwater:

- Solid-phase partitioning (Section 1.3.1)
- Volatilization into air (Section 1.3.2)
- Diffusion in air and water (Section 1.3.3)
- Air-Water interface partitioning (Section 1.3.4)
- Supramolecular aggregations (Section 1.3.5)
- Surfactant-induced flow (Section 1.3.6)
- Transformation (Section 1.3.7)

This background information provides context for various discussions in this report, including the Section 2 model review and selection, the Section 3 model parameter selection, and the sensitivity analysis included in Section 5.

1.3.1 Solid-Phase Partitioning

Chemical-specific solid-phase partitioning for site characterization, remediation, and risk assessment is typically represented by a solid-liquid partition coefficient (K_d). K_d values are a function of chemical properties, aqueous solution, and solid-phase properties. Lower K_d values relate to faster leaching from soil, so assuming lower K_d values results in the calculation of more protective leaching-based soil values. Solid-liquid partitioning coefficients may be estimated from physical and chemical properties, experimentally derived in such a way that they are assumed to be applicable across a certain range of conditions, or empirically derived through field or laboratory measurements.

Appendix A includes additional discussion of solid-phase partitioning and the U.S. Geological Survey (USGS) research to study occurrence and leachability of PFAS in shallow soils in New Hampshire (hereafter referred to as the 2023 USGS NH Study) (Tokranov et al., 2023).

The following factors that can affect solid-phase partitioning are discussed in the following subsections:

- Soil organic carbon adsorption (Section 1.3.1.1)
- Soil texture and mineralogy (Section 1.3.1.2)
- Electrostatic interactions (Section 1.3.1.3)
- Non-linear Sorption (Section 1.3.1.4)
- Kinetics (Section 1.3.1.5)
- Hysteresis (Section 1.3.1.6)

In a review of published PFAS K_d and K_{oc} values, Rovero et al. (2021) found that values for PFOA, PFNA, PFHxS, and PFOS ranged over four orders of magnitude or more, and interquartile ranges for K_d and K_{oc} were roughly one order of magnitude. In the conclusions of the review, Rovero et al. noted that the variability in literature K_d values make them inadequate for modeling leaching-based soil values and suggested using a site-specific K_d that reflects field conditions would be a better predictive tool. The following discussions include identification of modeling limitations in respect to factors that can affect solid-phase partitioning, considerations that may address or reduce those limitations, and if factors may tend to result in the calculation of more protective or less protective leaching-based soil values. The ITRC Technical and Regulatory Guidance Document Section 5.2.3 contains additional information regarding solid-phase partitioning (ITRC, 2022).

1.3.1.1 Soil Organic Carbon Adsorption

A common adaptation of the K_d approach is to normalize to soil organic carbon, resulting in an organic carbon-liquid partition coefficient (K_{oc}). This relationship is represented by the formula $K_d = K_{oc} \times f_{oc}$, where f_{oc} is the fraction of organic carbon in soil. This K_{oc} approach is discussed extensively in the USEPA 1996 Soil Screening Guidance (USEPA, 1996a; USEPA, 1996b), and it is the approach that is used in the USEPA Regional Screening Levels (RSLs) that include calculated leaching-based soil values for PFOA, PFNA, and PFOS.

When solid-phase partitioning is scaled directly to soil organic carbon using the $K_d = K_{oc} \times f_{oc}$ function, the implicit assumptions include: (i) partitioning is principally associated with sorption to organic carbon; and (ii) organic carbon scales directly with sorption to organic carbon (basically the more organic carbon present the more sorption that occurs, and all organic carbon has the same effect in terms of its ability to sorb the contaminant).

Assumptions implicit in the K_{oc} approach may not be met for solid-liquid partitioning of PFOA, PFNA, PFHxS, and PFOS. Numerous studies on PFAS sorption suggest a wide range of sorption mechanisms and variables are important beyond simple sorption to organic carbon (Rovero et al., 2021). For example, in a review of peer-reviewed literature by Li et al. (2018), organic carbon, pH, and clay content were noted as significant factors. The authors stressed the potential importance of electrostatic interactions and limitations of describing sorption only in terms of K_{oc}. Further, some PFAS have a greater affinity for certain types of organic matter (ITRC, 2022), so K_{oc} values may be a function of organic carbon constituents.

Lower K_{oc} values and lower f_{oc} in soil relate to faster leaching from soil, so assuming lower K_{oc} and f_{oc} result in the calculation of more protective leaching-based soil values. If soil organic carbon adsorption is sufficiently accounted for by using representative K_{oc} and f_{oc} values, then soil organic carbon adsorption does not tend to result in the calculation of a more protective or less protective leaching-based soil values.

1.3.1.2 Soil Texture and Mineralogy

Soil properties that may affect solid-phase partitioning for PFAS include grain size distribution; mineral and organic carbon content; nature of organic carbon; soil pH, ion exchange capacity, and other surface chemistry; and water pH and aqueous chemistry (ITRC, 2022). In general, these soil properties were included as potential factors in the 2023 USGS NH Study, and the K_{oc} selection approach provided as Appendix A includes additional discussion of the USGS Study data. The ITRC Technical and Regulatory Guidance Document Section 5.2.3 contains additional information regarding partitioning to solid phases (ITRC, 2022).

If soil texture and mineralogy are sufficiently accounted for by using a representative K_d or K_{oc}, then these factors do not tend to result in the calculation of a more protective or less protective leaching-based soil value.

1.3.1.3 Electrostatic Interactions

Partitioning of PFOA, PFNA, PFHxS, and PFOS from water onto solids is affected by both hydrophobic and electrostatic interactions. The fluorinated alkyl moiety of PFOA, PFNA, PFHxS, and PFOS lends hydrophobic properties to these PFAS. The functional groups of these four PFAS, which are largely anionic in water at typical environmental pHs, increase solubility in water (i.e., decrease hydrophobic tendencies). Electrostatic interactions involving the functional groups may also facilitate or hinder adsorption to a solid. For example, adsorption may be hindered if a solid surface is negatively charged because the negatively charged, anionic PFAS may be repulsed by the negative charge on the surface (ITRC, 2022). If there are adsorption sites on the solid surface that are positively charged, then adsorption may be facilitated.

If electrostatic interactions are sufficiently accounted for by using a representative K_d or K_{oc}, then these factors do not tend to result in the calculation of a more protective or less protective leaching-based soil values.

1.3.1.4 Non-linear Sorption

Both the K_d and K_{oc} approaches assume that those partitioning coefficients are constant over some range of conditions. In addition to the soil and liquid properties discussed above, the relationship between solid-phase and liquid-phase concentrations may also be a function of concentration, time, and past conditions or concentrations.

The Freundlich equation is commonly used for modeling partitioning as a function of concentration. The Freundlich equation relates K_d to the solid-phase concentration (C_S) and the liquid-phase concentration (C_L) using the equation $K_d = C_S / C_L^n$, where “n” is the Freundlich exponent. If the Freundlich exponent is found to be equal to 1 for a range of conditions, for example through empirical study, then the sorption is considered linear and partitioning is not a function of concentration. This linear Freundlich equation, which is equivalent to $K_d = C_S / C_L$, is the most common approach for describing PFAS partitioning. If a better fit is found using a Freundlich exponent not equal to 1 or if an entirely different equation is considered more appropriate, then sorption is considered non-linear, and typically the partitioning between solid and liquid phases is a function of concentration.

If non-linear sorption is significant and not accounted for, then the unaccounted-for effect may either result in the calculation of a more protective or less protective leaching-based soil values, depending on the type of non-linearity and model assumptions. If the linear K_d or K_{oc} values are representative of the range model concentrations, then that model would not tend to result in the calculation of a more protective or less protective leaching-based soil values.

1.3.1.5 Kinetics

Consideration of kinetics, or partitioning as a function of time, is stressed in the ITRC PFAS Technical and Regulatory Guidance Document (2022). Empirical partitioning coefficients are typically based on laboratory samples measured when they are assumed to be at equilibrium, and models that use those coefficients also assume equilibrium. Environmental systems are dynamic and may often not be at equilibrium, and mass transfer between solids and the mobile portion of the aqueous phase may control concentrations. For example, if clean water were infiltrated quickly through PFAS impacted soil, then mass transfer limitations could result in less PFAS leaching into the water than an equilibrium model would predict.

Although it may depend on the specific conceptual site model and relative importance of adsorption/desorption on transport and fate, the assumption of equilibrium tends to result in the calculation of a more protective leaching-based soil value because there is faster leaching from the source area soils.

1.3.1.6 Hysteresis

Hysteretic partitioning can result in partitioning depending on past concentrations and whether solid-phase concentrations are increasing (net sorption) or decreasing (net desorption). Most approaches to modeling partitioning, including K_d and K_{oc} approaches, assume sorption is reversable. In a review of published PFAS K_d and K_{oc} values, Rovero et al. (2021) identified increased partitioning to solids reported for desorption studies. This suggests that there is some observed partitioning that does not align with the typical models, likely including multiple partitioning mechanisms with different associated partitioning capacity, equilibrium constants, and kinetics.

If hysteresis is significant and not accounted for, then the unaccounted-for effect could be complex and may either result in the calculation of more protective or less protective leaching-based soil values, depending on the specific conceptual site model, relative importance of adsorption/desorption on transport and fate, and other factors. If hysteresis is sufficiently accounted for by using a representative K_d or K_{oc}, then these factors do not tend to result in the calculation of a more protective or less protective leaching-based soil values.

1.3.2 Volatilization to Soil Gas

Available literature values for the acidic forms of PFOA, PFNA, PFHxS, and PFOS Henry's Law constants are variable over many orders of magnitude. Most available information indicates low volatility for these PFAS at environmentally relevant pHs, although atmospheric transport can be a mechanism for release. There is a great deal of uncertainty in the modeling and measurement of volatilization for these PFAS, and it is complicated by the differing volatility of these PFAS as a function of pH (ITRC, 2022). The ITRC Technical and Regulatory Guidance Document Sections 4.2 and 5.2.4 contain additional information regarding volatilization (ITRC, 2022).

Volatility of organic acids, assuming negligible volatilization of the anionic species and a given Henry's Law constant (such as K_H') for the acidic species, can be calculated using an air-water distribution coefficient (D_{AW}). The D_{AW} describes the distribution of the total species concentrations between air and water as a function of the fraction of total species concentration in acidic form (α) using the equation $D_{AW} = \alpha K_H'$ (Rodenburg, 2020). The fraction of total species concentration in acidic form can be calculated using the acid dissociation constant (pK_a) and pH. At typical environmental pHs, PFOA, PFNA, PFHxS, and PFOS tend to be largely anionic; only a relatively small portion of PFOA, PFNA, PFHxS, and PFOS will be present as the more volatile undissociated acid.

Most models are unable to accommodate dynamic calculation of α and D_{AW}, and a simplifying assumption is to use the total aqueous concentration of the individual PFAS as the value for the concentration of the individual PFAS in acidic form. This assumption is anticipated to overestimate volatilization because at least some portion of aqueous PFAS would be present in the anionic form and assumed unavailable for volatilization.

Volatilization acts as a retention mechanism that tends to slow leaching. Therefore, assuming the PFAS are in their acidic form in a model would tend to result in the calculation of a less protective leaching-based soil value than if some or all of the PFAS were assumed to be in the non-volatile, ionic form.

1.3.3 Diffusion in Water and Air

Diffusion is the movement of constituents from areas of higher concentration to lower concentration. Diffusion-based mass flux can be modeled using the concentration gradient and a solute-solvent-specific diffusion coefficient (Sahimi, 1995). For modeling transport in the vadose zone, water and air diffusion coefficients are needed as model input parameters.

If representative diffusion coefficients are used, then these factors do not tend to result in the calculation of a more protective or less protective leaching-based soil values.

1.3.4 Air-Water Interface Partitioning

As discussed in relation to solid-phase partitioning, the fluorinated alkyl moiety of PFOA, PFNA, PFHxS, and PFOS lends hydrophobic properties to these PFAS, and the acidic functional groups of these four PFAS, which are largely anionic in water at typical environmental pHs, increase solubility in water. With the combined hydrophobic and hydrophilic properties, these PFAS can act as surfactants and partition from water to air-water interfaces. Accounting for or quantifying air-water interface partitioning of PFAS, including modeling and observation of field-scale effects, is an area of active research (Brusseau et al., 2019a; Anderson et al., 2019; Guo et al., 2020; Silva et al., 2020; Anderson et al., 2022). The ITRC Technical and Regulatory Guidance Document Section 5.2.4.1 contains additional information regarding air-water interface partitioning (ITRC, 2022).

The degree of air-water interfacial partitioning in the vadose zone is a function of PFAS physiochemical properties, PFAS concentration range, and soil properties, including soil texture and degree of saturation (Brusseau et al., 2019a). The importance of air-water interfacial partitioning as a mechanism significantly affecting retention in the vadose zone is also a function of how dominant solid-phase partitioning is for a given system (Guo et al. 2020; Silva et al., 2020). Solid-phase partitioning and air-water partitioning for modeling retention are additive, so air-water interfacial partitioning may have little effect on retention in systems dominated by solid-phase partitioning, and air-water interfacial partitioning may be an important retention mechanism in systems with little solid-phase partitioning.

If present in a system or a model, then air-water interfacial partitioning acts as a retention mechanism that tends to slow leaching. Therefore, not accounting for air-water interfacial partitioning in a model would tend to result in the calculation of a more protective leaching-based soil value than if air-water interfacial partitioning were included in the model.

1.3.5 Supramolecular Aggregations

The surfactant properties of PFOA, PFNA, PFHxS, and PFOS may increase the tendency for these PFAS to form supramolecular aggregations. Aggregations may include other PFAS and other constituents, such as natural organic matter. There is no consensus in the literature as to the extent or significance of supramolecular aggregations for these PFAS, and there is likely some dependence on solution chemistry and concentration of both PFAS and other constituents that may form supramolecular aggregations. The ITRC Technical and Regulatory Guidance Document Section 5.2.2.2 contains additional information regarding supramolecular aggregations (ITRC, 2022).

Solid-phase and liquid-phase supramolecular aggregations, if significant, are assumed to be reflected in the empirically derived solid-liquid partition coefficients from the 2023 USGS NH Study. If there are other supramolecular aggregations, for example at the air-water interface, then those aggregations may act as a retention mechanism because the aggregations are not traveling through the soil in the more mobile liquid-phase. Therefore, not specifically accounting for supramolecular aggregations in a model would tend to result in the calculation of a more protective leaching-based soil value than if supramolecular aggregations were included in the model.

1.3.6 Surfactant-Induced Flow

Unsaturated porewater flow can be affected by surface tension. For example, reduced surface tension reduces capillary pressures, which may increase drainage and reduce water-filled porosity available for aqueous transport. As surfactants, increased concentrations of PFOA, PFNA, PFHxS, and PFOS in soil porewater may reduce surface tension and induce drainage. The potential effect of surfactant-induced flow is smaller at lower PFAS soil porewater concentrations.

Surfactant-induced flow was included in a vadose zone model for PFAS by Guo et al. (2020). In the research article discussing the model, Guo et al. noted some apparent effects on surface tension and water content possibly due to surfactant-induced flow, with greater porewater concentrations (i.e., greater leaching) shown when surfactant-induced flow was included. The effects were relatively small for the modeled soils. For example, some simulations of soil columns with 1,000 milligram per liter (mg/L) PFOS added showed resulting peak porewater concentrations of about 25 mg/L if surfactant-induced flow was not included. The concentration increased by about 2 mg/L or less (8% increase or less) if surfactant-induced flow was included. For simulations using 100 mg/L PFOS in soil, the increased leaching effect from surfactant-induced flow was smaller. Guo et al. anticipated effects could be greater in soils where capillary pressure had stronger influence, such as finer-grained soils and soils near to the groundwater table.

The leaching-based soil values conceptual site model uses coarser-grained soils, which is a generally protective assumption, and leaching-based soil values will be applied to situations with much lower concentrations based on release site sample data from across the state, for example typically less than 1,000 nanogram per liter (ng/L) (0.001 mg/L). Based on the available information, the effect of omitting surfactant-induced flow in the calculation of a leaching-based soil value is potentially less protective but likely negligible.

1.3.7 Transformation

Some chemicals, referred to as precursors, may degrade to PFOA, PFNA, PFHxS, and PFOS. Precursors have been identified in numerous studies, and the presence of precursors can significantly complicate fate and transport considerations (ITRC, 2022). Some precursors are included in some commercially available PFAS analytical lists, but many are not. Although precursors are important to include in the conceptual model for some sites, the potentially wide-ranging and site-specific fate and transport characteristics and transformation potential of precursors make them infeasible to include in model scenarios at this time. Not accounting for

PFOA, PFNA, PFHxS, and PFOS precursors results in the calculation of a less protective leaching-based soil value than if precursors of those PFAS were included in the model.

PFOA, PFNA, PFHxS, and PFOS have not been found to degrade or transform in typical environmental conditions (ITRC, 2022). Not accounting for degradation of PFOA, PFNA, PFHxS, and PFOS results in the calculation of a more protective leaching-based soil value than if degradation of those PFAS were included in the model and is consistent with the current understanding that these compounds do not degrade in the subsurface.

The ITRC Technical and Regulatory Guidance Document Section 5.4 contains additional information regarding transformations of PFAS (ITRC, 2022).

2.0 REVIEW OF AVAILABLE MODELS FOR PFAS FATE AND TRANSPORT IN THE SUBSURFACE

This section of the report identifies and evaluates potentially applicable models that can be used to generate leaching-based soil values for PFAS. Our review and evaluation of models that could be used to generate leaching-based soil concentrations for PFAS is limited to the following five models listed below. These five models are selected to represent a variety of approaches, including two more simplified, one-dimensional models (e.g., SEVIEW and PRZM), two recently developed models that incorporate PFAS-specific transport processes [e.g., HYDRUS (1-D/2-D Modified with PFAS package) and PFAS-LEACH], and a more complex three-dimensional model that is able to represent spatial variability of vadose zone soils (e.g., MODFLOW-USG Transport).We note that MODFLOW-USG Transport and HYDRUS 3-D have somewhat similar capabilities, however, preference was given to MODFLOW-USG Transport because MODFLOW is considered an international standard for simulating and predicting groundwater conditions and groundwater/surface-water interactions (USGS, 2022). Other potentially applicable models are also available, but are beyond the scope of this report and have not been individually evaluated.

- SESOIL/AT123D (SEVIEW) (see Section 2.2.1),
- PRZM (see Section 2.2.2),
- HYDRUS (Modified) (see Section 2.2.3),
- PFAS-LEACH (Guo et al., 2022) (see Section 2.2.4), and
- MODFLOW-USG Transport (see Section 2.2.5).

This report reviews available fate and transport models for the leaching to groundwater migration pathway for a PFAS source located in soil in the vadose zone, including at the ground surface. Please note that review of models and approaches to calculating leaching-based soil values resulting from the application of biosolids to the ground surface or related land application processes were not evaluated as part of this effort. The report also does not include a review of other fate and transport models that are used for surface water runoff, and plant uptake migration pathways.

Model validation is used to evaluate if a theoretically derived model is capable of adequately replicating experimental data, and therefore provides confidence in the model predictions. The experimental dataset should be representative of the scale of interest, and test the same transport-dependent variables used by the model. A review of scientific literature by Silva et al., (2020), highlighted that there was a limited number of published unsaturated (or vadose zone) transport data for PFAS that could be used to validate model performance, in particular in relation to PFAS-specific fate and transport processes (e.g., effects of the air-water interface and surfactant-induced flow). Based on our review, it is our understanding that none of the models reviewed in this report have been validated specifically for PFAS fate and transport. As noted by Silva et al., (2020), additional experimental data is likely still needed to allow testing and validation of models against pilot-scale and field-scale PFAS datasets under representative conditions.

Review of models that may be used to generate leaching-based soil concentrations for PFAS has recently been performed by other organizations including The National Council for Air and Stream Improvement, Inc. (NCASI, June 2020), and Michigan Department of Environment, Great Lakes, and Energy (EGLE, July 2020):

- The document published by NCASI (June 2020) includes a review of models that may be used to evaluate fate and transport of PFAS in land-applied residuals and biosolids. The review considered models that may be suitable for modeling of PFAS fate and transport along three primary pathways including leaching to groundwater, surface water runoff, and plant uptake. NCASI has also published a guidance document for use of the USEPA Pesticide Root Zone Model (PRZM, Young and Frye, 2020) in screening-level PFAS leaching assessments (NCASI, 2021).

- The document published by Michigan Department of Environment, Great Lakes, and Energy (July 2020) includes a review of available software for modeling of PFAS fate and transport within the vadose zone.

The information and conclusions presented in these documents have been considered, but not relied upon, as part of our evaluation of the five models, and the conclusions presented in this report are based on the professional opinion of Sanborn Head.

Our evaluation of the above list of models considered the following criteria, each of which is assigned an equal weighting in terms of importance:

1. General ability of the model to simulate fate and transport processes that are applicable to most sites and contaminants including: the ability of the model to simulate the hydrologic cycle using realistic representation of processes; the number of spatial dimensions that are able to be simulated (i.e., one-, two-, or three-dimensions) and ability to represent heterogeneity through spatial discretization of properties; degree and flexibility of temporal discretization (i.e., ability of a model to perform calculations and provide results for different time-steps, such as hourly, daily, monthly, annually); the ability to simulate partitioning between different phases (air, water, solid, and pure phase); and the ability to simulate general physical, chemical, or biological processes (e.g., advection, dispersion, diffusion, volatilization, and transformation).

2. Ability of the model to simulate processes that are more specific to fate and transport of PFAS (e.g., air-water interface partitioning; electrostatic adsorption; surfactant-induced flow; non-linear and non-equilibrium sorption; and supramolecular aggregations).

3. Ease of Implementation (e.g., availability of graphical user interface to set up a model simulation; the minimum number of model parameters required to run a model simulation; the ability to obtain the data required for all relevant input parameters; the run-time of the model; and the ability to view and post-process results).

4. Documented model limitations, calibration/verification and peer review, software licensing and availability, and software maintenance and user support.

2.1 General Concepts for Selection of Models

There are several different approaches to modeling fate and transport of contaminants in the environment. Three common approaches include general, realistic, and precise and accurate. Each approach to modeling has advantages and challenges depending on the intended application of the model. To develop leaching-based soil values that are applicable across a wide range of conditions we typically need to use a general model, which can provide useful results across a broad range of conditions based on unrealistic or partially realistic processes as described below. However, to provide context for a general model, a variety of more specific, realistic situations may be modeled with a greater focus on precision and accuracy. By doing so, the performance of the general model can be judged against that of the non-general. Models cannot be simultaneously general, precise, and realistic (Levins, 1966). When selecting a suitable model, it is necessary to sacrifice at least one of the three characteristics to accomplish the others. The importance of each characteristic will depend on the goal(s) of the model.

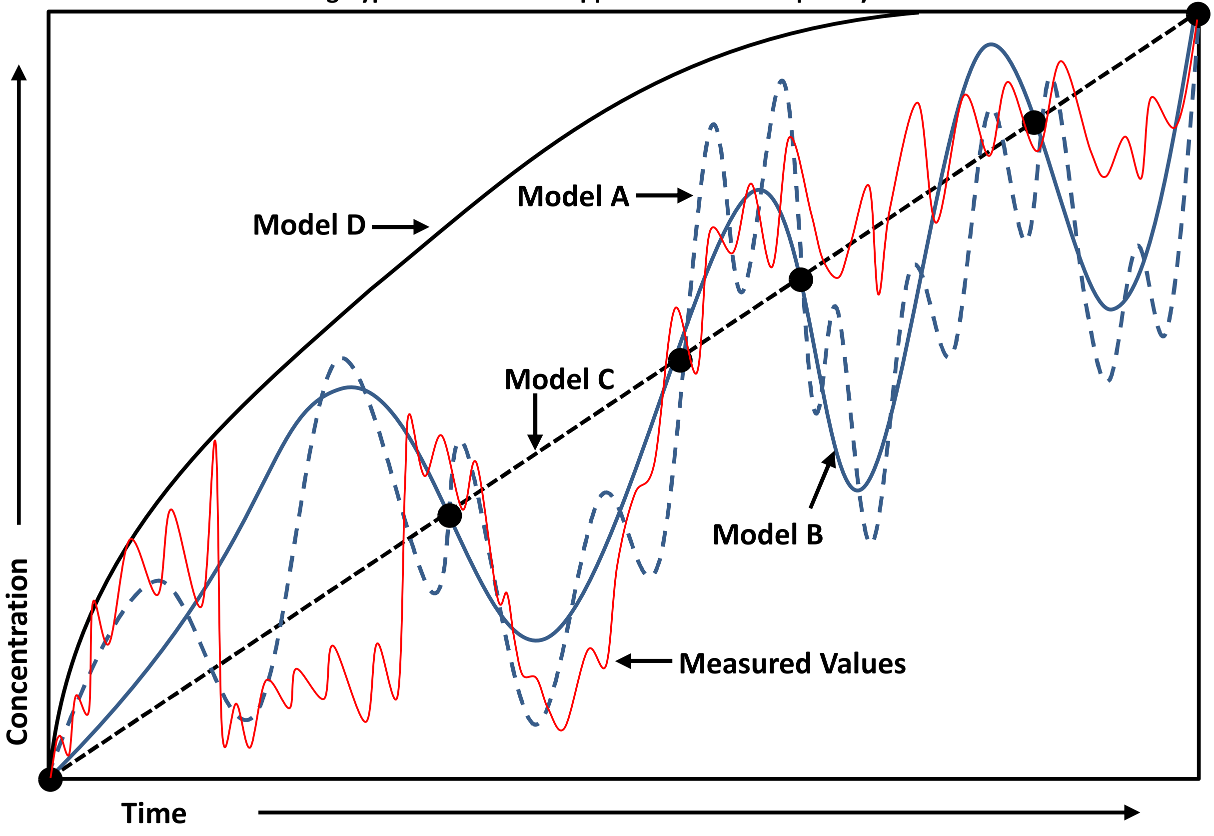
General – general models may provide useful results across a broad range of conditions, but they have equations that are based on unrealistic, or only partially realistic, processes. For example, when modeling the flow of water through soil, we can aim to have a precise and realistic model that accurately simulates how quickly the water moves and is able to describe the observed path of water molecules around each grain of soil using equations that represent realistic processes. In contrast, we can have a general model that is able to correctly predict how quickly the water moves between two distant points, but only generally predicts the direction that water is moving rather than simulating the exact flow path. A general model will use a relatively simple equation with fewer parameters that are not based on realistic processes but may just recognize that the path broadly follows a linear direction over longer distances.

Realistic – realistic models tend to use mathematical equations representing the laws of nature to predict an outcome. This is contrasted with a model that is still able to predict the outcome but arrives at the answer using a more empirical mathematical equation that is not based on underlying physical processes.

Precise and Accurate – precise and accurate models consistently provide results close to those observed in nature. Models that are accurate and precise generally work under very limited and specific conditions. For example, we may have a very accurate model representing the soil and climate in one area, but we are not able to translate the result of that model to other areas that may have different soil properties or different climate conditions.

The choice between using a realistic or general model is typically a balance of simplicity versus complexity, and it is also affected by the ability to measure or estimate the parameter values used to setup and run a model. General models are often used because they require less time to setup, require less computing power and time, and require measurement or estimation of fewer parameters. In the context of modeling the fate and transport of PFAS, there are also processes that are still the subject of ongoing research. With limited or developing understanding, it is not always possible to directly represent all potentially relevant processes in existing models. Even when a new process is incorporated into a model it may be the case that there is only a limited amount of research to verify the accuracy of the new model. In addition, the data needed to run the model may not be available, or may be difficult, time consuming, or costly to obtain. If data are available, then they may only be applicable to specific situations.

Exhibit 2-1: Schematic showing hypothetical model approaches and complexity.



To illustrate the concepts of general, realistic and precise models, Exhibit 2-1 above presents a time series of artificial concentrations (red line), and includes conceptual representation of four different hypothetical models. Brief description of the characteristics and relevance of each model is summarized below.

- **Model A** is a model that can simulate multiple processes using a realistic approach and provides detailed results calculated on a daily time interval.
- **Model B** is the same as Model A but provides less detail because results are calculated on a weekly time interval.
- **Model C** is a general model and different from Model A/B. It is a more simplified model that does not incorporate realistic processes but is able to match experimentally observed values on a monthly time interval.
- **Model D** is a general model, different from Model A/B and Model C, and it is generally incorrect because it only occasionally matches the observed values. However, it may be more applicable over a wider range of observations and captures the broad pattern of increased concentration with time. Model D initially increases at a faster rate and tends to predict concentrations that are higher than observed concentrations.

None of the four models can correctly simulate the observed values at every point in time, but even so, each of the four models can be useful. The choice of which model to select is then based on the question that is being asked and for what purpose the results are being used. When selecting a model for calculating a generic risk-based leaching-based soil value, a more general model may be preferred. The more general model can be protective over a broader range of scenarios, but it is less specific, realistic, and accurate for any specific scenario.

2.2 Review of Individual Models

The following sections describe each of the five models reviewed. Table 1 provides a summary of the key elements of each of the five models and summarizes advantages and challenges of each.

2.2.1 SEVIEW (SESOIL/AT123D)

SEVIEW is a graphical user interface developed by ESCI, LLC, that couples the SESOIL vadose zone model with the AT123D saturated zone model. SESOIL was originally developed for the USEPA in 1981 by Bonazountas and Wagner, and AT123D was developed by G. T. Yeh (1981) at Oak Ridge National Laboratory. Both models have been updated and modified since the original development.

SESOIL (Seasonal SOIL compartment model) is a finite difference, one-dimensional, vertical model for vadose zone flow and contaminant transport. SESOIL can simulate seasonal climatic variation using monthly data and results are also calculated on a monthly time-step. Other than the ability to vary the climate variable, SESOIL assumes steady-state boundary conditions for flow. Flow in the vadose zone is represented by a vertical, one-dimensional, water-balance approach to calculate soil moisture. The rate at which downward movement of water occurs is controlled by the hydraulic conductivity of the vadose zone soil, which is time-dependent and varies in response to changing soil moisture content. In SESOIL, the vadose zone hydraulic conductivity is calculated using the Brooks and Corey (1966) relationship which accounts for soil moisture content, and includes an exponent-term called the soil pore disconnectedness index that accounts for the soil-specific “wetting” and “drying” soil moisture characteristics (Eagleson, 1978; Eagleson and Tellers, 1982). The soil pore disconnectedness index is a lumped parameter which applies a simplified representation of the physical system by combining several vadose zone soil parameters into a single parameter. The lumped parameter approach can be an advantage by simplifying the data estimation process and reducing computational time needed to run a model. The soil pore disconnectedness index parameter is not commonly found in the literature (ESCI, 2023). SEVIEW provides default values for different soil types based on the work of Eagleson (1978) and Bonazountas and Wagner (1981, 1984). The SESOIL model domain can be split with up to four main layers that each can have up to 10 sub-layers. SESOIL can be used to simulate time-dependent releases from one or more source areas. The size of the source areas, and the depth of release, can be varied. SESOIL uses a multiphase partitioning approach that considers distribution among soil, water, air, and pure phase. Contaminant fate and transport is based on the processes of advection, diffusion, adsorption, volatilization, biodegradation, cation exchange and hydrolysis. SESOIL is used by several states including Hawaii, Massachusetts, New Jersey, Oregon, and Wisconsin, and the USEPA as a vadose zone model for the development of soil remediation standards (NJDEP, 2008). The results calculated by SESOIL for the leaching concentration at the base of the vadose zone are subsequently passed as an input to AT123D to provide the initial concentration in groundwater beneath the soil source.

AT123D is an analytical model that simulates one-dimensional horizontal flow in the saturated zone and incorporates three-dimensional spreading of contaminant by dispersion. The AT123D model assumes steady-state boundary conditions for flow. Fate and transport processes that are simulated in AT123D include advection, dispersion, diffusion, adsorption, and biological decay.

2.2.2 PRZM

The Pesticide Root Zone Model (PRZM) is a model developed by the USEPA primarily for regulation of pesticide uses in agriculture. The original version was released in October 1992 and has been updated on multiple occasions. PRZM 5 Revision B is the most recent version of the model and includes a number of modifications to the model code compared to earlier versions (Young & Fry, 2020). PRZM is currently distributed by the USEPA as part of the Pesticide Water Calculator (PWC) which links PRZM and the Variable Volume Water Model (VVWM) to simulate pesticide applications to land surfaces and subsequent transport to and fate in water bodies, including surface water bodies as well as simple groundwater aquifers. PWC version 2.001 is the version currently approved for regulatory use in the Office of Pesticide Programs (USEPA website accessed June 2023) (USEPA, 2023b).

PRZM is a one-dimensional, finite-difference model developed to simulate pesticide fate and transport in agricultural soils. Multiple soil layers can be simulated with parameters describing different properties of the soil layers including layer thickness, porosity, range of soil capacity (i.e., wilting point and field capacity), and organic carbon content. Temperature-related soil properties can also be activated and specified. Hydrologic processes that are simulated in the model include precipitation and snowmelt, surface runoff, infiltration/percolation, evapotranspiration, and irrigation. Flow in the vadose zone is always modeled to occur in a vertical downward direction. PRZM uses a “tipping bucket” approach to calculate downward flow (i.e., flow is modeled to occur from an upper soil zone to a lower soil zone when the upper soil zone is filled to a maximum capacity). PRZM is designed to simulate agricultural settings and therefore several agronomic practices and characteristics can be represented to simulate land application of chemicals. Contaminant is added to the model in a source area using a defined daily loading rate that can be fixed or variable. Contaminant load can be applied to the ground surface or at depth within the soil column. The model uses a daily time-step for calculation and presentation of results. PRZM uses a multiphase partitioning approach that simulates contaminant distribution among soil, water, and air phases. PRZM simulates contaminant fate and transport based on the processes of surface runoff, soil erosion, microbial and chemical degradation (first-order rate with capability to simulate up to two daughter products), volatilization, foliar wash off, plant uptake, leaching, dispersion, and equilibrium and non-equilibrium sorption with linear and non-linear (Freundlich) isotherms. These transport attributes simulated in the PRZM are not specifically designed for PFAS but are designed to address contaminants more generally. Not all of these attributes are relevant to PFAS (such as degradation). The model also includes simulation of crop growth which influences movement of water at the surface and in shallow soil. Soil erosion resulting from surface runoff is simulated and accounts for topography, soil erodibility, and vegetation coverage. These two processes can influence fate and transport of contaminants in the vadose zone (i.e., plant growth will alter the overall water balance and change how much water infiltrates into the soil column, and for simulations where contaminant is present in surface soils some of the contaminant can be transported to surface water through soil erosion).

2.2.3 Modified HYDRUS

HYDRUS is a Windows-based graphical user interface application for simulating water, heat, and solute movement in one-, two-, and three-dimensional variably saturated media. The one-dimensional version (HYDRUS-1D) is free, public-domain software that is well documented. The two- and three-dimensional versions (HYDRUS-2D/3D) are distributed commercially by PC-Progress (a private software development vendor), and the program can be extended with special add-on modules. HYDRUS is validated/peer reviewed, well maintained, and updated regularly (PC-Progress website, June 2023). The current commercial version of software (HYDRUS V5.02, PC-Progress, November 2022) merges HYDRUS-1D with HYDRUS-2D/3D.

The HYDRUS program numerically solves the Richards equation for water flow in the vadose zone. The Richards equation incorporates the effects of variable moisture content and pressure head on the vadose zone hydraulic conductivity using the Darcy principals for saturated (groundwater) flow. Application of the Richards equation allows for flow to be represented by a physically based process with measurable parameters in lieu of general assumptions to account for these processes. Flow and transport can be simulated to occur in the vertical, horizontal, or inclined directions (for 2D and 3D versions), and multiple model layers can be incorporated to represent variable soil properties. Both flow and transport can be simulated with steady-state or transient boundary conditions. Fate and transport of contaminants is simulated in HYDRUS using convection-dispersion type equations for heat and solute transport. HYDRUS is capable of accounting for multiple processes influencing contaminant fate and transport, including non-linear, non-equilibrium reactions between the solid and liquid phases, linear equilibrium reaction between the liquid and gaseous phases, zero-order production, first-order degradation independent of other solutes, and first-order decay/production reactions that provide the required coupling between the solutes involved in the sequential first-order chain. The transport models can simultaneously account for convection and dispersion in the liquid phase, and diffusion in the gas phase. HYDRUS can currently simulate up to fifteen separate contaminants, which can either be coupled in a unidirectional chain or move independently of each other. Physical non-equilibrium solute transport can be simulated using a two-region, dual porosity type formulation, which partitions the liquid phase into mobile and immobile regions (Šimůnek et al., 2022).

As well as the above fate and transport processes, additional capabilities are available as add-on packages. HYDRUS can be coupled with the USGS PHREEQC program to simulate geochemical reactions. In addition, a "PFAS" add-on module provided by PC-Progress is currently available for use with HYDRUS-1D and HYDRUS-2D. The PFAS module includes options to consider sorption to the air-water interface and the concentration effects on surface tension and viscosity (Silva et al., 2020). We note that use of the PFAS module in 1D and 2D projects also requires a license for the H1D-Pro add-on module package adding additional costs and adapting code is needed to use these modules which requires advanced techniques and calibration. Further, the literature reviewed indicate that the PFAS module has not been validated or verified by field collected empirical data to date.

2.2.4 PFAS-LEACH

PFAS-LEACH is a US Department of Defense (DoD) Environmental Security Technology Certification Program (ESTCP) funded research and development project (Project ER21-5041, Principal Investigator – Bo Guo, Ph.D., anticipated project completion in 2024) that is intended to result in a decision support platform designed specifically to determine PFAS leaching in source zones. It comprises three tiers of simulators decreasing in model complexity, and a comprehensive parameter selection module to support the simulators. The most complex simulator (Tier 1) referred to as PFAS-LEACH-COMP is understood to include a numerical code that incorporates a comprehensive representation of PFAS transport and transformation processes with variably saturated flow based on the Richards equation. A series of research papers have been produced in conjunction with the PFAS-LEACH project (Guo et al., 2022; Zeng and Guo, 2021). Zeng and Guo, 2021 describes the mathematical model that is being developed for the PFAS-LEACH project to simulate PFAS release, transport, and retention based on equations that calculate fluid flow, adsorption, solute transport, and includes an approach to soil heterogeneity. The paper demonstrates (using laboratory studies) that the model accurately simulates PFAS flow and retention in vadose zone soil, and the paper indicates that the model is the first model to account for surfactant-induced flow and solid-phase and air-water interfacial adsorption. However, the literature reviewed indicate that the PFAS module has not been validated or verified by field collected empirical data to date.

Although the more complex model (PFAS-LEACH-COMP) is not yet available, the simplified, one-dimensional version of the model (PFAS-LEACH-Screening model) is available as an analytical solution. Computer code for PFAS-LEACH-Screening is currently only available in two versions (one in Python and the other in MATLAB), and they require that the user has a basic understanding of programing in Python or MATLAB. We understand that a Microsoft Excel-based version is being developed that will make the program more accessible to users that do not have prior coding experience (Personal Communication, Guo B., 2023). It is anticipated that the Microsoft Excel-based version will be made available to the public by the end of 2023 (Personal Communication, Guo B., 2023.)

2.2.5 MODFLOW-USG TRANSPORT

MODFLOW is a modular, finite-difference hydrologic model developed by USGS with multiple versions available as the software has been updated and additional capabilities added. MODFLOW is a command line executable program written in FORTRAN that reads ASCII text and binary input files and writes ASCII text and binary output files.

The MODFLOW program itself does not generate graphical output; however, USGS distributes several free pre- and post-processors for MODFLOW, and commercial graphical user interfaces are also available for sale by private vendors.

- One of these versions, MODFLOW-USG uses an unstructured-grid approach to simulate steady-state and/or transient groundwater flow and tightly coupled processes using a control volume finite-difference formulation (Panday et al., 2013).

- MODFLOW-USG-Transport, released by GSI Environmental, is an additional module that includes advancements to the MODFLOW-USG software. The transport model simulates heterogeneous, three-dimensional solute transport of multiple chemical constituents in the subsurface, caused by advection; hydrodynamic dispersion (which includes both mechanical dispersion and molecular diffusion); mixing (or dilution) from fluid sources; simple reactions including first-order and zero-order decay; linear or Freundlich equilibrium adsorption; and non-equilibrium retardation via a dual-porosity representation. Density-dependent flow and transport processes are also accommodated as is heat transport, matrix diffusion, and dissolution/precipitation of solutes to/from the solution. Other enhancements include saturated/unsaturated flow, dual porosity flow, and water distribution modules along with several convenient features and enhancements that assist with smooth modeling of flow and transport in the subsurface (Panday, S., 2022). Vadose zone flow is simulated by solving the Richards equation.

2.3 Model Review – Summary and Recommendations

There are multiple advantages and challenges with each of the models that have been reviewed as summarized in Table 1. In situations where significant site-specific data are available and variability of input parameters is more constrained such as for purposes of site characterization, risk assessment, and remedial action, use of more comprehensive models (e.g., HYDRUS with PFAS add-on module, or PFAS-LEACH-COMP) may provide more representative predictions than use of general models. However, models can still be used if their limitations are appropriately accounted for, either by stating the limitation when presenting the results, or by adjusting the model setup to implicitly account for a process that is explicitly included in other models. For example, SESOIL does not directly simulate partitioning of PFAS at the air-water interface, however, by reviewing the results of a different model that does include air-water interfacial partitioning, the resulting effect on retention in the vadose zone may be pseudo-replicated by appropriately modifying solid-water partitioning values, and therefore demonstrate the influence that the process would have if it was included in the model.

In summary:

- One-dimensional models (e.g., SEVIEW, PRZM, PFAS-LEACH-Screening) have the limitation of artificially constraining contaminants to move in a single direction. Two- or three-dimensional models (e.g., HYDRUS-2D/3D, MODFLOW-USG Transport, and PFAS-LEACH-COMP) may result in a more accurate prediction relative to observed conditions, but are more challenging to use over larger areas such as state-wide due to the significant variability in site conditions. Therefore, use of the one-dimensional model will likely be more protective by calculating a lower leaching-based soil value.
- None of the models reviewed are currently able to simulate all processes that are emerging as variables that may potentially affect PFAS leaching from soils. Two of the models reviewed (HYDRUS and PFAS-LEACH) can simulate partitioning of PFAS to the air-water interface. However, these models have yet to be validated by specific field data for PFAS transport simulations. Models that do not include this mechanism may underestimate retention in vadose zone soil and overestimate concentrations in leachate that may reach groundwater.
- Research and development of models that incorporate PFAS-specific transport mechanisms is an on-going process, and the literature reviewed indicate that additional research, calibration, and development of model code is needed to provide full functionality and to confirm that each of the models being developed to incorporate PFAS-specific transport mechanisms have the ability to provide accurate predictions under a variety of field conditions.
- Each model applies a different approach to simulate flow of water in the vadose zone. The general models (e.g., SESOIL, PZRM, PFAS-LEACH Screening) simulate downward flow of water using a water balance approach, lumped parameter, or similar, while the more complex (or realistic) models (e.g., HYDRUS, PFAS-LEACH-COMP, MODFLOW USG Transport) simulate flow of water through the vadose zone by solving the Richards Equation. Application of the Richards equation allows for flow to be represented by a physically based process with measurable parameters. However, to obtain the necessary parameter values requires collection of additional site data, or estimation from reported values in research literature to average over varying site conditions. In contrast, the use of a lumped parameter or water balance approach reduces the amount of data needed and simplifies the model calculations, but is not physically based and directly measurable. We note that although a general model may not be able to accurately match observed values on a short time scale (e.g., days), if considered over a longer time scale (e.g., months or years), then the modeled values may be sufficiently accurate for the intended purpose, which in this instance would be development of protective leaching-based soil values.

Based on our review, SEVIEW was selected to model leaching-based soil values because it provides:

- Efficient approach to effectively simulate state-wide conditions and address large-scale variability in site conditions for multiple input parameters.

- Simulates protective leaching-based soil values despite the limitations of one-dimensional flow, simulating flow through the vadose zone using a water balance approach and lumped parameter, and not simulating air-water interface PFAS partitioning, since these limitations tend to increase the PFAS leached from the soil, downward transport of the contaminant will be quicker and at higher concentrations, and leaching of the contaminant will occur for a shorter period of time.
- Use of a general model reduces the complexity of obtaining voluminous site-specific data or conducting substantial analysis of literature values to provide representative results over a wide variation of site conditions.
- Consistency with the process previously used by NHDES to develop existing leaching-based soil values and used by several other states and USEPA to develop remediation soil standards.

In addition, we have selected MODFLOW-USG Transport as a secondary model to compare to results of SEVIEW modeling. As previously noted, although MODFLOW-USG Transport and HYDRUS 3-D have similar capabilities, preference was given to MODFLOW in selecting a secondary model because it is considered the industry-standard (USGS, 2022). This model assesses more complex situations (e.g., three-dimensional soil heterogeneity) while incorporating the same key fate and transport processes as SEVIEW. However, based on inputs requiring more site-specific criteria which needs to be estimated over a wide range of variable site conditions for the purpose of simulating state-wide conditions, MODFLOW-USG Transport is less likely to provide results that are protective and could result in actual individual sites where leaching-based soil values developed using MODFLOW-USG Transport are not representative of actual leaching conditions.

3.0 CHEMICAL-SPECIFIC MODEL INPUT PARAMETER SELECTION

This section describes the chemical-specific data used as input parameters to SEVIEW and MODFLOW-USG Transport. A tabulated summary of the selected input parameters is provided below in Exhibit 3-1.

Exhibit 3-1: Tabulated Chemical-Specific Model Input Parameters.

Chemical	PFHxS	PFNA	PFOS	PFOA
K_{oc}	64	203	804	64
K_{oc} Source	2023 USGS NH Study – further discussed in Appendix A			
Molecular Weight (MW) (g/mol)	4.00E+02	4.60E+02	5.00E+02	4.10E+02
MW Source	RSL Supporting Table (EPA 2023)			
Henry's Law Constant (HLC) (atm-m^3/mol)	6.1E-05	1.9E-03	4.43E-07	3.57E-06
HLC Source	ITRC (2022)	ITRC (2022)	RSL Supporting Table (EPA 2023)	
Water Solubility (mg/L)	239.43	11.66	6.80E+02	9.50E+03
Solubility Source	ITRC (2022)	ITRC (2022)	RSL Supporting Table (EPA 2023)	
Air Diffusion Coefficient D_{ia} (cm^2/s)	2.33E-02	2.13E-02	2.07E-02	2.26E-02
D_{ia} Source	RSL Supporting Table (EPA 2023)			

Water Diffusion Coefficient D_{iw} (cm²/s)	6.01E-06	5.43E-06	5.25E-06	5.79E-06
D_{iw} Source	RSL Supporting Table (EPA 2023)			
Water Diffusion Coefficient D_{iw} (m²/hr)	2.164E-06	1.955E-06	1.890E-06	2.084E-06

Additional discussion of the selection process for the following chemical-specific input parameters is provided in this section:

- Organic carbon partitioning coefficient (k_{oc}) (Section 3.1)
- Henry's law constant (Section 3.2)
- Water solubility (Section 3.3)
- Air and water diffusion coefficients (Section 3.4)

Given the range in some of the input parameter values, a sensitivity analysis was completed to identify the potential impact the variables have on the calculation of leaching-based soil values. A summary of the input parameters used in the sensitivity analysis is provided in Section 5.

3.1 Solid-Phase Partitioning

The NHDES partnered with the USGS for the 2023 USGS NH Study. A stated purpose of the 2023 USGS NH Study was to investigate partitioning for New Hampshire soils. The soil isotherm K_d values, and associated K_{oc} values, were screened by Sanborn Head to select samples that were (i) representative of the soils and conditions included in the conceptual site models (CSMs) used for the leaching-based soil value model scenarios, and (ii) provided relatively stable partitioning values. Solid phase partitioning coefficients are summarized in Table 2. The approach for selecting K_{oc} values from the 2023 USGS NH Study is discussed in Appendix A.

3.2 Volatilization to Soil Gas

The selected Henry's Law constants for PFOA and PFOS were those included in the USEPA RSLs chemical specific parameters generic table, which cited "ATSDR Profile" as the original source for the PFOA Henry's Law constant and "3M" as the original source for the PFOS Henry's Law constant (USEPA, 2023a). PFNA and PFHxS volatility parameters are not available in the USEPA RSLs chemical-specific parameters generic table or the 2021 ATSDR Tox Profile (ATSDR, 2021). Selected Henry's Law constants for PFNA and PFHxS were based on median of literature values compiled by ITRC (2022).

3.3 Solubility

The selected solubility values for PFOA and PFOS were those included in the USEPA RSLs chemical specific parameters generic table, which cited "3M" as the original source (USEPA, 2023a). PFNA and PFHxS solubility values are not available in the USEPA RSLs chemical-specific parameters generic table or the 2021 ATSDR Tox Profile (ATSDR, 2021). Selected solubility values for PFNA and PFHxS were based on median of literature values compiled by ITRC (2022).

3.4 Diffusion in Water and Air

The selected water and air diffusion coefficients for PFOA, PFNA, PFHxS, and PFOS were those included in the USEPA RSLs chemical specific parameters generic table, which cited "WATER 9" as the original source (USEPA, 2023). WATER9 is a USEPA software for estimating air emissions from wastewater.

4.0 DEVELOPMENT OF A GENERIC CONCEPTUAL SITE MODEL

To derive leaching-based soil values, it is necessary to develop a generic release site (i.e., generic conceptual site model) that is representative of generic site conditions (e.g., soils/geology of the region, climate, and depth to groundwater) and generic contaminant release scenarios. For the generic site, it is assumed that following a release, the contaminant leaches over a period of time from the source area, migrates through soil to underlying groundwater, and reaches the receptor well (point of compliance [POC] well). To be protective for this scenario, a leaching-based soil value is set at a value so that the contaminant concentration at the POC (e.g., drinking water well) is not greater than the applicable AGQS. The generic CSM needs to represent a typical release scenario and incorporate conservative assumptions that are representative of statewide conditions because the leaching-based soil values are designed to be protective at sites across the state.

Release scenarios common to many contaminants, including PFAS, can include situations like a leaking underground storage tank (UST), leaking pipeline, discharge to a dry well or drain field, or surface spill with release to soil. The CSM previously used by NHDES to develop leaching-based soil values is a subsurface discharge scenario (e.g., a leaking UST or leaking pipeline) (NHDES, 1998). There are also release scenarios for many contaminants including PFAS that result in direct discharge to the ground surface. Examples of surface release scenarios for PFAS include application of aqueous film forming foam (AFFF) and air deposition.

The CSM applied by NHDES to develop existing leaching-based soil values for other contaminants is summarized in the following section. Subsequently, we present and discuss an alternative CSM that can be applied to represent the PFAS-specific surface release scenarios described above. Finally, we review and discuss general aspects of the CSM (parameters and assumptions) that could be updated or modified to either be more protective (e.g., source area size, distance to receptor), or be more representative of current conditions (e.g., climate).

4.1 Existing NHDES CSM Summary (Subsurface Release CSM)

The generic CSM established by NHDES to develop existing leaching-based soil values protective of groundwater quality is summarized in Appendix B (Revised September 2018) of the RCMP (NHDES, 1998) (referred to hereafter as the Subsurface Release CSM). Consistent with the types of contaminants being widely investigated and remediated at the time of initial development, the Subsurface Release CSM is a generic scenario intended to simulate a site with a leaking UST or pipeline. Although the Subsurface Release CSM does not represent all possible release scenarios, it represents a typical release scenario and is considered protective for groundwater because the source release occurs below ground nearer to the groundwater table. As such, there will be less contaminant dilution and attenuation as the contaminant travels the shorter vertical distance to the groundwater table, and therefore a lower leaching-based soil value is needed to be protective of groundwater.

The Subsurface Release CSM assumes:

- The water table is static at 3 meters (approximately 10 feet) below the ground surface, and a drinking water well is located 10 meters from the downgradient edge of the contaminated soil area.
- The area of contaminated soil is 10 meters by 10 meters.
    - The first meter below the ground surface (Model Layer 1) is not contaminated.
    - From one to two meters below ground (Model Layer 2), the soil is contaminated.[5]
    - From two to three meters (consisting of Model Layers 3 and 4) the soil is initially not contaminated but becomes contaminated as the model simulates transport of the contaminant downward through the vadose zone to the groundwater.

Unless specifically discussed in the following sections, parameter input values applied for the Subsurface CSM are model simulations are kept consistent with the values described in RCMP Appendix B (NHDES, 2018). A schematic of the Subsurface Release CSM is provided below in Exhibit 4-1.

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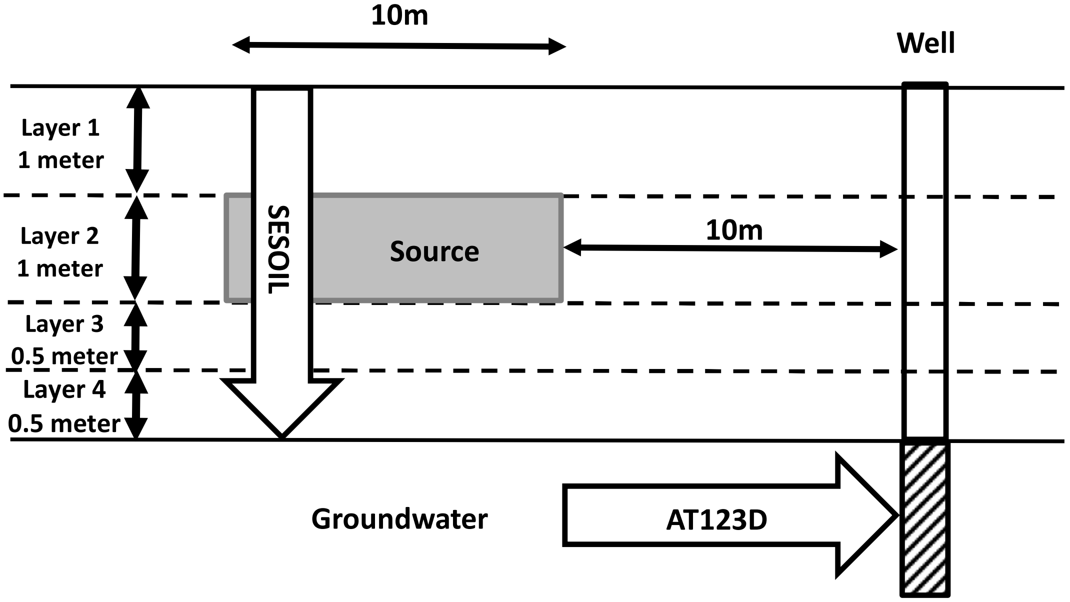
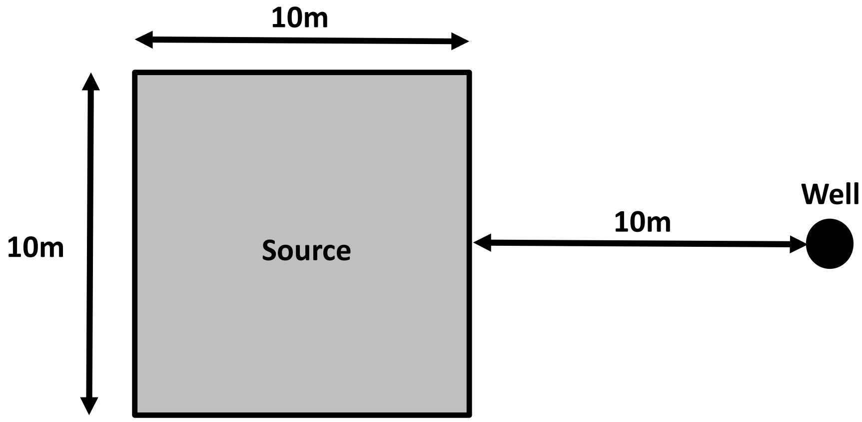
[5] The model assumes that the source soil is contaminated at a concentration of 10 parts per million (ppm) by weight, equivalent to 10 milligrams per kilogram (mg/kg). The concentration of 10 ppm is used as a place-holder value and does not affect the calculated DAF used for deriving the leaching-based soil values because the processes included in the model do not change with concentration. For example, neither the linear K_{oc} approach for solid-phase partitioning nor the Henry's Law approach for volatility change with changing concentration. If a process that depends on concentration were included, such as non-linear partitioning, then the approach would need to be updated to use more representative concentrations for PFAS transport modeling.

Exhibit 4-1: Schematics for the Conceptual Site Model for the Subsurface Release CSM

Subsurface Release Conceptual Site Model (Vertical Cross-Section)
(Adapted from Liptak and Lombardo, 1996)



Subsurface Release Conceptual Site Model (Horizontal Plan View)



4.1.1 Thickness of Vadose Zone

The Subsurface Release CSM assumes that the water table is static at 3 meters (approximately 10 feet) below the ground surface (NHDES, 1998). Based on review of available data, we concluded that the Subsurface Release CSM depth to groundwater of 3 meters was still representative. The analysis and review of New Hampshire specific data that supports this conclusion is summarized below.

To confirm the typical thickness of the vadose zone in New Hampshire, we reviewed data from the approximately 104,000 water well records contained in the NHDES' electronic database of records[6]. The database comprises installation records for approximately 97,000 bedrock wells and 7,000 overburden wells, of which approximately 93,000 well records have been classified as domestic water supply wells. The remaining 11,000 wells were classified as test wells, geothermal wells, or other water supply wells (e.g., municipal, commercial, industrial, agricultural).

After splitting the water well records into two groups by aquifer type (overburden or bedrock), the records were subsequently grouped by month of well installation. Summary statistics were then calculated for each of the 24 groups and reviewed relative to the Subsurface Release CSM release scenario.

Box plots representing the monthly statistics for each of the overburden and bedrock groups are shown below in Exhibit 4-3. Although there is some monthly variation as expected based on natural processes such as precipitation, the relative change between months was not considered significant, particularly given the uncertainty in the accuracy and precision of the recorded data as the data are only field observations during drilling installation of the wells, and the overall variability in the reported depths to groundwater amongst the wells was substantially greater than the seasonal variation in the mean depths to groundwater. Calculated statistics for median, lower quartile, and upper quartile are summarized below in Exhibit 4-2 for the separate overburden and bedrock groups. Based on review of these data, we concluded that the Subsurface Release CSM depth to groundwater of 3 meters was still representative. The range in depths to groundwater based on the upper and lower quartiles was also used for sensitivity testing as described in Section 5.

Exhibit 4-2 Summary Statistics of Approximate Depth to Groundwater for Overburden and Bedrock Wells in New Hampshire [feet below ground surface (ft bgs) – values rounded to nearest foot]

	Quartile 1	Median	Quartile 3
Overburden wells	6 ft bgs	10 ft bgs	20 ft bgs
Bedrock wells	13 ft bgs	20 ft bgs	33 ft bgs

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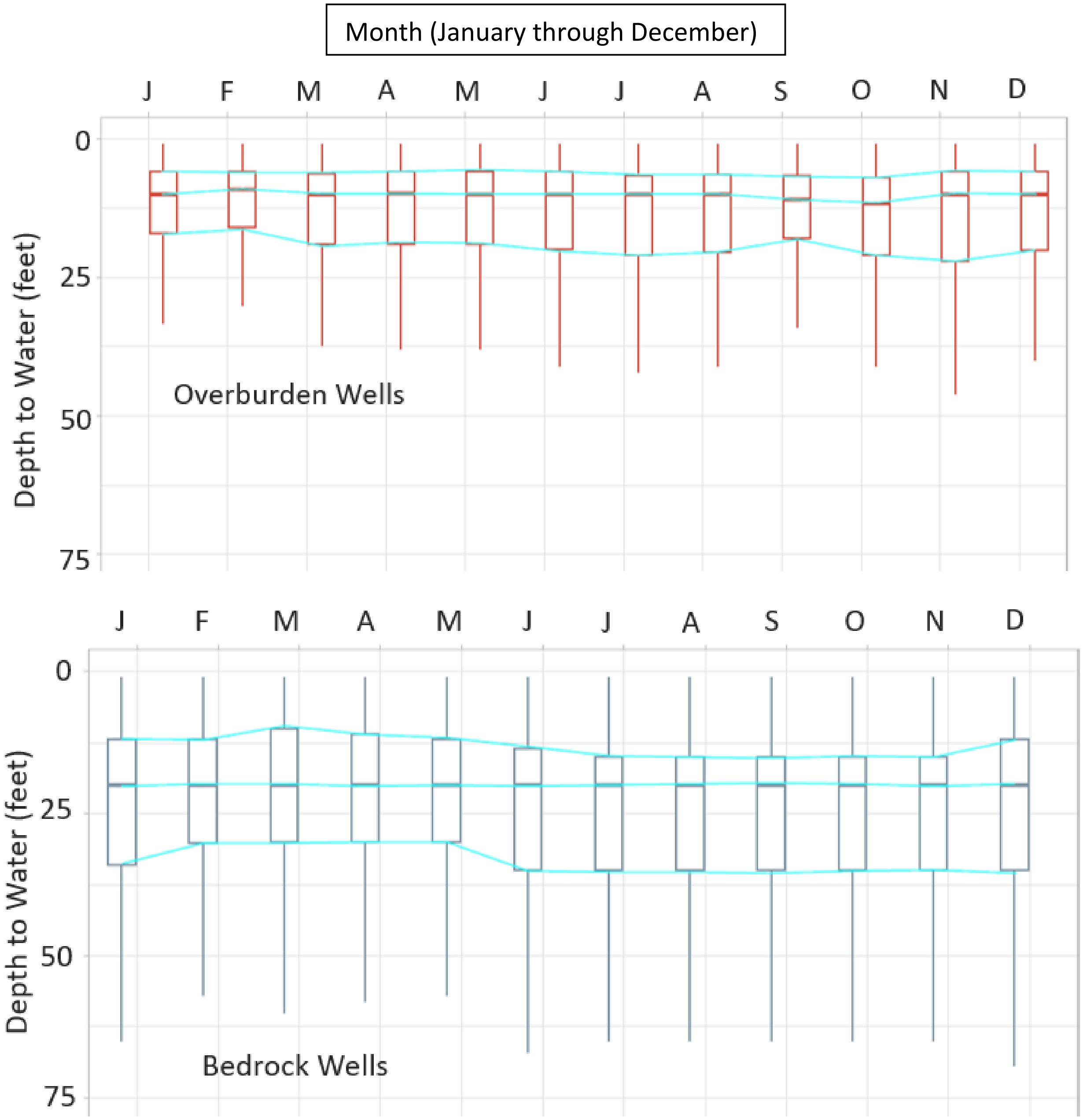
[6] NHDES Onestop Database - https://www4.des.state.nh.us/DESOnestop/BasicSearch.aspx

Exhibit 4-3: Graphical summary of monthly statistics of depth to groundwater for overburden and bedrock wells in New Hampshire [feet below ground surface (ft bgs).



4.1.2 *Soil Type*

In the Subsurface Release CSM, the entire soil column is modeled as sand soil with organic carbon content set at 0.1% throughout the entire thickness of the vadose zone. A soil organic carbon content of 0.1% is considered representative of sub-surface glacial sand soils and was previously selected by NHDES for soil-to-groundwater leaching modeling as representative of New Hampshire soils (Liptak and Lombardo, 1996; NHDES, 1998)[7]. Use of sand as the soil type

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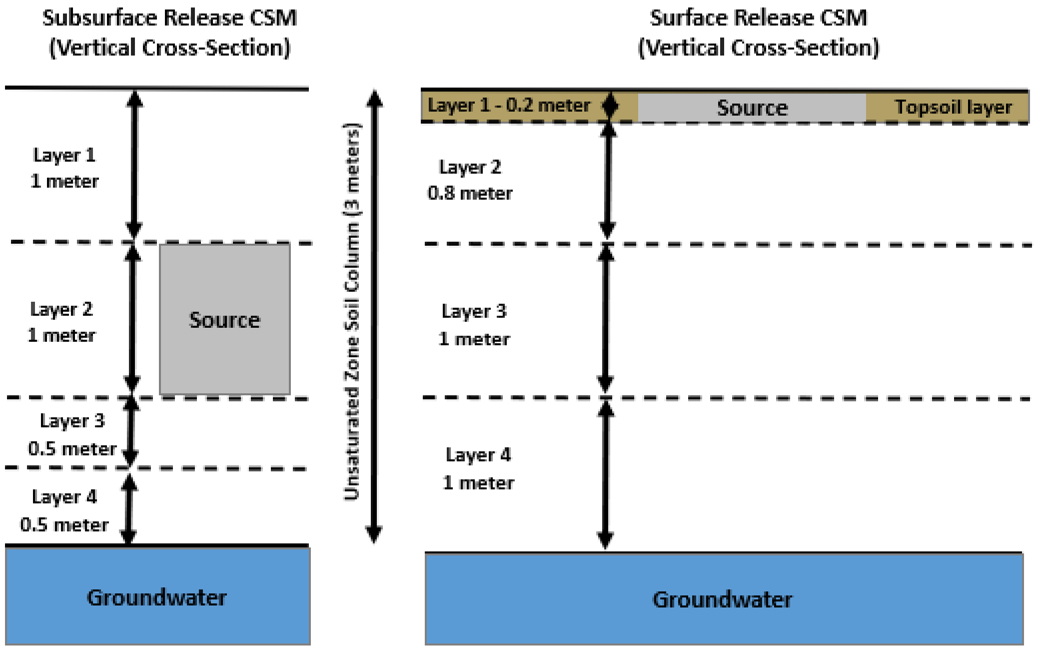
[7] An attempt was also made to evaluate the type of overburden soils recorded on the water well record (for both overburden and bedrock wells). Around 5,000 records did not include a soil type. After grouping the records by soil type, the groups were ranked by soil types with highest number of data entries to lowest number of data entries. Review of the ranked data

is a typical approach in developing leaching-based soil values because the sand soil has a relatively high hydraulic conductivity and typically low organic carbon content, both of which tend to result in more rapid leaching and transport of contaminants from soil to groundwater.

4.2 Development of Alternative CSM (Surface Release CSM)

Given the potential for PFAS releases to occur to the ground surface, an alternative surface release CSM (hereafter referred to as the Surface Release CSM, and referenced in Table 4 as simulation # 13 to 16 for each of the four PFAS) that assumes the contaminant release occurs in the upper 0.2 meters of the soil column was modeled, which is represented by a topsoil with higher organic carbon content of 5% although the model runs also varied this to 0.1% total organic carbon. This organic carbon content value (5%) is representative of the upper range of organic carbon content measured in the soil included in the 2023 USGS NH Study discussed in Appendix A. No change is made to the thickness of the vadose zone (3 meters) because the analysis presented above in Section 4.1.1 indicates this is representative of the median depth to groundwater for overburden soils in New Hampshire. The Surface Release CSM is visually represented below in Exhibit 4-4 and includes a comparison to the Subsurface Release CSM.

Exhibit 4-4: Schematic of Surface Release CSM compared to the Subsurface Release CSM in cross-section view.



Other aspects of the CSM discussed herein (e.g., climate, source area size, and depth to groundwater) remain the same because the parameters are generally applicable to both the Subsurface Release CSM and the Surface Release CSM. For example, the Surface Release CSM

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shows that approximately 70% of records can be classified by a single soil type with 25% of the well records stating till as the only soil type, 17% gravel, 10% sand, 9% clay, and 8% sand and gravel. The remaining 30% of records could be split into around 1,800 unique groups based on two or more recorded soil types.

uses the same 10 x 10 meter source area size for SEVIEW model simulations (Simulations #13-16). Due to the types of surface releases that are common to PFAS (application of AFFF, air deposition), the source area size for the Surface Release CSM was also varied to 25 x 25 meters (Simulations #17-20) since these types of surface releases can be found over larger areas. However, due to model set up and limitations of one-dimensional flow models in general, the size of the source area will not materially change the leaching-based soil value after a certain point (i.e., source area size dimensions). This point of departure was estimated at 25 x 25 meters for the Surface Release CSM.

4.3 Updates to Subsurface Release CSM

This section provides a discussion of analysis of climate data, precipitation infiltration, and the size of the source area for inputs within the CSM and selected model. Note that SEVIEW uses location specific climate data to calculate the water balance to address recharge in the model. However, MODLFOW USG Transport does not use a calculation of water balance and instead uses direct input of estimated recharge for the area being modeled and is intended for this to be a site-specific input. To provide consistency between SEVIEW and MODFLOW USG Transport, the calculated groundwater recharge input used in the SEVIEW model based on the climate analysis presented below was also used as the direct groundwater recharge input for the MODLFOW USG Transport simulations.

4.3.1 Climate Data and Infiltration of Precipitation

Water from precipitation infiltrates at the ground surface into the soil and moves downward through the soil towards the groundwater table. As water moves downward through the soil, contaminants coming into contact with the water are transported through the vadose zone to groundwater. This is the primary mechanism of PFAS leaching and therefore the magnitude and timing of when infiltration of precipitation occurs is a key component of vadose zone leaching models.

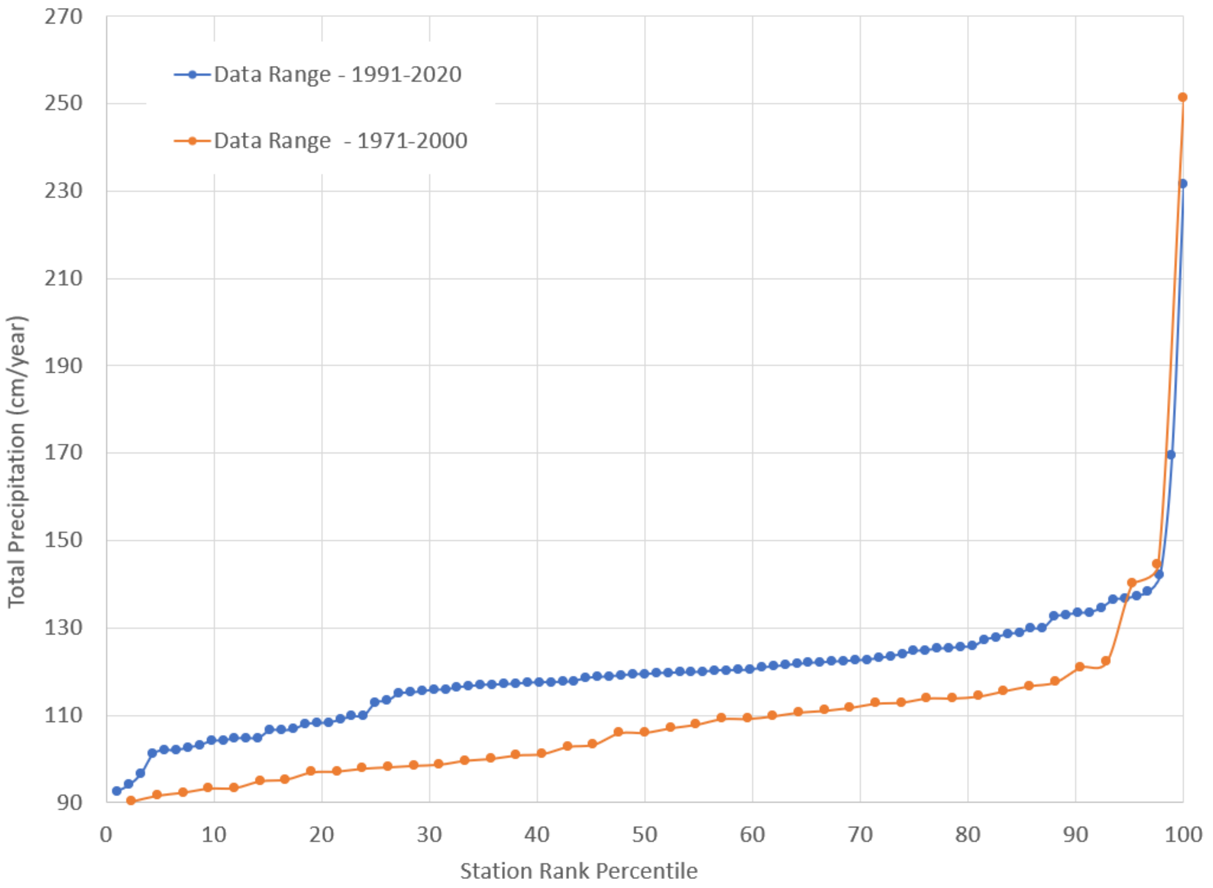
As indicated above, the SESOIL model uses location specific climate data to calculate the water balance including surface water runoff, evaporation, and infiltration. The climate data used in the SESOIL model includes monthly air temperature, cloud cover fraction, relative humidity, short wave albedo, rainfall depth, mean storm duration, number of storms per month, and length of rainy season within a month. The SEVIEW software program is preloaded with climate data from weather stations for use with SESOIL model simulations. Following the previous SEVIEW modeling completed by NHDES in 2013 and 2018 and as described in Appendix B of the RCMP, climate data are included for two different meteorological periods (1971 to 2000, and 1991 to 2020), with 1971-2000 data available for 42 stations located throughout New Hampshire, and data for 92 New Hampshire stations for the period 1991 to 2020.

As described in Appendix B of the RCMP, NHDES has previously applied a "representative" climate dataset for New Hampshire based on the climate station (Massabesic Station) that has an annual total precipitation closest to the New Hampshire annual average, excluding the stations with the highest and lowest precipitation values. After excluding the data from New Hampshire's highest and lowest precipitation stations, the average value was calculated by the NHDES using data from the 42 stations with 1971 to 2000 data.

As part of this work, we have assessed climate data available for New Hampshire to evaluate if there has been a change in precipitation with time, and if there is a spatial component to climate in New Hampshire that might warrant an update to the Subsurface Release CSM input parameters.

To assess change with time, we compared the data available in SEVIEW from the two time periods (i.e., the 1971 to 2000 and 1991 to 2020 datasets). Review of the datasets shows an overall higher total annual precipitation in the more recent dataset. Review of the data shows that for the two climate stations representing the median of each respective dataset, total annual precipitation increased from 106 cm/year (41.7 inches/year) to 119 cm/year (46.9 inches/year). Due to the difference in the sizes of the datasets (42 versus 92 stations) and the increased complexity of comparing the two datasets, the median value was selected as a more representative comparison point as average values typically are skewed by higher and lower values. Graphical comparison of the precipitation data for the two datasets is presented below in Exhibit 4-5.

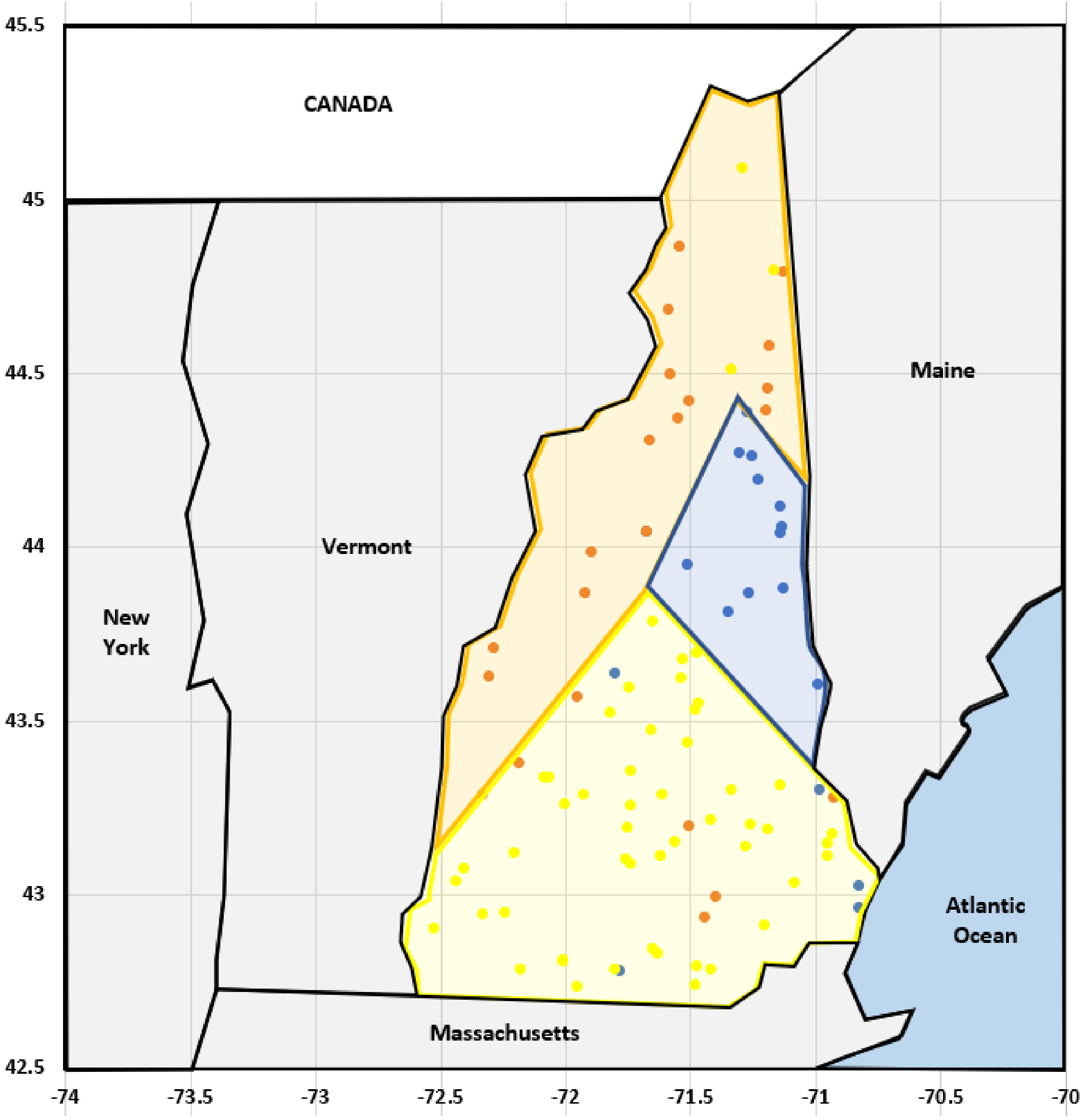
Exhibit 4-5: Total New Hampshire precipitation by station 1971-2000 and 1991-2020



To assess spatial variability in climate across New Hampshire, we ranked the climate stations with data for 1991 to 2020 using total annual precipitation. We then separated the ranked stations into three groups representing the bottom 20%, top 20%, and the remaining middle

60%. The climate station locations were plotted on a map of the State and assigned a symbol color based on their respective percentile. As shown in Exhibit 4-6, in general, the groups form three distinct areas. The stations with the lowest total annual precipitation are typically located in the region north and west of the White Mountains (orange symbols). The group with the highest annual precipitation is located within the White Mountain region (blue symbols), and the middle group representing the remaining precipitation range is generally located in the southern region of New Hampshire (yellow symbols).

Exhibit 4-6: Map of New Hampshire climate station locations (geographical boundaries are approximate). Stations with low total annual precipitation (orange symbols). Stations with high annual precipitation (blue symbols). Stations representing the middle of the precipitation range (yellow symbols). See text for additional explanation of symbols.



For the Subsurface Release CSM (Simulations #1-4) and Surface Release CSM (Simulations #13-16) simulations, the climate data used were kept consistent with the climate data stated in Appendix B of RCMP 2018. The modified Surface Release CSM (Simulations #17-20) was adjusted to consider snow melt (described below). Recognizing that there are variations in the climate data, climate stations from both time periods and representative of the range of precipitation observed were assessed (Simulations #75-82) as part of the sensitivity analysis described in Section 5.3.

Snow Melt

The climate data applied in SESOIL do not automatically account for build-up, and subsequent melting, of a snowpack during the winter season (i.e., precipitation recorded as snow is treated as rainfall and infiltrates in the month it is recorded and not during the month when it melts). Melting of snowpack is an important mechanism that influences seasonal infiltration of precipitation. The proportion of monthly precipitation that is rain or snow can be estimated using mean monthly temperature. As described in the USGS Open-File Report 2007–1088 (McCabe and Markstrom, 2007), when mean monthly temperature is below a specified threshold, all precipitation can be considered to be snow. If temperature is greater than an additional upper temperature threshold, then all precipitation can be considered to be rain. Within the range defined by these two temperatures, the amount of precipitation that is snow can be linearly proportioned from 100 percent to 0 percent of total precipitation. Using this model, precipitation that is considered to be snow is stored until temperatures increase sufficiently to cause complete melting. The result of this process is that less infiltration of precipitation will occur during cold months when precipitation is stored as snow, and an increased amount will subsequently infiltrate during the warmer spring months. To test the influence of snowpack and snow melt on the derivation of leaching-based soil values, we used the above approach to modify the precipitation data from the 1991-2020 Massabesic climate station data to simulate melting of snowpack. The result of this modification is that less infiltration occurs in the months of January to March, and a larger quantity infiltrates in the month of April relative to the unmodified data. As noted above, the modified precipitation data is applied in Simulations #17-20, and Simulation #76.

4.3.2 Depth to Groundwater

Model simulations addressed the depth to groundwater based on the estimated or modeled thickness of the vadose zone as described in Section 4.1.1. As noted in Section 4.1.1, the selected depth to groundwater is 3 meters (10 feet).

4.3.3 Size of the Source Area

The Subsurface Release CSM tends to be restricted to a smaller subsurface area in contrast to common PFAS-specific surface release scenarios, which may represent releases over a larger area. In general, as the source area size increases, the contaminant load to groundwater also increases, and thus the leaching-based soil value decreases. As such, the Subsurface Release CSM assumes that the size of the source area is 10 meters-by-10 meters (approximately 0.025 acres). A range of source area dimensions from 5 meters-by-5 meters up to 150 meters-by-150 meters were considered, as described below. For context, we note that the median parcel size in New Hampshire where a water well is present on the property is approximately 2.3 acres (corresponding to an area of approximately 100-by-100 meters).

Exhibit 4-6: Schematic of Subsurface Release CSM with the size of the source area varied.

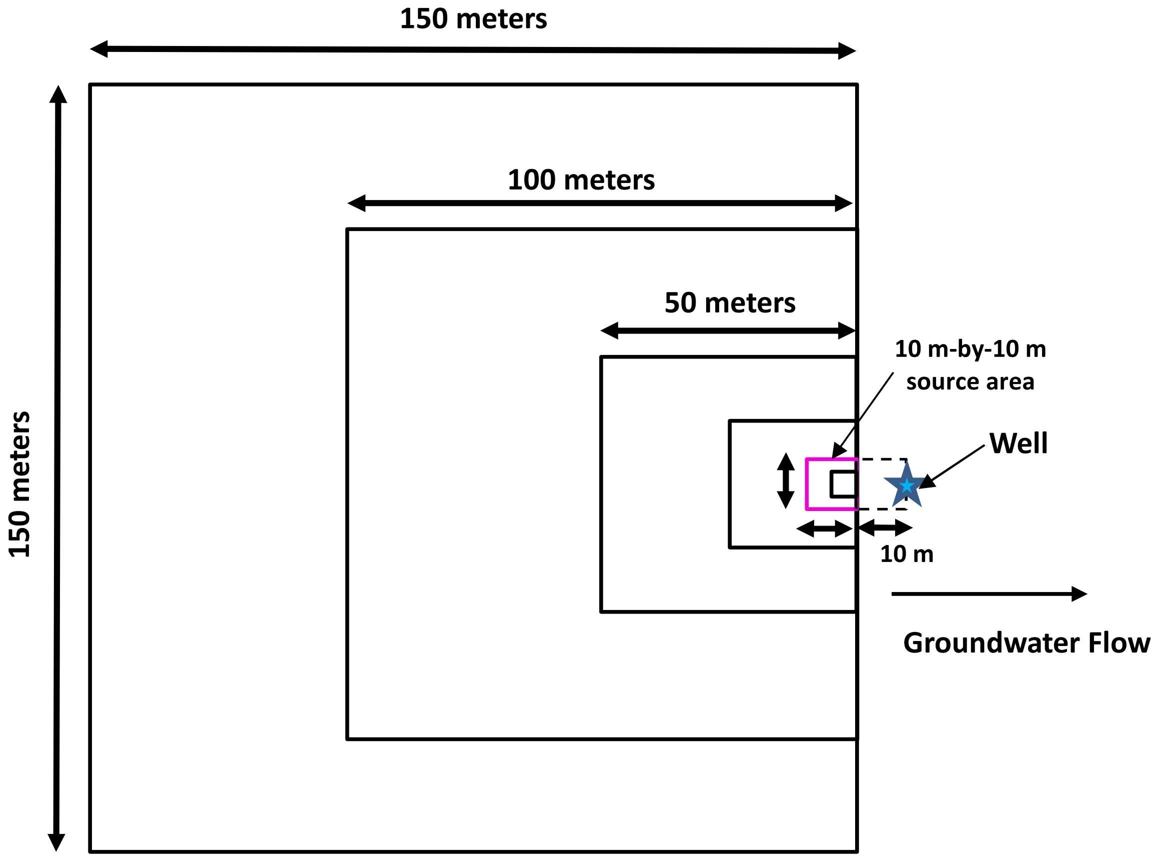


Exhibit 4-7: Varied Source Area Sizes by CSM

Conceptual Site Model (CSM)	Source Area Size (in meters)					
Subsurface Release CSM	5 x 5	10 x 10	25 x 25	50 x 50	100 x 100	150 x 150
Surface Release CSM	Not Used	10 x 10	25 x 25	Not Used	Not Used	Not Used

The simulations also included other soil types which cover a range of soil physical properties beyond the sand soil.

4.4 Parameter Values Selected for SEVIEW Model Simulations

Based on review of parameters described in Section 3 and the CSM and related input information described previously in this Section, input parameters were selected for use in the model simulations. A range of input parameter values were used for both chemical specific and non-chemical specific input parameters due to the state-wide variability in site conditions and the complexity of chemical transport in the subsurface. Unless specifically discussed in the prior sections, parameter input values applied for the Subsurface CSM model simulations are summarized in Table 3, and have been kept consistent with the values described in RCMP Appendix B (NHDES, 2018).

Table 3 summarizes the input parameters selected for use in the SEVIEW Model. Table 3 also specifies the input parameters used as a reference point or baseline for the Subsurface Release and Surface Release CSM model simulations. Table 4 provides a comparison of selected input parameters and the simulation results from the SEVIEW model with discussion of simulation results provided in Section 5.

4.5 MODFLOW-USG Transport Model Setup and Parameter Selection

As discussed in Section 2.3, MODFLOW-USG Transport model was also constructed to compare to the results of the SEVIEW model as described in Section 2.3. MODFLOW-USG Transport model setup and parameter information for the six model scenarios are included in Table 5 and discussed below.

Scenario One – Model design consists of homogeneous, anisotropic sand with a subsurface release from 1 to 2 meters below ground level. Model parameter values, grid construction, and the size and depth of release are intended to replicate the Subsurface Release CSM used in the SEVIEW model. The vadose zone thickness is approximately 3 meters while the saturated zone is approximately 20 meters thick.
Scenario Two – This simulation is a modification of Scenario One and is intended to demonstrate the influence of aquifer thickness and dispersivity values. The soil continues to be represented by a homogeneous, anisotropic sand. The vadose zone thickness is again approximately 3 meters thick, but the saturated zone thickness is reduced to approximately 10 meters. Dispersivity values are based on the Xu & Eckstein (1995) empirical relationship to flow path length.
Scenario Three – Model design consists of homogeneous sand with a surface release in a 10 meter-by-10 meter area, and grid construction and soil organic carbon representative of the SEVIEW Surface Release CSM. Aquifer thickness is again limited to 10 meters thick, and dispersivity values are based on the Xu & Eckstein (1995) empirical relationship to flow path length.
Scenario Four – Model design consists of a heterogeneous sand with the range of conductivity values generated randomly as described in Section 4.6. Other input parameters are similar to Scenario Three.
Scenario Five – Model design consists of a layered, heterogeneous silt and sand soil with the range conductivity values generated randomly as described in Section 4.6. Other input parameters are similar to Scenario 3.
Scenario Six – Model design consists of a layer of sand over low permeability heterogenous till soil (sandy clay) layer. The range of conductivity values were generated randomly, and other input parameters were kept consistent with Scenario 3.

5.0 MODEL SIMULATIONS AND RESULTS

Development of leaching-based soil values for the PFAS for which NHDES has adopted AGQS (i.e., PFOS, PFHxS, PFNA, and PFOA), has been performed by modeling the leaching potential of the select PFAS using SEVIEW (SESOIL and AT123D) and MODFLOW-USG Transport.
The results are summarized in the following:

- Table 3 provides a summary of the input parameter values for the surface and subsurface CSM model simulations performed using SEVIEW. Table 4 provides a summary of the SEVIEW model simulated results, including maximum groundwater concentration, DAF, time to reach the maximum groundwater concentration, AGQS, and the leaching-based soil value for each of the contaminants modeled.
- Table 5 provides a summary of the assumptions, input parameter values, and model predicted results for each simulation of PFOA fate and transport performed using MODFLOW-USG Transport.
- Review and discussion are provided in Section 5.1 for the SEVIEW model results and in Section 5.2 for MODFLOW-USG Transport model results.

5.1 SEVIEW Results

Approximately 145 simulations were completed using the SEVIEW model including sensitivity analysis simulations. A comparison of simulated leaching-based soil value results based on input parameter variations within the model runs is provided in Figure 1 and summarized in Table 4. As a reference point, model simulation #4 (PFOA with subsurface CSM) is used as the baseline for comparison to other model simulations, and is highlighted on Figure 1 by a vertical dotted line. With reference to the model simulation numbers listed in Table 4, and as illustrated on Figure 1, the leaching-based soil value results for each of the SEVIEW model simulations performed are generally summarized and discussed as follows:

- **Subsurface Release CSM** simulations for PFOS, PFHxS, PFNA, and PFOA (**Simulation #1 – 4**);
- Interim simulations performed (for PFOS, PFHxS, PFNA, and PFOA) to demonstrate the relative effect of changes made to the model in the transition from subsurface to surface CSM (Simulation # 5- 15). Changes made in a step-wise approach included modification of the model grid (Simulation # 5- 8), change in fraction of organic carbon in the near-surface soil (Simulation # 9 - 12), and change to release depth, which is reference in the bullet below as the Surface Release CSM simulations (Simulation #13 – 16);
- **Surface Release CSM** simulations for PFOS, PFHxS, PFNA, and PFOA (**Simulation #13 – 16**);
- Surface Release CSM simulations for PFOS, PFHxS, PFNA, and PFOA, with alternative input parameter values applied for source area size, climate data, distance to compliance point, and aquifer dispersivity (Simulation #17 – 20); and
- Sensitivity Analysis of Individual Model Parameters (Simulation #21 – 145), which is reviewed in Section 5.3.

The modeling work described in this report considered two CSMs including the Subsurface Release CSM and the Surface Release CSM). Simulations completed for PFOS, PFHxS, PFNA, and PFOA using the Subsurface Release CSM (Simulation # 1 – 4 as indicated in Table 4), showed a range of leaching-based soil value results between 0.16 to 0.89 ng/g (i.e., approximately one order of magnitude - 0.1 to 1.0 ng/g). In contrast, simulations completed for PFOS, PFHxS, PFNA, and PFOA using the Surface Release CSM (Simulation # 13 – 16 as indicated in Table 4), showed a range of leaching-based soil value results between about 6.67 to 195.38 ng/g (i.e., a range that is about two orders of magnitude higher than the range using the Subsurface Release CSM). Tabulated results for two simulations including the four PFAS and two CSMs are provided in Exhibit 5-1 below for comparative purposes. Values are reported in ng/g and rounded to the hundredth place. Other simulations are summarized in Table 4.

Exhibit 5-1: Summary of Leaching-Based Soil Values for Simulation of PFOS, PFHxS, PFNA, and PFOA Using Both the Subsurface Release and Surface Release CSMs.

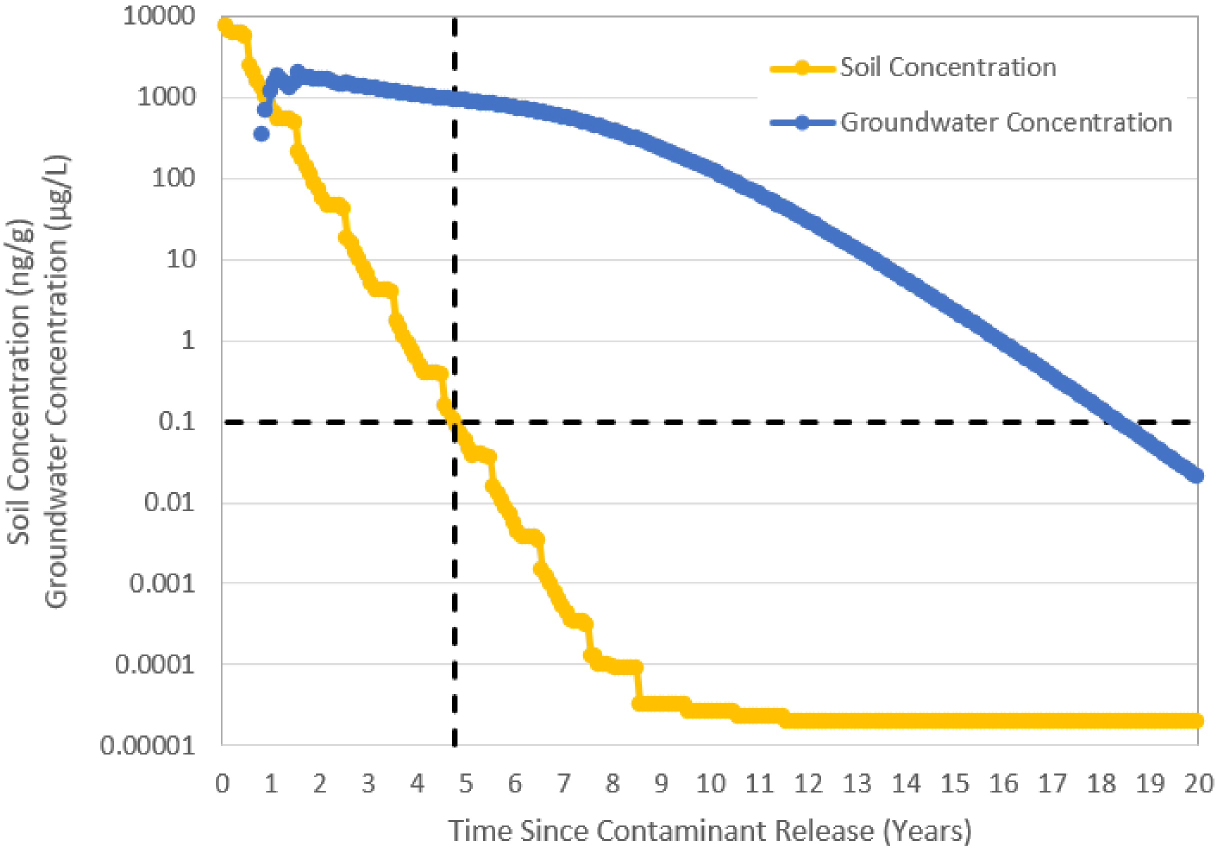
Chemical	PFOA	PFNA	PFHxS	PFOS	Simulation #[1]
Subsurface Release CSM Source area soil foc = 0.1%	0.16	0.53	0.24	0.89	1-4
Surface Release CSM (release at surface, 10 m x 10 m source area) Source area soil foc = 5%	6.67	195.38	10.91	99.34	13-16

Notes: [1] indicates that there is an individual simulation for each of the four PFAS modeled as presented in Exhibit 5-1.

The Subsurface Release CSM (Simulations #1-4) resulted in lower leaching-based soil values than the Surface Release CSM (Simulations #13-16) primarily because (i) the subsurface releases were associated with relatively low organic carbon content soil, which is modeled to be more leachable, and (ii) the subsurface release occurs nearer to the groundwater table, so there is less vertical distance for attenuation in the vadose zone.

Both CSMs used model parameters that tended to be either values used previously by NHDES for the Subsurface Release CSM, were chemical parameters selected as discussed in Section 3, or were protective values. As previously stated, a set of simulations for PFOS, PFHxS, PFNA, and PFOA was performed using the modified version of the Surface Release CSM that included an alternative set of potentially representative conditions. The alternative set of conditions included a surface release in an area of 25-by-25 meters, lower aquifer dispersivity, point of compliance at edge of source, and climate with spring snowmelt. This alternative set of parameters can be considered representative and/or more protective. Exhibit 5-2 below shows a chart of model predicted results from the simulation of PFOA with the alternative Surface Release CSM (simulation # 20), including near-surface (0 - 10 cm – model layer 1, sublayer 1) soil concentrations, and model predicted groundwater concentrations at the point of compliance well. The results show that with a starting concentration of 10 ppm (10,000 ng/g) in the near surface soils (0 -20 cm), the model predicts that it will take slightly less than 5 years for surface soil concentrations to decline to around 0.1 ng/g, which is a decrease of five orders of magnitude. The peak groundwater concentration just under 2,000 ug/L occurs after approximately a year and a half following the initial release.

Exhibit 5-2: Comparison of predicted near-surface soil (0-10 cm) and groundwater concentrations at the compliance point over time for simulation of PFOA with the alternative Surface Release CSM (Simulation #20).



5.2 MODFLOW-USG Transport Results

The objectives of the MODFLOW-USG Transport simulations were as follows:

- Compare the influence that each model (i.e., SEVIEW and MODFLOW-USG Transport) has on the results of analogous CSMs (i.e., the Subsurface Release CSM is applied to both SEVIEW and MODFLOW-USG Transport simulations to allow direct comparison of model predicted results).
- Evaluate the difference in model results when comparing model simulations that include different aquifer thicknesses.
- Evaluate influence of three-dimensional fate and transport relative to the one-dimensional results of the SEVIEW model.
- Compare model results for simulations that include homogeneous and heterogeneous soils.
- Evaluate the differences in model results when simulating different overburden soil types.
- Evaluate the differences in model results when simulating a static water table and a variable water table.

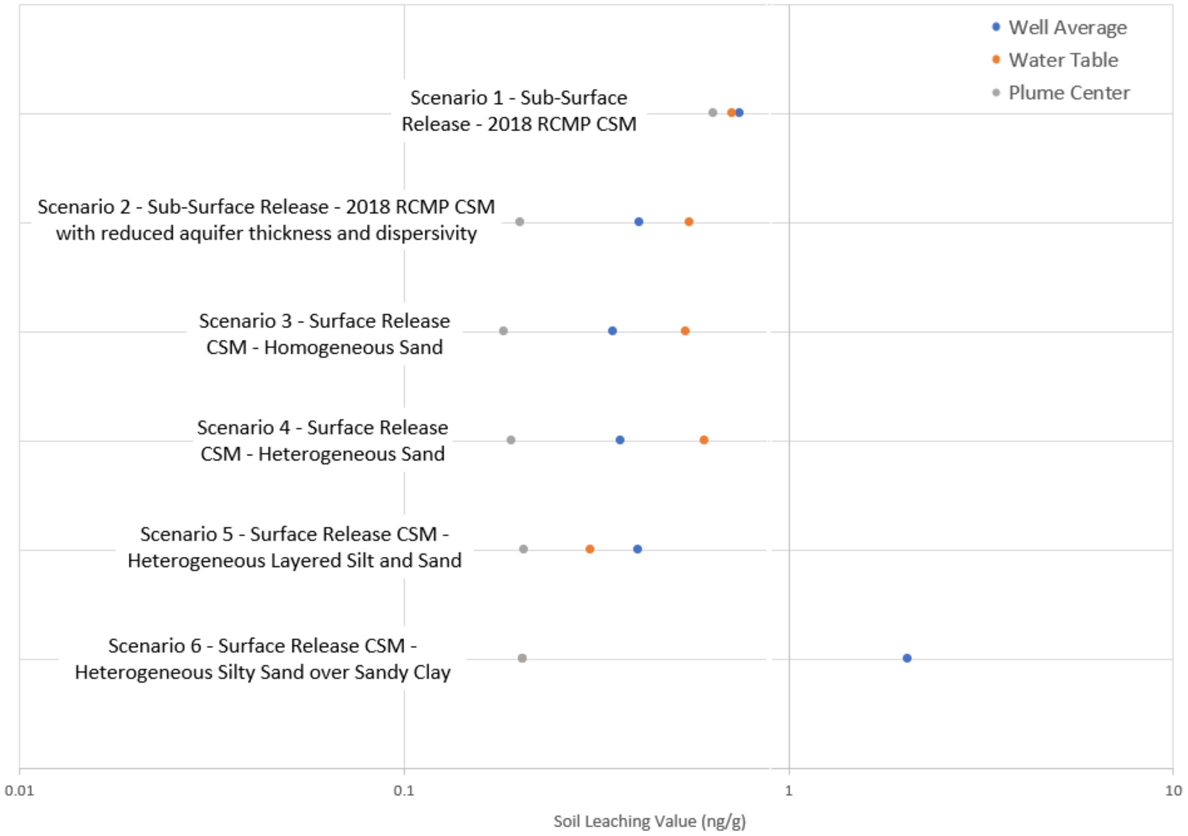
Most of the MODFLOW-USG Transport calculated leaching-based soil values for PFOA, provided in Table 5, fall within the same 0.1 to 1.0 ng/g range as seen with the SEVIEW model results. Scenario 1 includes simulation of PFOA fate and transport with the Subsurface Release CSM, and is comparable to simulation # 4 in the SEVIEW model. Scenario 3 includes simulation of PFOA fate and transport with the Surface Release CSM, and is comparable to simulation # 16 in the SEVIEW model. Comparison of the leaching-based soil value calculated using the MODFLOW-USG Transport result for Scenario 1, water table receptor well, (maximum concentration: 252 ug/L, time to maximum: 1.5 years, calculated leaching-based soil value: 0.72 ng/g) with that of the analogous SEVIEW result (770 ug/L, 0.33 years, 0.16 ng/g) demonstrates the difference in modeling one dimensional and three dimensional transport. MODFLOW-USG Transport predicts a lower peak concentration (and thus a higher leaching-based soil value) than SEVIEW. This is likely because fate and transport can occur in all three dimensions of the MODFLOW-USG model domain, while in SEVIEW the transport mechanism is primarily one-dimensional and therefore limits dispersion of the contaminant during simulated transport vertically downward. Another aspect that results in additional dispersion is the seasonal rise and fall of the water table which aids in the upward dispersion into the vadose zone above the water table.

As shown on Exhibit 5-3, the model simulated leaching-based soil values for Scenarios 2 through 5 are similar to each other, and results fall within a range of 0.1 to 1.0 ng/g. These similarities are likely due to similar input parameters except for the soil layering and randomly generated conductivities. Although heterogeneity is expected to have an effect on values, the model does not appear to be sensitive to this parameter. Also, lower dispersivity values were used in contrast to Scenario 1 resulting in higher mass transport to the groundwater.

For Scenario 6 the plume center and water table condition have the same predicted leaching-based soil value (0.2 ng/g). However, the well average concentration condition value is more than two times higher than the next highest predicted value (well average concentration condition for Scenario 1). This is likely due to the significantly lower hydraulic conductivities and location of the sandy clay unit (till) which is placed is the deepest layer in this scenario resulting in a longer travel time in the aquifer to achieve the concentration of concern in groundwater. However, the water table concentration is highest in this scenario due to higher conductivities in the sand (similar to Scenario 1 except heterogeneous) and lower dispersivity values than Scenario 1 allowing for more rapid leaching of mass to groundwater.

Exhibit 5-3 provides a visual summary of the leaching-based soil values for PFOA simulated using MODFLOW-USG Transport for Scenario 1 to 6. Results in Exhibit 5-3 are presented for three potential groundwater measurement points (i.e., well average, water table, plume center), to demonstrate the relative difference in the results when considering alternative measurement approaches. Since SEVIEW only simulates groundwater flow in one dimension, the highest groundwater concentration is constrained to the water table. However, MODFLOW USG Transport simulates groundwater flow in three dimensions, the highest groundwater concentration may not be at the water table so the well average and plume center conditions were also identifed in the simulation results and used to calculate leaching-based soil values.

Exhibit 5-3: Summary of leaching-based soil values resulting from the six scenarios modeled using MODFLOW-USG Transport.



5.3 Sensitivity Analysis

Sensitivity analysis is the evaluation of model input parameters to see how much they affect model outputs when the input is varied over a range of values. Sensitivity analysis was conducted on the model results for the range of input parameters varied in the model simulations presented in Section 4.4, using the Subsurface Release CSM for PFOA as the reference point (or point of comparison) for the analysis. Since the only chemical specific variable that showed substantial variation that might result in potentially less protective leaching-based soil values in the model runs was K_{oc}, PFOA was used as an example to understand variations in the non-chemical specific parameters.

Figure 1 graphically depicts the range in model predicted leaching-based soil values for PFOA for each input parameter that was varied in the SEVIEW model during sensitivity analysis, and results are discussed further below. Sensitivity analysis was conducted to better understand how specific input parameters varied over a range of values would influence the predicted or simulated leaching-based soil values. This process provides for a better understanding which input parameters have the most influence on the simulated leaching-based soil values predicted by the model.

Variations of most input parameters yielded leaching-based soil values that ranged less than an order of magnitude. For example, sensitivity analysis performed by individually varying soil types, soil pore disconnectedness indices, and hydraulic gradients, generated results of less than an order of magnitude range in model values (i.e., ranging from approximately 0.1 to 0.5 ng/g). The model displayed even less sensitivity to other parameters (e.g., soil porosity, bulk density, effective porosity, etc.), with resulting leaching-based soil values clustered around their respective median value.

Several input parameters showed greater variability than an order of magnitude, including source area size, soil dispersivity, aquifer hydraulic conductivity, and K_{oc}. The lower dispersivity values included in the sensitivity analyses resulted in leaching-based soil values up to about two orders of magnitude lower. The tested source area sizes had a more balanced effect, with about half an order of magnitude higher and lower for smaller and larger source areas, respectively. The tested K_{oc} values resulted in up to about an order of magnitude increase in leaching-based soil values. The model was also very sensitive when varying the groundwater hydraulic conductivity parameter, with model simulated values ranging over four orders of magnitude. It should be noted that not all parameters are independent of one another and, as a result, the observed range in model simulated values may be larger than would be expected if parameter dependency was accounted for in the sensitivity analysis. For example, the hydraulic gradient is not independent of the hydraulic conductivity of an aquifer since there is a negative correlation between the two parameters. Low hydraulic gradients are typically associated with higher values of hydraulic conductivity, and steeper hydraulic gradients associated with lower values of hydraulic conductivity.

Of the input parameters with the greatest associated variability (i.e., input parameters that showed a larger range of leaching-based soil values when varied), K_{oc} was the only parameter specific to PFAS. Previously modeled leaching-based soil values for other contaminants were likely subject to similar sensitivity to input parameter selection such that the other input parameters that demonstrated larger variation in the simulated results likely had a similar effect on other contaminants and therefore are likely not specific to PFAS transport characteristics (e.g., increasing hydraulic conductivity in the aquifer).

6.0 CONCLUSIONS

A review of available approaches that can be used to model PFAS fate and transport in vadose zone soil, and in groundwater, was performed. The SEVIEW modeling software was selected for modeling and development of leaching-based soil values. Each of the reviewed models had noted limitations. In relation to SEVIEW, those limitations tend to result in more protective leaching-based soil values for protection of groundwater, which is the appropriate approach to developing leaching-based soil values designed to be protective at a variety of site conditions across the state. The SEVIEW model was selected based on the following:

- Efficient approach to effectively simulate state-wide conditions and address large-scale variability in site conditions for multiple input parameters,
- Protective leaching-based soil values despite the limitations of one-dimensional flow, simulating flow through the vadose zone using a water balance approach and a lumped parameter, and not simulating air-water interface PFAS partitioning since these limitations tend to increase the PFAS leached from the soil, downward transport of the contaminant will be quicker, and leaching of the contaminant will occur for a shorter period of time.

- Use of a general model reduces the complexity of obtaining voluminous site-specific data or conducting substantial analysis of literature values to provide representative results over a wide variation of site conditions needed for this effort.
- Consistency with the process previously used by NHDES and used by other states to develop existing leaching-based soil values.

Approximately 145 SEVIEW model simulations were completed as part of this work. The central tendency of the values for the Subsurface Release CSM simulations is in the range of 0.2 to 0.3 ng/g, with most of the simulations falling between about 0.1 to 1.0 ng/g. Results indicated that the central tendency for the Surface Release CSM appeared to be higher at about 1 to 2 ng/g, with a range between about 0.06 to 195 ng/g.

The MODFLOW-USG Transport results indicated consistency with the SEVIEW results in most instances ranging between 0.1 to 1.0 ng/g. However, the results do demonstrate the differences between modeling in one and three dimensions. When comparing individual simulations between the two models (same input parameters, CSM, etc.), MODFLOW-USG Transport tends to predict a lower peak concentration (and thus a higher leaching-based soil value) than SEVIEW. This indicates that use of the MODFLOW-USG Transport results may be less protective for developing state-wide leaching-based soil values considering there are similar limitations in each model with respect to PFAS transport (e.g., air-water interface partitioning, Koc, etc.)

Sensitivity analysis indicated that several parameters were found to have significant influence, and of the input parameters with the greatest associated variability, K_{oc} was the only parameter specific to PFAS. Previously modeled leaching-based soil values for other contaminants were likely subject to similar sensitivity to input parameter selection.

Some of the key limitations of the SEVIEW model and primary CSMs were related to chemical-specific modeling and parameter selection. PFAS transport and fate is an area of active research and evolving understanding. As discussed in Section 1.3, some PFAS transport and fate considerations may be addressed by the use of representative K_{oc} values, and there was significant effort made to select representative K_{oc} values using the New Hampshire-specific values from the 2023 USGS NH Study. Some other PFAS transport and fate considerations, such as solid-phase partitioning kinetics, air-water interface partitioning, and precursor transformation, were not included in the model sensitivity analysis. New models that are described in recently published literature (Silva et al., 2020 and Guo et al., 2022) provide a process to simulate one or more of these transport processes, but they still require further development, testing, and validation. The SEVIEW model does not include partitioning to the air-water interface, and the limitations of the K_{oc} model for solid-phase partitioning is discussed in Section 1.3, above. Those limitations include extrapolation of laboratory data for use in modeling field conditions, which may not reflect partitioning in lower f_{oc} soils, kinetics, and hysteresis. Most of these chemical-specific limitations involve the SEVIEW model predicting greater leachability from soil than might be observed for some field conditions.

7.0 LIMITATIONS

This Report and Attachments were prepared by Sanborn Head in accordance with generally accepted environmental evaluation practices for the exclusive use of the NHDES for the specific application of calculating leaching-based soil values for four (4) PFAS: PFOS, PFHxS, PFNA, and PFOA. No other party may rely on these opinions and evaluations without the express written consent of Sanborn Head. Accuracy, completeness, and currency of the information are not guaranteed. No warranty, express or implied, is made.

The conceptual model scenarios and selected parameters included in the model scenarios are not intended to reflect specific releases or sites, and the model scenario results are not necessarily indicative of actual concentrations that might be observed if site-specific conditions are considered.

This Report and Attachments were based on various types of information developed by previous investigators. Interpretations, conclusions, or recommendations that rely on that information are contingent on the validity of such information. Sanborn Head did not independently confirm this information and relied upon the information as provided.

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Tables

Table 1
Model Review Summary
Development of Leaching-Based Soil Values for PFAS
New Hampshire Department of Environmental Services

Model Reviewed	Analytical	Numerical	Dimesional Complexity	Soil Layering Complexity	Time Element	Equilibrium Soprtion/ Desorption	Air-Water Interface Partitioning	Surfactant Induced Flow	Precursor Transformations	Volatilization	Advantages	Disadvantages
SESOIL/AT123D (SEVIEW)	Yes*	Yes*	SESOIL - 1D AT123D - 1D flow/3D transport	Multiple for SESOIL,** Single for AT123D	Transient (monthly time-step)	Yes	No	No	No	Yes	Long history of use in New Hampshire and other states for developing leaching-based soil values and has been validated by peer review with software maintenance and user support. Can simulate seasonal climate variation and includes an extensive database of climate data. Includes most of the primary processes that influence fate and transport of contaminants. Graphical user interface and includes post-processing of results. Run times for a single model simulation require signifcantly less time than more complicated models.	Does not directly simulate air-water interface partitioning or surfactant-induced flow. Assumes equilibrium conditions for partitioning process. Does not represent heterogeneous soil or groundwater flow conditions. Uses a single layer averaged value to calculate flow. Simulates only one-dimensional vertical flow. Conditions are steady-state.[1] Does not allow for time-steps. Does not simulate breakdown of precursors. Uses a simplification of vadose zone flow equations with lumped parameter that has limited documentation in literature. Groundwater flow in AT123D is limited to steady-state, horizontal one-dimensional flow and assumes homogeneity.
PRZM[2]		Yes	1D	Multiple	Transient (daily time-step)	Yes	No	No	No	Yes	Currently approved for regulatory use by USEPA and has been validated by peer review with software maintenance and user support. Simulates multiple soil layers having variable media properties, including effective porosity and fraction of organic carbon. Also, has time-step features. Includes most of the primary processes that influence fate and transport of contaminants. Climate data for use in the model can be downloaded from the US EPA website. For surface release scenarios the model includes additional fate and transport pathways and processes (e.g., surface runoff, root zone, and plant uptake) that are not typically simulated by vadose zone models.	Unsaturated zone flow is estimated using a "tipping bucket" model. Does not directly simulate air-water interface partitioning or surfactant-induced flow. Additional fate and transport pathways and processes included (e.g., surface runoff, root zone, and plant uptake) are only directly relevant to fate and transport of contaminants when considering a shallow surface release scenario and are not relevant to a deeper subsurface release scenario.
HYDRUS (modified)		Yes	1D, 2D, or 3D	Multiple	Steady State and Transient (user-defined time steps)	Yes	Yes (add-on module to 1D and 2D versions only)	No	No	Yes	Model is well-maintained and updated regularly with user support. Graphical interface and post-processing of results. Includes most of the primary processes that influence fate and transport of contaminants. Can be modified to accommodate additional code to represent PFAS-related fate and transport. Can be coupled with PHREEQC[3] for modeling of additional geochemical processes. Unstructured grid design allows for more efficient refinement and representation of heterogeneous properties in areas of interest. Allows for representation of multiple boundary conditions. Time-step can be varied as needed to represent processes. Simulates heterogeneous conditions in three dimensions. Can represent preferential pathways, dual porosity, and dual permeability flow conditions.	Packages necessary for complex sites and modeling of additional fate and transport processes/parameters need to be purchased at additional cost. Adapting code is needed to effectively use the PFAS packages and requires advanced techniques and calibration. PFAS add-on module is currently only available for one- and two-dimensional models. Effects of the air-water interface and surfactant-induced flow that are available in the PFAS add-on module still need to be tested and validated against pilot-scale and field-scale datasets under representative conditions.
PFAS-LEACH-Screening	Yes	In Development	1D available, 3D version in development	3D version in development	Unknown	Yes	Yes	No	No	Yes	When completed, the PFAS-LEACH-COMP is anticipated to include a relatively comprehensive representation of flow (including heterogeneous conditions), transport processes (including surfactant-induced flow, and solid-phase and air-water interfacial adsorption), and transformation processes. The products from the PFAS-LEACH project, including the computer codes, will be made available to the public when the project is completed.	Model development and testing are part of a multi-part project that is not yet complete. The currently-available PFAS-LEACH-Screening Model is a simplified version of the model based on analytical solutions and is therefore much less complex and does not provide for many of the attributes of the other models. The other model tiers, including PFAS-LEACH-COMP, are currently being tested and validated against pilot-scale and field-scale datasets by researchers, and it is estimated that the models will not be available for approximately 1.5 to 2 years (Dr. Guo, personal communication, March 2023).
MODFLOW-USG Transport		Yes	3D	Multiple	Steady State and Transient (user-defined time steps)	Yes	No	No	No	No	Model is well-maintained and updated regularly with user support. Graphical user interface and post-processing of results. Can be modified to accommodate additional code to simulate PFAS fate and transport. Unstructured grid design allows for more efficient refinement and representation of heterogeneous properties in areas of interest. Allows for representation of multiple boundary conditions. Time-step can be varied as needed to represent processes. Simulates heterogeneous conditions in three dimensions. Can represent preferential pathways, dual porosity, and dual permeability flow conditions. Can be coupled with PHREEQC for modeling of additional geochemical processes.	Setup of more complicated simulations can be time-consuming. Model run-time is relatively long for more complex simulations. Does not currently account for air-water interface partitioning, surfactant-induced flow, or volatilization. Code modification is possible but has not yet been completed and will require advanced knowledge and calibration.

Notes:
1. Steady-state conditions do not allow for change over time for key input parameters (e.g., climate input data are limited to a single annual dataset that does not vary from year to year, and water table depths are fixed throughout the simulation).
2. PRZM indicates USEPA Pesticide Root Zone Model (Young and Frye, 2020).
3. PHREEQC is a computer program developed by the USGS for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations.
4. "*" indicates that the SEVIEW model contains both analytical (ATD123) and numerical (SESOIL) methods for similuating transport in the subsurface.
"**" indicates that the SESOIL model, from an average of multiple layers, uses a single layer averaged value to calculate flow.

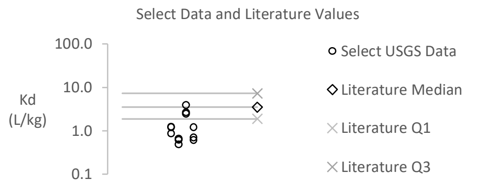
Table 2
Solid-Phase Partitioning Coefficient Summary
Development of Leaching-Based Soil Values for PFAS
New Hampshire Department of Environmental Services

PFOA Select USGS Partitioning Data

Sample	PFAS	Soil Concentration (ng/g)	Replicate ID	Kd (L/kg)	foc (kg-oc/kg)	Koc (L/kg-oc)
BTW-U-1	PFOA	2.15	07-BTW-U1-SH-PF-L0-R1	1.237	0.0229	54.0
BTW-U-1	PFOA	2.15	08-BTW-U1-SH-PF-L0-R2	1.192	0.0229	52.0
BTW-U-1	PFOA	2.15	09-BTW-U1-SH-PF-L0-R3	0.866	0.0229	37.8
BTW-U-2	PFOA	1.6	28-BTW-U2-DP-PF-L0-R1	0.618	0.0129	47.9
BTW-U-2	PFOA	1.6	29-BTW-U2-DP-PF-L0-R2	0.655	0.0129	50.8
BTW-U-2	PFOA	1.6	30-BTW-U2-DP-PF-L0-R3	0.481	0.0129	37.3
NHF-U-1	PFOA	0.655	58-NHF-U1-SH-PF-L0-R1	2.637	0.0583	45.2
NHF-U-1	PFOA	0.655	59-NHF-U1-SH-PF-L0-R2	2.454	0.0583	42.1
NHF-U-1	PFOA	0.655	60-NHF-U1-SH-PF-L0-R3	3.889	0.0583	66.7
WND-U-1	PFOA	0.335	37-WND-U1-SH-PF-L0-R1	0.701	0.0108	64.7
WND-U-1	PFOA	0.335	38-WND-U1-SH-PF-L0-R2	0.608	0.0108	56.1
WND-U-1	PFOA	0.335	39-WND-U1-SH-PF-L0-R3	1.199	0.0108	111

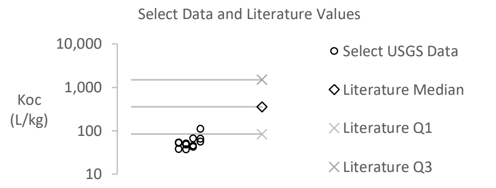
PFOA Kd (L/kg) Literature Value Comparison

Select Data Minimum	Select Data Median	Select Data Maximum	Literature Q1	Literature Median	Literature Q3
0.481	1.029	3.889	1.88	3.49	7.32


Select Data and Literature Values

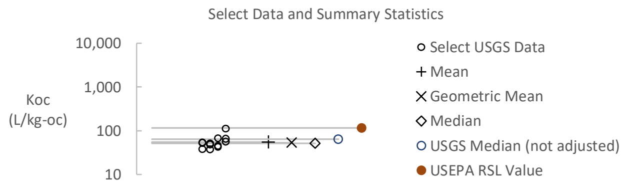
PFOA Koc (L/kg-oc) Literature Value Comparison

Select Data Minimum	Select Data Median	Select Data Maximum	Literature Q1	Literature Median	Literature Q3
37	51	111	84	357.1	1500


Select Data and Literature Values

PFOA Koc (L/kg-oc) 2023 USGS NH Study Select Data Summary Statistics

USGS Maximum	USGS Minimum	USGS Mean	USGS Geometric Mean	USGS Median	USGS Linear Freundlich	USGS Kd-foc linear correlation	USGS Median (foc not adjusted for soil moisture)	USEPA RSL Value
111	37.3	55.4	53.0	51.4	52.5	51.4	64	115

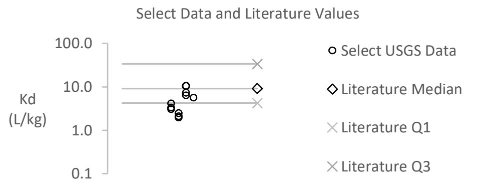

Select Data and Summary Statistics

PFNA Select USGS Partitioning Data

Sample	PFAS	Soil Concentration (ng/g)	Replicate ID	Kd (L/kg)	foc (kg-oc/kg)	Koc (L/kg-oc)
BTW-U-1	PFNA	0.46	07-BTW-U1-SH-PF-L0-R1	3.343	0.0229	146
BTW-U-1	PFNA	0.46	08-BTW-U1-SH-PF-L0-R2	4.167	0.0229	182
BTW-U-1	PFNA	0.46	09-BTW-U1-SH-PF-L0-R3	3.059	0.0229	133
BTW-U-2	PFNA	0.23	28-BTW-U2-DP-PF-L0-R1	2.481	0.0129	192
BTW-U-2	PFNA	0.23	29-BTW-U2-DP-PF-L0-R2	2.120	0.0129	164
BTW-U-2	PFNA	0.23	30-BTW-U2-DP-PF-L0-R3	1.962	0.0129	152
NHF-U-1	PFNA	0.25	58-NHF-U1-SH-PF-L0-R1	7.361	0.0583	126
NHF-U-1	PFNA	0.25	59-NHF-U1-SH-PF-L0-R2	6.368	0.0583	109
NHF-U-1	PFNA	0.25	60-NHF-U1-SH-PF-L0-R3	10.479	0.0583	180
WND-U-1	PFNA	0.053 J	37-WND-U1-SH-PF-L0-R1	NA	0.0108	NA
WND-U-1	PFNA	0.053 J	38-WND-U1-SH-PF-L0-R2	NA	0.0108	NA
WND-U-1	PFNA	0.053 J	39-WND-U1-SH-PF-L0-R3	5.637	0.0108	520

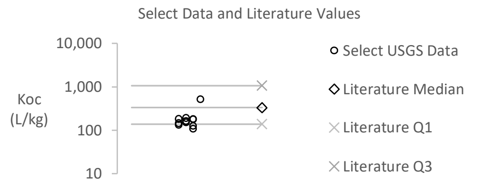
PFNA Kd (L/kg) Literature Value Comparison

Select Data Minimum	Select Data Median	Select Data Maximum	Literature Q1	Literature Median	Literature Q3
1.962	3.755	10.479	4.24	9.12	34.0


Select Data and Literature Values

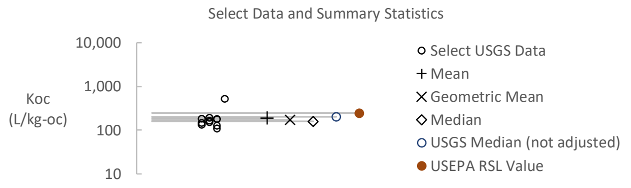
PFNA Koc (L/kg-oc) Literature Value Comparison

Select Data Minimum	Select Data Median	Select Data Maximum	Literature Q1	Literature Median	Literature Q3
109	158	520	139	331.9	1072


Select Data and Literature Values

PFNA Koc (L/kg-oc) 2023 USGS NH Study Select Data Summary Statistics

USGS Maximum	USGS Minimum	USGS Mean	USGS Geometric Mean	USGS Median	USGS Linear Freundlich	USGS Kd-foc linear correlation	USGS Median (foc not adjusted for soil moisture)	USEPA RSL Value
520	109	190	171	158	171	145	203	246

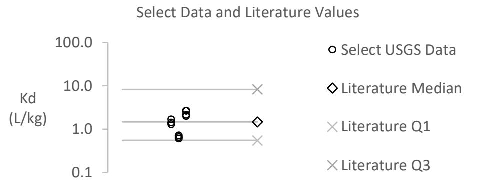

Select Data and Summary Statistics

PFHxS Select USGS Partitioning Data

Sample	PFAS	Soil Concentration (ng/g)	Replicate ID	Kd (L/kg)	foc (kg-oc/kg)	Koc (L/kg-oc)
BTW-U-1	PFHxS	0.395	07-BTW-U1-SH-PF-L0-R1	1.691	0.0229	73.8
BTW-U-1	PFHxS	0.395	08-BTW-U1-SH-PF-L0-R2	1.419	0.0229	61.9
BTW-U-1	PFHxS	0.395	09-BTW-U1-SH-PF-L0-R3	1.302	0.0229	56.8
BTW-U-2	PFHxS	0.355	28-BTW-U2-DP-PF-L0-R1	0.609	0.0129	47.2
BTW-U-2	PFHxS	0.355	29-BTW-U2-DP-PF-L0-R2	0.708	0.0129	54.9
BTW-U-2	PFHxS	0.355	30-BTW-U2-DP-PF-L0-R3	0.650	0.0129	50.4
NHF-U-1	PFHxS	0.18	58-NHF-U1-SH-PF-L0-R1	2.016	0.0583	34.6
NHF-U-1	PFHxS	0.18	59-NHF-U1-SH-PF-L0-R2	2.127	0.0583	36.5
NHF-U-1	PFHxS	0.18	60-NHF-U1-SH-PF-L0-R3	2.654	0.0583	45.5
WND-U-1	PFHxS	ND	37-WND-U1-SH-PF-L0-R1	NA	0.0108	NA
WND-U-1	PFHxS	ND	38-WND-U1-SH-PF-L0-R2	NA	0.0108	NA
WND-U-1	PFHxS	ND	39-WND-U1-SH-PF-L0-R3	NA	0.0108	NA

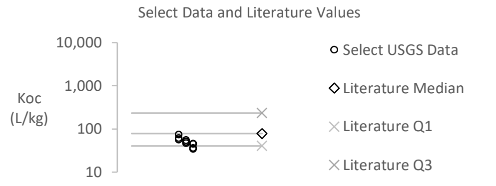
PFHxS Kd (L/kg) Literature Value Comparison

Select Data Minimum	Select Data Median	Select Data Maximum	Literature Q1	Literature Median	Literature Q3
0.609	1.419	2.654	0.548	1.47	8.29


Select Data and Literature Values

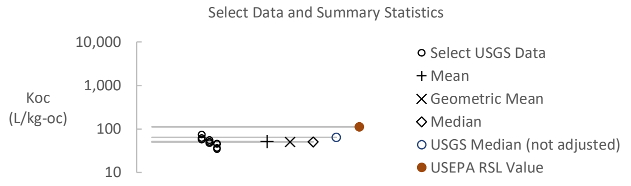
PFHxS Koc (L/kg-oc) Literature Value Comparison

Select Data Minimum	Select Data Median	Select Data Maximum	Literature Q1	Literature Median	Literature Q3
35	50	74	40.4	78.4	232.8


Select Data and Literature Values

PFHxS Koc (L/kg-oc) 2023 USGS NH Study Select Data Summary Statistics

USGS Maximum	USGS Minimum	USGS Mean	USGS Geometric Mean	USGS Median	USGS Linear Freundlich	USGS Kd-foc linear correlation	USGS Median (foc not adjusted for soil moisture)	USEPA RSL Value
73.8	34.6	51.3	50.0	50.4	50.1	42.6	64	112

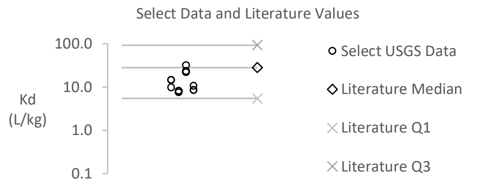

Select Data and Summary Statistics

PFOS Select USGS Partitioning Data

Sample	PFAS	Soil Concentration (ng/g)	Replicate ID	Kd (L/kg)	foc (kg-oc/kg)	Koc (L/kg-oc)
BTW-U-1	PFOS	4.35	07-BTW-U1-SH-PF-L0-R1	14.707	0.0229	642
BTW-U-1	PFOS	4.35	08-BTW-U1-SH-PF-L0-R2	14.497	0.0229	632
BTW-U-1	PFOS	4.35	09-BTW-U1-SH-PF-L0-R3	9.829	0.0229	429
BTW-U-2	PFOS	1.65	28-BTW-U2-DP-PF-L0-R1	8.111	0.0129	629
BTW-U-2	PFOS	1.65	29-BTW-U2-DP-PF-L0-R2	8.206	0.0129	636
BTW-U-2	PFOS	1.65	30-BTW-U2-DP-PF-L0-R3	7.528	0.0129	584
NHF-U-1	PFOS	2.05	58-NHF-U1-SH-PF-L0-R1	23.238	0.0583	398
NHF-U-1	PFOS	2.05	59-NHF-U1-SH-PF-L0-R2	21.901	0.0583	375
NHF-U-1	PFOS	2.05	60-NHF-U1-SH-PF-L0-R3	32.103	0.0583	550
WND-U-1	PFOS	0.33	37-WND-U1-SH-PF-L0-R1	8.418	0.0108	776
WND-U-1	PFOS	0.33	38-WND-U1-SH-PF-L0-R2	8.525	0.0108	786
WND-U-1	PFOS	0.33	39-WND-U1-SH-PF-L0-R3	10.668	0.0108	984

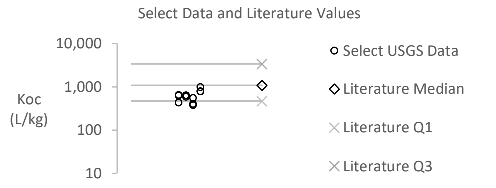
PFOS Kd (L/kg) Literature Value Comparison

Select Data Minimum	Select Data Median	Select Data Maximum	Literature Q1	Literature Median	Literature Q3
7.528	10.249	32.103	5.44	28.2	92.9


Select Data and Literature Values

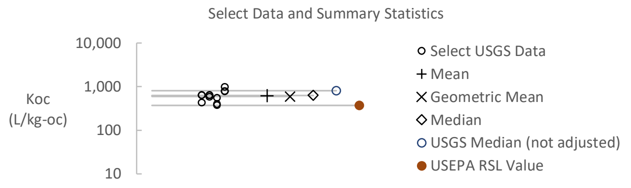
PFOS Koc (L/kg-oc) Literature Value Comparison

Select Data Minimum	Select Data Median	Select Data Maximum	Literature Q1	Literature Median	Literature Q3
375	631	984	467.7	1081	3357


Select Data and Literature Values

PFOS Koc (L/kg-oc) 2023 USGS NH Study Select Data Summary Statistics

USGS Maximum	USGS Minimum	USGS Mean	USGS Geometric Mean	USGS Median	USGS Linear Freundlich	USGS Kd-foc linear correlation	USGS Median (foc not adjusted for soil moisture)	USEPA RSL Value
984	375	619	596	631	596	475	804	372


Select Data and Summary Statistics

Notes:

1. Select data were obtained or calculated from the U.S. Geological Survey (USGS) publication: *Tokranov, A.K., Welch, S.M., Santangelo, L.M., Kent, D.B., Repert, D.A., Perkins, K., Bliznik, P.A., Roth, D.A., Drouin, A.F., Lincoln, T.A., Deyette, N.A., Schlosser, K.E.A., and Marts, J.M. (2023), Solid/Water Partitioning of Per- and Polyfluoroalkyl Substances (PFAS) in New Hampshire Soils and Biosolids: Results from Laboratory Experiments at the U.S. Geological Survey: U.S. Geological Survey data release, https://doi.org/10.5066/P9TKSM8S.* The select samples were uncontaminated samples with no spiked PFAS. The USGS Median (foc not adjusted for soil moisture) values were calculated for and used in the modeling prior to Sanborn Head being aware that soil organic content data were reported on a wet-weight basis. See Appendix A for discussion of sample and experimental condition selection. Soil concentrations are based on an average of primary and duplicate environmental soil results.
2. Literature value summary statistics were obtained from the publication: Rovero, M., Cutt, D., Griffiths, R., Filipowicz, U., Mishkin, K., White, B., Goodrow, S. and Wilkin, R.T. (2021), Limitations of Current Approaches for Predicting Groundwater Vulnerability from PFAS Contamination in the Vadose Zone. Groundwater Monit R, 41: 62-75. https://doi.org/10.1111/gwmr.12485.
3. "Replicate ID" indicates a unique value for the solid/water experimental sample, referred to as Kd_ID in the USGS publication.
   "Kd (L/kg)" indicates solid/water partitioning coefficient as reported by the USGS in units of liters of water per kilogram of solid.
   "foc (kg-oc/kg)" indicates fraction of organic carbon in units of kilograms organic carbon per kilogram solid. Fraction of organic carbon values were calculated from USGS-provided total organic carbon concentrations (wet weight basis) and percent moisture. The primary and duplicate total organic carbon and percent moisture values were averaged before calculating foc.
   "Koc (L/kg-oc)" indicates organic carbon/water partitioning coefficient as calculated from Kd and foc values in units of liters of water per kilogram of organic carbon.
   "USEPA RSL Value" indicates the organic carbon/water partitioning coefficient for the corresponding PFAS obtained from the U.S. Environmental Protection Agency Regional Screening Levels chemical specific parameters generic table. The reported values are based on *Higgins, C.P. and Luthy, R.G. (2003), Sorption of Perfluorinated Surfactants on Sediments, Environmental Science & Technology 2006 40 (23), 7251-7256, DOI: 10.1021/es061000n* for PFOA, PFNA, and PFOS or *Guelfo, J.L. and Higgins, C.P. (2013), Subsurface Transport Potential of Perfluoroalkyl Acids at Aqueous Film-Forming Foam (AFFF)-Impacted Sites, Environmental Science & Technology 2013 47 (9), 4164-4171, DOI: 10.1021/es3048043* for PFHxS.
4. "ND" indicated the analyte was not detected.
   "J" indicates the analyte was detected at a concentration below the reporting limit, and the indicated value is an estimated concentration.
   "NA" indicates not applicable because the analyte was not detected in either the experimental solid or water fraction.
   Blank indicates a Koc value was not calculated because a Kd value was not applicable.
5. Displayed significant figures for Kd generally match those for corresponding data provided in the USGS publication. Calculated foc values, Koc values, and Koc summary statistics are generally presented with three significant figures.
6. Refer to Appendix A for additional notes and discussion.

Table 3

Summary of SEVIEW Model Input Parameters for Surface and Subsurface CSMs

Development of Leaching-Based Soil Values for PFAS

New Hampshire Department of Environmental Services

Parameter	Units	Subsurface Release CSM	Reference	Surface Release CSM	Reference
Total Soil Column Thickness and Depth to Groundwater	(cm)	300	Section 4.1 and 4.1.1	300	Section 4.2 and 4.3.2
Soil Input	(ppm)	10	Section 4.1	10	Section 4.2
Input Method	(-)	Sublayer	Section 4.1	Sublayer	Section 4.2
Release Top Depth	(cm)	100	Section 4.1	0	Section 4.2
Release Bottom Depth	(cm)	200	Section 4.1	20	Section 4.2
Source Area Size	(m)	10 x 10	Section 4.1	25 x 25	Section 4.3.3
Climate File	(-)	Massabesic (71-00)	Section 4.2.1	Massabesic (91-20) Snowmelt	Section 4.3.1
Soil Type	(-)	SAND	Section 4.1.2	SAND	Section 4.2
Soil Vertical Hydraulic Conductivity (SESOIL)	(cm/s)	1.00E-03	Section 4.4	1.00E-03	Section 4.4
Permeability (SESOIL)	(cm^2)	1.00E-08	Section 4.4	1.00E-08	Section 4.4
Porosity (SESOIL)	(-)	0.30	Section 4.4	0.30	Section 4.4
Bulk Density (SESOIL)	(g/cm^3)	1.30	Section 4.4	1.30	Section 4.4
Disconnectedness Index (SESOIL)	(-)	3.7	Section 4.4	3.7	Section 4.4
f$_{oc}$ (model layer 1)	(%)	0.1	Section 4.1.2	5	Section 4.2
f$_{oc}$ (model layers 2 to 4)	(%)	0.1	Section 4.1.2	0.1	Section 4.2
PFOA K$_{oc}$	(L/kg)	64	Section 3.1	64	Section 3.1
PFNA K$_{oc}$	(L/kg)	203	Section 3.1	203	Section 3.1
PFHxS K$_{oc}$	(L/kg)	64	Section 3.1	64	Section 3.1
PFOS K$_{oc}$	(L/kg)	804	Section 3.1	804	Section 3.1
Freundlich Exponent	(-)	1	Section 1.3.1.4	1	Section 1.3.1.4
PFOA Water Solubility	(mg/L)	9500	Section 3.3	9500	Section 3.3
PFNA Water Solubility	(mg/L)	11.66	Section 3.3	11.66	Section 3.3
PFHxS Water Solubility	(mg/L)	239.43	Section 3.3	239.43	Section 3.3
PFOS Water Solubility	(mg/L)	680	Section 3.3	680	Section 3.3
PFOA Water Diffusion Coefficient	(cm^2/s)	5.79E-06	Section 3.4	5.79E-06	Section 3.4
PFNA Water Diffusion Coefficient	(cm^2/s)	5.43E-06	Section 3.4	5.43E-06	Section 3.4
PFHxS Water Diffusion Coefficient	(cm^2/s)	6.01E-06	Section 3.4	6.01E-06	Section 3.4
PFOS Water Diffusion Coefficient	(cm^2/s)	5.25E-06	Section 3.4	5.25E-06	Section 3.4
PFOA Water Diffusion Coefficient	(m^2/hr)	2.08E-06	Section 3.4	2.08E-06	Section 3.4
PFNA Water Diffusion Coefficient	(m^2/hr)	1.95E-06	Section 3.4	1.95E-06	Section 3.4
PFHxS Water Diffusion Coefficient	(m^2/hr)	2.16E-06	Section 3.4	2.16E-06	Section 3.4
PFOS Water Diffusion Coefficient	(m^2/hr)	1.89E-06	Section 3.4	1.89E-06	Section 3.4
PFOA Air Diffusion Coefficient	(cm^2/s)	2.26E-02	Section 3.4	2.26E-02	Section 3.4
PFNA Air Diffusion Coefficient	(cm^2/s)	2.13E-02	Section 3.4	2.13E-02	Section 3.4
PFHxS Air Diffusion Coefficient	(cm^2/s)	2.33E-02	Section 3.4	2.33E-02	Section 3.4
PFOS Air Diffusion Coefficient	(cm^2/s)	2.07E-02	Section 3.4	2.07E-02	Section 3.4
PFOA Henry's Law Constant	(m^3-atm/mol)	3.57E-06	Section 3.2	3.57E-06	Section 3.2
PFNA Henry's Law Constant	(m^3-atm/mol)	1.90E-03	Section 3.2	1.90E-03	Section 3.2
PFHxS Henry's Law Constant	(m^3-atm/mol)	6.10E-05	Section 3.2	6.10E-05	Section 3.2
PFOS Henry's Law Constant	(m^3-atm/mol)	4.43E-07	Section 3.2	4.43E-07	Section 3.2
PFOA Molecular Weight	(g/mol)	410	Section 3.0	410	Section 3.0
PFNA Molecular Weight	(g/mol)	460	Section 3.0	460	Section 3.0
PFHxS Molecular Weight	(g/mol)	400	Section 3.0	400	Section 3.0
PFOS Molecular Weight	(g/mol)	500	Section 3.0	500	Section 3.0
Volitilization Factor (all 4 PFAS)	(-)	1	protective assumed value	1	protective assumed value
Point of Compliance Top Depth	(m bWT)	0	Section 4.1	0	Section 4.2
Point of Compliance Bottom Depth	(m bWT)	0	Section 4.1	0	Section 4.2
Distance to Point of Compliance	(m)	10	Section 4.1	0	Section 4.2
Aquifer Horizontal Hydraulic Conductivity (AT123D)	(m/hr)	0.36	Section 4.4	0.36	Section 4.4
Hydraulic Gradient (AT123D)	(m/m)	0.005	Section 4.4	0.005	Section 4.4
Effective Porosity (AT123D)	(-)	0.30	Section 4.4	0.30	Section 4.4
Bulk Density (AT123D)	(g/cm^3)	1.30	Section 4.4	1.30	Section 4.4
Longitudinal Dispersivity (AT123D)	(m)	20	Liptak and Lombardo, 1996/ Xu and Eckstein, 1995	0.83	Liptak and Lombardo, 1996/ Xu and Eckstein, 1995
Transverse Dispersivity (AT123D)	(m)	2	Liptak and Lombardo, 1996/ Xu and Eckstein, 1995	0.083	Liptak and Lombardo, 1996/ Xu and Eckstein, 1995
Vertical Dispersivity (AT123D)	(m)	2	Liptak and Lombardo, 1996/ Xu and Eckstein, 1995	0.0083	Liptak and Lombardo, 1996/ Xu and Eckstein, 1995
Aquifer Width (AT123D)	(m)	Inf		Inf	
Aquifer Thickness (AT123D)	(m)	Inf		Inf	

Notes:

1. Units of parameters are as follows:

(cm) - centimeter
(ppm) - parts per million which is equivalent to milligrams per liter (mg/L)
(m) - meter
(cm/s) - centimeters per second
(cm^2) - square centimeter
(g/cm^3) - grams per cubic centimeter
(L/kg) - liters per kilogram
(mg/L) - milligrams per liter
(cm^2/s) - square centimeters per second
(m^2/hr) - square meters per hour
(m^3-atm/mol) - atmosphere cubic meters per mole
(g/mol) - grams per mole
(m bWT) - meters below water table
(m/hr) - meters per hour
(m/m) - meters per meter

2. "SESOIL" indicates parameter is applied in the SESOIL (vadose zone model) portion of the SEVIEW model.

3. "f$_{oc}$" is organic carbon content of soil.

4. "K$_{oc}$" is soil organic carbon-water partition coefficient.

5. "AT123D" indicates parameter is applied in the AT123D (saturated zone model) portion of the SEVIEW model.

Table 4
Summary of SEVIEW Model Input Parameters and Simulation Results
Development of Leaching-Based Soil Values for PFAS
New Hampshire Department of Environmental Services

Conceptual Model (name)	Simulation Number	Sensitivity Analysis Parameter	Subsurface Release CSM Parameter Value	Surface Release CSM Parameter Value	Sensitivity Analysis Run Parameter Value
Subsurface Release CSM	1	not applicable	-	-	-
Subsurface Release CSM	2	not applicable	-	-	-
Subsurface Release CSM	3	not applicable	-	-	-
Subsurface Release CSM	4	not applicable	-	-	-
Surface Release CSM	5	not applicable	-	-	-
Surface Release CSM	6	not applicable	-	-	-
Surface Release CSM	7	not applicable	-	-	-
Surface Release CSM	8	not applicable	-	-	-
Surface Release CSM	9	not applicable	-	-	-
Surface Release CSM	10	not applicable	-	-	-
Surface Release CSM	11	not applicable	-	-	-
Surface Release CSM	12	not applicable	-	-	-
Surface Release CSM	13	not applicable	-	-	-
Surface Release CSM	14	not applicable	-	-	-
Surface Release CSM	15	not applicable	-	-	-
Surface Release CSM	16	not applicable	-	-	-
Surface Release CSM	17	not applicable	-	-	-
Surface Release CSM	18	not applicable	-	-	-
Surface Release CSM	19	not applicable	-	-	-
Surface Release CSM	20	not applicable	-	-	-
Sensitivity Analysis	21	Soil Organic Carbon-Liquid Partition Coefficient	64	64	43
Sensitivity Analysis	22	Soil Organic Carbon-Liquid Partition Coefficient	64	64	64
Sensitivity Analysis	23	Soil Organic Carbon-Liquid Partition Coefficient	64	64	99
Sensitivity Analysis	24	Soil Organic Carbon-Liquid Partition Coefficient	64	64	40
Sensitivity Analysis	25	Soil Organic Carbon-Liquid Partition Coefficient	64	64	78
Sensitivity Analysis	26	Soil Organic Carbon-Liquid Partition Coefficient	64	64	233
Sensitivity Analysis	27	Soil Organic Carbon-Liquid Partition Coefficient	203	203	135
Sensitivity Analysis	28	Soil Organic Carbon-Liquid Partition Coefficient	203	203	203
Sensitivity Analysis	29	Soil Organic Carbon-Liquid Partition Coefficient	203	203	587
Sensitivity Analysis	30	Soil Organic Carbon-Liquid Partition Coefficient	203	203	139
Sensitivity Analysis	31	Soil Organic Carbon-Liquid Partition Coefficient	203	203	332
Sensitivity Analysis	32	Soil Organic Carbon-Liquid Partition Coefficient	203	203	1072
Sensitivity Analysis	33	Soil Organic Carbon-Liquid Partition Coefficient	804	804	466
Sensitivity Analysis	34	Soil Organic Carbon-Liquid Partition Coefficient	804	804	804
Sensitivity Analysis	35	Soil Organic Carbon-Liquid Partition Coefficient	804	804	1111
Sensitivity Analysis	36	Soil Organic Carbon-Liquid Partition Coefficient	804	804	468
Sensitivity Analysis	37	Soil Organic Carbon-Liquid Partition Coefficient	804	804	1081
Sensitivity Analysis	38	Soil Organic Carbon-Liquid Partition Coefficient	804	804	3357
Sensitivity Analysis	39	Soil Organic Carbon-Liquid Partition Coefficient	64	64	47
Sensitivity Analysis	40	Soil Organic Carbon-Liquid Partition Coefficient	64	64	64
Sensitivity Analysis	41	Soil Organic Carbon-Liquid Partition Coefficient	64	64	125
Sensitivity Analysis	42	Soil Organic Carbon-Liquid Partition Coefficient	64	64	84
Sensitivity Analysis	43	Soil Organic Carbon-Liquid Partition Coefficient	64	64	357
Sensitivity Analysis	44	Soil Organic Carbon-Liquid Partition Coefficient	64	64	1500
Sensitivity Analysis	45	Total Soil Column Thickness and Depth to Groundwater (cm)	300	300	300
Sensitivity Analysis	46	Total Soil Column Thickness and Depth to Groundwater (cm)	300	300	200
Sensitivity Analysis	47	Total Soil Column Thickness and Depth to Groundwater (cm)	300	300	600
Sensitivity Analysis	48	Release Top Depth / Release Bottom Depth	100 / 200	0 / 20	100 / 200
Sensitivity Analysis	49	Release Top Depth / Release Bottom Depth	100 / 200	0 / 20	0 / 100
Sensitivity Analysis	50	Release Top Depth / Release Bottom Depth	100 / 200	0 / 20	200 / 300
Sensitivity Analysis	51	Release Top Depth / Release Bottom Depth	100 / 200	0 / 20	0 / 50
Sensitivity Analysis	52	Release Top Depth / Release Bottom Depth	100 / 200	0 / 20	0 / 100
Sensitivity Analysis	53	Release Top Depth / Release Bottom Depth	100 / 200	0 / 20	0 / 150
Sensitivity Analysis	54	Release Top Depth / Release Bottom Depth	100 / 200	0 / 20	0 / 200
Sensitivity Analysis	55	Release Top Depth / Release Bottom Depth	100 / 200	0 / 20	0 / 250
Sensitivity Analysis	56	Release Top Depth / Release Bottom Depth	100 / 200	0 / 20	0 / 300
Sensitivity Analysis	57	Source Area Size	10 x 10	25 x 25	5 x 5
Sensitivity Analysis	58	Source Area Size	10 x 10	25 x 25	10 x 10
Sensitivity Analysis	59	Source Area Size	10 x 10	25 x 25	25 x 25
Sensitivity Analysis	60	Source Area Size	10 x 10	25 x 25	50 x 50
Sensitivity Analysis	61	Source Area Size	10 x 10	25 x 25	100 x 100
Sensitivity Analysis	62	Source Area Size	10 x 10	25 x 25	150 x 150
Sensitivity Analysis	63	Source Area Size (compliance point at edge of source)	-	-	5 x 5
Sensitivity Analysis	64	Source Area Size (compliance point at edge of source)	-	-	10 x 10
Sensitivity Analysis	65	Source Area Size (compliance point at edge of source)	-	-	25 x 25
Sensitivity Analysis	66	Source Area Size (compliance point at edge of source)	-	-	50 x 50
Sensitivity Analysis	67	Source Area Size (compliance point at edge of source)	-	-	100 x 100
Sensitivity Analysis	68	Source Area Size (compliance point at edge of source)	-	-	150 x 150
Sensitivity Analysis	69	Source Area Size (compliance point at edge of source, low dispersivity)	-	-	5 x 5
Sensitivity Analysis	70	Source Area Size (compliance point at edge of source, low dispersivity)	-	-	10 x 10
Sensitivity Analysis	71	Source Area Size (compliance point at edge of source, low dispersivity)	-	-	25 x 25
Sensitivity Analysis	72	Source Area Size (compliance point at edge of source, low dispersivity)	-	-	50 x 50
Sensitivity Analysis	73	Source Area Size (compliance point at edge of source, low dispersivity)	-	-	100 x 100
Sensitivity Analysis	74	Source Area Size (compliance point at edge of source, low dispersivity)	-	-	150 x 150
Sensitivity Analysis	75	Climate File	Massabesic (71-00)	Massabesic (91-20) Snowmelt	Massabesic (71-00)
Sensitivity Analysis	76	Climate File	Massabesic (71-00)	Massabesic (91-20) Snowmelt	Massabesic (91-20) Snowmelt
Sensitivity Analysis	77	Climate File	Massabesic (71-00)	Massabesic (91-20) Snowmelt	Franklin Falls Dam (71-00)
Sensitivity Analysis	78	Climate File	Massabesic (71-00)	Massabesic (91-20) Snowmelt	Berlin Muni AP (91-20)
Sensitivity Analysis	79	Climate File	Massabesic (71-00)	Massabesic (91-20) Snowmelt	Massabesic (91-20)
Sensitivity Analysis	80	Climate File	Massabesic (71-00)	Massabesic (91-20) Snowmelt	Laconia 2.8S (91-20)
Sensitivity Analysis	81	Climate File	Massabesic (71-00)	Massabesic (91-20) Snowmelt	Lincoln NEPP (91-20)
Sensitivity Analysis	82	Climate File	Massabesic (71-00)	Massabesic (91-20) Snowmelt	Mt Washington (91-20)

Note: The Subsurface Release CSM was used as the reference point (or point of comparison) for the sensitivity analysis because the Subsurface Release CSM parameters, such as release depth and soil fraction of organic carbon, were set at values nearer the middle of the range of values tested in the sensitivity analysis.
Refer to previous tables for additional notes.

Table 4
Summary of SEVIEW Model Input Parameters and Simulation Results
Development of Leaching-Based Soil Values for PFAS
New Hampshire Department of Environmental Services

Conceptual Model (name)	Simulation Number	Sensitivity Analysis Parameter	Subsurface Release CSM Parameter Value	Surface Release CSM Parameter Value	Sensitivity Analysis Run Parameter Value
Sensitivity Analysis	83	Soil Type	SAND	SAND	SAND
Sensitivity Analysis	84	Soil Type	SAND	SAND	SILTY SAND
Sensitivity Analysis	85	Soil Type	SAND	SAND	TILL/CLAY
Sensitivity Analysis	86	Soil Vertical Hydraulic Conductivity (SESOIL)	0.001	0.001	1.00E-01
Sensitivity Analysis	87	Soil Vertical Hydraulic Conductivity (SESOIL)	0.001	0.001	1.00E-03
Sensitivity Analysis	88	Soil Vertical Hydraulic Conductivity (SESOIL)	0.001	0.001	1.00E-06
Sensitivity Analysis	89	Porosity (SESOIL)	0.3	0.3	0.4
Sensitivity Analysis	90	Porosity (SESOIL)	0.3	0.3	0.3
Sensitivity Analysis	91	Porosity (SESOIL)	0.3	0.3	0.2
Sensitivity Analysis	92	Porosity (SESOIL)	0.3	0.3	0.1
Sensitivity Analysis	93	Bulk Density (SESOIL)	1.3	1.3	1.3
Sensitivity Analysis	94	Bulk Density (SESOIL)	1.3	1.3	1.5
Sensitivity Analysis	95	Bulk Density (SESOIL)	1.3	1.3	1.7
Sensitivity Analysis	96	Disconnectedness Index (SESOIL)	3.7	3.7	3.7
Sensitivity Analysis	97	Disconnectedness Index (SESOIL)	3.7	3.7	6
Sensitivity Analysis	98	Disconnectedness Index (SESOIL)	3.7	3.7	12
Sensitivity Analysis	99	Fraction of Organic Carbon (model layers 1 to 4)	0.1	5	0.01
Sensitivity Analysis	100	Fraction of Organic Carbon (model layers 1 to 4)	0.1	5	0.1
Sensitivity Analysis	101	Fraction of Organic Carbon (model layers 1 to 4)	0.1	5	1
Sensitivity Analysis	102	Water Diffusion Coefficient	5.79E-06	5.79E-06	5.21E-06
Sensitivity Analysis	103	Water Diffusion Coefficient	5.79E-06	5.79E-06	5.79E-06
Sensitivity Analysis	104	Water Diffusion Coefficient	5.79E-06	5.79E-06	6.37E-06
Sensitivity Analysis	105	Air Diffusion Coefficient	2.26E-02	2.26E-02	2.03E-02
Sensitivity Analysis	106	Air Diffusion Coefficient	2.26E-02	2.26E-02	2.26E-02
Sensitivity Analysis	107	Air Diffusion Coefficient	2.26E-02	2.26E-02	2.49E-02
Sensitivity Analysis	108	Henry's Law Constant	3.57E-06	3.57E-06	3.57E-03
Sensitivity Analysis	109	Henry's Law Constant	3.57E-06	3.57E-06	3.57E-06
Sensitivity Analysis	110	Henry's Law Constant	3.57E-06	3.57E-06	3.57E-09
Sensitivity Analysis	111	Volitilization Factor	1	1	1
Sensitivity Analysis	112	Volitilization Factor	1	1	0.5
Sensitivity Analysis	113	Volitilization Factor	1	1	0
Sensitivity Analysis	114	Point of Compliance Bottom Depth	0	0	0
Sensitivity Analysis	115	Point of Compliance Bottom Depth	0	0	2
Sensitivity Analysis	116	Point of Compliance Bottom Depth	0	0	4
Sensitivity Analysis	117	Point of Compliance Bottom Depth	0	0	6
Sensitivity Analysis	118	Point of Compliance Bottom Depth	0	0	8
Sensitivity Analysis	119	Point of Compliance Bottom Depth	0	0	10
Sensitivity Analysis	120	Distance to Point of Compliance	10	0	10
Sensitivity Analysis	121	Distance to Point of Compliance	10	0	5
Sensitivity Analysis	122	Distance to Point of Compliance	10	0	0
Sensitivity Analysis	123	Aquifer Horizontal Hydraulic Conductivity (AT123D)	0.36	0.36	0.00036
Sensitivity Analysis	124	Aquifer Horizontal Hydraulic Conductivity (AT123D)	0.36	0.36	0.0036
Sensitivity Analysis	125	Aquifer Horizontal Hydraulic Conductivity (AT123D)	0.36	0.36	0.036
Sensitivity Analysis	126	Aquifer Horizontal Hydraulic Conductivity (AT123D)	0.36	0.36	0.36
Sensitivity Analysis	127	Aquifer Horizontal Hydraulic Conductivity (AT123D)	0.36	0.36	3.6
Sensitivity Analysis	128	Aquifer Horizontal Hydraulic Conductivity (AT123D)	0.36	0.36	36
Sensitivity Analysis	129	Hydraulic Gradient (AT123D)	0.005	0.005	0.01
Sensitivity Analysis	130	Hydraulic Gradient (AT123D)	0.005	0.005	0.005
Sensitivity Analysis	131	Hydraulic Gradient (AT123D)	0.005	0.005	0.003
Sensitivity Analysis	132	Hydraulic Gradient (AT123D)	0.005	0.005	0.001
Sensitivity Analysis	133	Effective Porosity (AT123D)	0.3	0.3	0.4
Sensitivity Analysis	134	Effective Porosity (AT123D)	0.3	0.3	0.3
Sensitivity Analysis	135	Effective Porosity (AT123D)	0.3	0.3	0.2
Sensitivity Analysis	136	Effective Porosity (AT123D)	0.3	0.3	0.1
Sensitivity Analysis	137	Bulk Density (AT123D)	1.3	1.3	1.3
Sensitivity Analysis	138	Bulk Density (AT123D)	1.3	1.3	1.5
Sensitivity Analysis	139	Bulk Density (AT123D)	1.3	1.3	1.7
Sensitivity Analysis	140	Longitudinal / Transverse / Vertical Dispersivity (AT123D)	20 / 2 / 2	0.83 / 0.083 / 0.0083	20 / 2 / 2
Sensitivity Analysis	141	Longitudinal / Transverse / Vertical Dispersivity (AT123D)	20 / 2 / 2	0.83 / 0.083 / 0.0083	20 / 2 / 0.01
Sensitivity Analysis	142	Longitudinal / Transverse / Vertical Dispersivity (AT123D)	20 / 2 / 2	0.83 / 0.083 / 0.0083	20 / 0.1 / 0.01
Sensitivity Analysis	143	Longitudinal / Transverse / Vertical Dispersivity (AT123D)	20 / 2 / 2	0.83 / 0.083 / 0.0083	1 / 0.1 / 0.01
Sensitivity Analysis	144	Longitudinal / Transverse / Vertical Dispersivity (AT123D)	20 / 2 / 2	0.83 / 0.083 / 0.0083	0.83 / 0.083 / 8.30E-03
Sensitivity Analysis	145	Longitudinal / Transverse / Vertical Dispersivity (AT123D)	20 / 2 / 2	0.83 / 0.083 / 0.0083	1.00E-02 / 1.00E-09 / 1.00E-09

Note: The Subsurface Release CSM was used as the reference point (or point of comparison) for the sensitivity analysis because the Subsurface Release CSM parameters, such as release depth and soil fraction of organic carbon, were set at values nearer the middle of the range of values tested in the sensitivity analysis.
Refer to previous tables for additional notes.

Table 4
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Development of Leaching-Based Soil Values for PFAS
New Hampshire Department of Environmental Services

Conceptual Model	Simulation Number	Layer 1		Layer 2		Layer 3		Layer 4		Total Soil Column Thickness and Depth to Groundwater (cm)	Chemical	Soil Input	Input Method	Release Top Depth	Release Bottom Depth	Source Area Size
(name)		No. of Sublayers	Layer Thickness (cm)	No. of Sublayers	Layer Thickness (cm)	No. of Sublayers	Layer Thickness (cm)	No. of Sublayers	Layer Thickness (cm)		(name)	(ppm)	(-)	(cm)	(cm)	(m)
Subsurface Release CSM	1	10	100	10	100	10	50	10	50	300	PFHxS	10	Sublayer	100	200	10 x 10
Subsurface Release CSM	2	10	100	10	100	10	50	10	50	300	PFNA	10	Sublayer	100	200	10 x 10
Subsurface Release CSM	3	10	100	10	100	10	50	10	50	300	PFOS	10	Sublayer	100	200	10 x 10
Subsurface Release CSM	4	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Surface Release CSM	5	2	20	8	80	10	100	10	100	300	PFHxS	10	Sublayer	100	200	10 x 10
Surface Release CSM	6	2	20	8	80	10	100	10	100	300	PFNA	10	Sublayer	100	200	10 x 10
Surface Release CSM	7	2	20	8	80	10	100	10	100	300	PFOS	10	Sublayer	100	200	10 x 10
Surface Release CSM	8	2	20	8	80	10	100	10	100	300	PFOA	10	Sublayer	100	200	10 x 10
Surface Release CSM	9	2	20	8	80	10	100	10	100	300	PFHxS	10	Sublayer	100	200	10 x 10
Surface Release CSM	10	2	20	8	80	10	100	10	100	300	PFNA	10	Sublayer	100	200	10 x 10
Surface Release CSM	11	2	20	8	80	10	100	10	100	300	PFOS	10	Sublayer	100	200	10 x 10
Surface Release CSM	12	2	20	8	80	10	100	10	100	300	PFOA	10	Sublayer	100	200	10 x 10
Surface Release CSM	13	2	20	8	80	10	100	10	100	300	PFHxS	10	Sublayer	0	20	10 x 10
Surface Release CSM	14	2	20	8	80	10	100	10	100	300	PFNA	10	Sublayer	0	20	10 x 10
Surface Release CSM	15	2	20	8	80	10	100	10	100	300	PFOS	10	Sublayer	0	20	10 x 10
Surface Release CSM	16	2	20	8	80	10	100	10	100	300	PFOA	10	Sublayer	0	20	10 x 10
Surface Release CSM	17	2	20	8	80	10	100	10	100	300	PFHxS	10	Sublayer	0	20	25 x 25
Surface Release CSM	18	2	20	8	80	10	100	10	100	300	PFNA	10	Sublayer	0	20	25 x 25
Surface Release CSM	19	2	20	8	80	10	100	10	100	300	PFOS	10	Sublayer	0	20	25 x 25
Surface Release CSM	20	2	20	8	80	10	100	10	100	300	PFOA	10	Sublayer	0	20	25 x 25
Sensitivity Analysis	21	10	100	10	100	10	50	10	50	300	PFHxS	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	22	10	100	10	100	10	50	10	50	300	PFHxS	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	23	10	100	10	100	10	50	10	50	300	PFHxS	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	24	10	100	10	100	10	50	10	50	300	PFHxS	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	25	10	100	10	100	10	50	10	50	300	PFHxS	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	26	10	100	10	100	10	50	10	50	300	PFHxS	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	27	10	100	10	100	10	50	10	50	300	PFNA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	28	10	100	10	100	10	50	10	50	300	PFNA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	29	10	100	10	100	10	50	10	50	300	PFNA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	30	10	100	10	100	10	50	10	50	300	PFNA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	31	10	100	10	100	10	50	10	50	300	PFNA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	32	10	100	10	100	10	50	10	50	300	PFNA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	33	10	100	10	100	10	50	10	50	300	PFOS	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	34	10	100	10	100	10	50	10	50	300	PFOS	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	35	10	100	10	100	10	50	10	50	300	PFOS	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	36	10	100	10	100	10	50	10	50	300	PFOS	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	37	10	100	10	100	10	50	10	50	300	PFOS	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	38	10	100	10	100	10	50	10	50	300	PFOS	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	39	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	40	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	41	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	42	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	43	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	44	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	45	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	46	10	100	10	100	N/A	N/A	N/A	N/A	200	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	47	10	100	10	100	10	200	10	200	600	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	48	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	49	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	0	100	10 x 10
Sensitivity Analysis	50	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	200	300	10 x 10
Sensitivity Analysis	51	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	0	50	10 x 10
Sensitivity Analysis	52	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	0	100	10 x 10
Sensitivity Analysis	53	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	0	150	10 x 10
Sensitivity Analysis	54	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	0	200	10 x 10
Sensitivity Analysis	55	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	0	250	10 x 10
Sensitivity Analysis	56	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	0	300	10 x 10
Sensitivity Analysis	57	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	5 x 5
Sensitivity Analysis	58	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	59	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	25 x 25
Sensitivity Analysis	60	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	50 x 50
Sensitivity Analysis	61	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	100 x 100
Sensitivity Analysis	62	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	150 x 150
Sensitivity Analysis	63	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	5 x 5
Sensitivity Analysis	64	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	65	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	25 x 25
Sensitivity Analysis	66	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	50 x 50
Sensitivity Analysis	67	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	100 x 100
Sensitivity Analysis	68	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	150 x 150
Sensitivity Analysis	69	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	5 x 5
Sensitivity Analysis	70	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	71	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	25 x 25
Sensitivity Analysis	72	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	50 x 50
Sensitivity Analysis	73	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	100 x 100
Sensitivity Analysis	74	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	150 x 150
Sensitivity Analysis	75	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	76	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	77	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	78	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	79	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	80	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	81	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	82	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10

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Conceptual Model	Simulation Number	Layer 1		Layer 2		Layer 3		Layer 4		Total Soil Column Thickness and Depth to Groundwater (cm)	Chemical	Soil Input	Input Method	Release Top Depth	Release Bottom Depth	Source Area Size
(name)		No. of Sublayers	Layer Thickness (cm)	No. of Sublayers	Layer Thickness (cm)	No. of Sublayers	Layer Thickness (cm)	No. of Sublayers	Layer Thickness (cm)		(name)	(ppm)	(-)	(cm)	(cm)	(m)
Sensitivity Analysis	83	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	84	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	85	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	86	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	87	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	88	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	89	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	90	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	91	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	92	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	93	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	94	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	95	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	96	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	97	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	98	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	99	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	100	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	101	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	102	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	103	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	104	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	105	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	106	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	107	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	108	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	109	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	110	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	111	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	112	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	113	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	114	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	115	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	116	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	117	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	118	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	119	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	120	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	121	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	122	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	123	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	124	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	125	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	126	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	127	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	128	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	129	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	130	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	131	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	132	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	133	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	134	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	135	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	136	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	137	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	138	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	139	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	140	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	141	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	142	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	143	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	144	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10
Sensitivity Analysis	145	10	100	10	100	10	50	10	50	300	PFOA	10	Sublayer	100	200	10 x 10

Table 4
Summary of SEVIEW Model Input Parameters and Simulation Results
Development of Leaching-Based Soil Values for PFAS
New Hampshire Department of Environmental Services

Conceptual Model (name)	Simulation Number	Climate File (name)	Soil Type (name)	Soil Vertical Hydraulic Conductivity (SESOIL) (cm/s)	Permeability (SESOIL) (cm^2)	Porosity (SESOIL) (-)	Bulk Density (SESOIL) (g/cm3)	Disconnectedness Index (SESOIL) (-)	Fraction of Organic Carbon (model layer 1) (%)	Fraction of Organic Carbon (model layers 2 to 4) (%)
Subsurface Release CSM	1	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Subsurface Release CSM	2	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Subsurface Release CSM	3	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Subsurface Release CSM	4	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Surface Release CSM	5	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Surface Release CSM	6	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Surface Release CSM	7	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Surface Release CSM	8	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Surface Release CSM	9	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	5	0.1
Surface Release CSM	10	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	5	0.1
Surface Release CSM	11	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	5	0.1
Surface Release CSM	12	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	5	0.1
Surface Release CSM	13	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	5	0.1
Surface Release CSM	14	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	5	0.1
Surface Release CSM	15	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	5	0.1
Surface Release CSM	16	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	5	0.1
Surface Release CSM	17	Massabesic (91-20) Snowmelt	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	5	0.1
Surface Release CSM	18	Massabesic (91-20) Snowmelt	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	5	0.1
Surface Release CSM	19	Massabesic (91-20) Snowmelt	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	5	0.1
Surface Release CSM	20	Massabesic (91-20) Snowmelt	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	5	0.1
Sensitivity Analysis	21	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	22	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	23	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	24	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	25	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	26	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	27	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	28	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	29	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	30	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	31	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	32	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	33	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	34	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	35	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	36	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	37	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	38	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	39	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	40	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	41	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	42	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	43	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	44	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	45	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	46	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	47	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	48	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	49	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	50	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	51	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	52	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	53	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	54	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	55	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	56	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	57	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	58	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	59	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	60	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	61	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	62	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	63	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	64	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	65	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	66	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	67	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	68	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	69	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	70	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	71	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	72	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	73	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	74	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	75	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	76	Massabesic (91-20) Snowmelt	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	77	Franklin Falls Dam (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	78	Berlin Muni AP (91-20)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	79	Massabesic (91-20)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	80	Laconia 2.8S (91-20)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	81	Lincoln NEPP (91-20)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	82	Mt Washington (91-20)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1

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New Hampshire Department of Environmental Services

Conceptual Model (name)	Simulation Number	Climate File (name)	Soil Type (name)	Soil Vertical Hydraulic Conductivity (SESOIL) (cm/s)	Permeability (SESOIL) (cm^2)	Porosity (SESOIL) (-)	Bulk Density (SESOIL) (g/cm3)	Disconnectedness Index (SESOIL) (-)	Fraction of Organic Carbon (model layer 1) (%)	Fraction of Organic Carbon (model layers 2 to 4) (%)
Sensitivity Analysis	83	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	84	Massabesic (71-00)	SILTY SAND	3.20E-05	3.20E-10	0.20	1.50	6	0.1	0.1
Sensitivity Analysis	85	Massabesic (71-00)	TILL/CLAY	1.00E-06	1.00E-11	0.10	1.70	12	0.1	0.1
Sensitivity Analysis	86	Massabesic (71-00)	SAND	1.00E-01	1.00E-06	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	87	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	88	Massabesic (71-00)	SAND	1.00E-06	1.00E-11	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	89	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.40	1.30	3.7	0.1	0.1
Sensitivity Analysis	90	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	91	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.20	1.30	3.7	0.1	0.1
Sensitivity Analysis	92	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.10	1.30	3.7	0.1	0.1
Sensitivity Analysis	93	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	94	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.50	3.7	0.1	0.1
Sensitivity Analysis	95	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.70	3.7	0.1	0.1
Sensitivity Analysis	96	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	97	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	6	0.1	0.1
Sensitivity Analysis	98	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	12	0.1	0.1
Sensitivity Analysis	99	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.01	0.01
Sensitivity Analysis	100	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	101	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	1	1
Sensitivity Analysis	102	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	103	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	104	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	105	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	106	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	107	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	108	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	109	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	110	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	111	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	112	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	113	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	114	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	115	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	116	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	117	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	118	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	119	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	120	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	121	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	122	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	123	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	124	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	125	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	126	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	127	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	128	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	129	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	130	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	131	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	132	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	133	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	134	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	135	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	136	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	137	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	138	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	139	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	140	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	141	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	142	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	143	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	144	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1
Sensitivity Analysis	145	Massabesic (71-00)	SAND	1.00E-03	1.00E-08	0.30	1.30	3.7	0.1	0.1

Table 4
Summary of SEVIEW Model Input Parameters and Simulation Results
Development of Leaching-Based Soil Values for PFAS
New Hampshire Department of Environmental Services

Conceptual Model (name)	Simulation Number	Soil Organic Carbon-Liquid Partition Coefficient (L/kg)	Freundlich Exponent (-)	Solid-Liquid Partition Coefficient (model layer 1) (m3/kg)	Solid-Liquid Partition Coefficient (model layers 2 to 4) (m3/kg)	Water Solubility (mg/L)	Water Diffusion Coefficient (cm2/s)	Water Diffusion Coefficient (m2/hr)	Air Diffusion Coefficient (cm2/s)	Henry's Law Constant (m3-atm/mol)	Molecular Weight (g/mol)	Volitilization Factor (-)
Subsurface Release CSM	1	64	1	6.4E-05	6.4E-05	239.43	6.01E-06	2.16E-06	2.33E-02	6.10E-05	400	1
Subsurface Release CSM	2	203	1	2.0E-04	2.0E-04	11.66	5.43E-06	1.95E-06	2.13E-02	1.90E-03	460	1
Subsurface Release CSM	3	804	1	8.0E-04	8.0E-04	680	5.25E-06	1.89E-06	2.07E-02	4.43E-07	500	1
Subsurface Release CSM	4	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Surface Release CSM	5	64	1	6.4E-05	6.4E-05	239.43	6.01E-06	2.16E-06	2.33E-02	6.10E-05	400	1
Surface Release CSM	6	203	1	2.0E-04	2.0E-04	11.66	5.43E-06	1.95E-06	2.13E-02	1.90E-03	460	1
Surface Release CSM	7	804	1	8.0E-04	8.0E-04	680	5.25E-06	1.89E-06	2.07E-02	4.43E-07	500	1
Surface Release CSM	8	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Surface Release CSM	9	64	1	3.2E-03	6.4E-05	239.43	6.01E-06	2.16E-06	2.33E-02	6.10E-05	400	1
Surface Release CSM	10	203	1	1.0E-02	2.0E-04	11.66	5.43E-06	1.95E-06	2.13E-02	1.90E-03	460	1
Surface Release CSM	11	804	1	4.0E-02	8.0E-04	680	5.25E-06	1.89E-06	2.07E-02	4.43E-07	500	1
Surface Release CSM	12	64	1	3.2E-03	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Surface Release CSM	13	64	1	3.2E-03	6.4E-05	239.43	6.01E-06	2.16E-06	2.33E-02	6.10E-05	400	1
Surface Release CSM	14	203	1	1.0E-02	2.0E-04	11.66	5.43E-06	1.95E-06	2.13E-02	1.90E-03	460	1
Surface Release CSM	15	804	1	4.0E-02	8.0E-04	680	5.25E-06	1.89E-06	2.07E-02	4.43E-07	500	1
Surface Release CSM	16	64	1	3.2E-03	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Surface Release CSM	17	64	1	3.2E-03	6.4E-05	239.43	6.01E-06	2.16E-06	2.33E-02	6.10E-05	400	1
Surface Release CSM	18	203	1	1.0E-02	2.0E-04	11.66	5.43E-06	1.95E-06	2.13E-02	1.90E-03	460	1
Surface Release CSM	19	804	1	4.0E-02	8.0E-04	680	5.25E-06	1.89E-06	2.07E-02	4.43E-07	500	1
Surface Release CSM	20	64	1	3.2E-03	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	21	43	1	4.3E-05	4.3E-05	239.43	6.01E-06	2.16E-06	2.33E-02	6.10E-05	400	1
Sensitivity Analysis	22	64	1	6.4E-05	6.4E-05	239.43	6.01E-06	2.16E-06	2.33E-02	6.10E-05	400	1
Sensitivity Analysis	23	99	1	9.9E-05	9.9E-05	239.43	6.01E-06	2.16E-06	2.33E-02	6.10E-05	400	1
Sensitivity Analysis	24	40	1	4.0E-05	4.0E-05	239.43	6.01E-06	2.16E-06	2.33E-02	6.10E-05	400	1
Sensitivity Analysis	25	78	1	7.8E-05	7.8E-05	239.43	6.01E-06	2.16E-06	2.33E-02	6.10E-05	400	1
Sensitivity Analysis	26	233	1	2.3E-04	2.3E-04	239.43	6.01E-06	2.16E-06	2.33E-02	6.10E-05	400	1
Sensitivity Analysis	27	135	1	1.4E-04	1.4E-04	11.66	5.43E-06	1.95E-06	2.13E-02	1.90E-03	460	1
Sensitivity Analysis	28	203	1	2.0E-04	2.0E-04	11.66	5.43E-06	1.95E-06	2.13E-02	1.90E-03	460	1
Sensitivity Analysis	29	587	1	5.9E-04	5.9E-04	11.66	5.43E-06	1.95E-06	2.13E-02	1.90E-03	460	1
Sensitivity Analysis	30	139	1	1.4E-04	1.4E-04	11.66	5.43E-06	1.95E-06	2.13E-02	1.90E-03	460	1
Sensitivity Analysis	31	332	1	3.3E-04	3.3E-04	11.66	5.43E-06	1.95E-06	2.13E-02	1.90E-03	460	1
Sensitivity Analysis	32	1072	1	1.1E-03	1.1E-03	11.66	5.43E-06	1.95E-06	2.13E-02	1.90E-03	460	1
Sensitivity Analysis	33	466	1	4.7E-04	4.7E-04	680	5.25E-06	1.89E-06	2.07E-02	4.43E-07	500	1
Sensitivity Analysis	34	804	1	8.0E-04	8.0E-04	680	5.25E-06	1.89E-06	2.07E-02	4.43E-07	500	1
Sensitivity Analysis	35	1111	1	1.1E-03	1.1E-03	680	5.25E-06	1.89E-06	2.07E-02	4.43E-07	500	1
Sensitivity Analysis	36	468	1	4.7E-04	4.7E-04	680	5.25E-06	1.89E-06	2.07E-02	4.43E-07	500	1
Sensitivity Analysis	37	1081	1	1.1E-03	1.1E-03	680	5.25E-06	1.89E-06	2.07E-02	4.43E-07	500	1
Sensitivity Analysis	38	3357	1	3.4E-03	3.4E-03	680	5.25E-06	1.89E-06	2.07E-02	4.43E-07	500	1
Sensitivity Analysis	39	47	1	4.7E-05	4.7E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	40	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	41	125	1	1.2E-04	1.2E-04	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	42	84	1	8.4E-05	8.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	43	357	1	3.6E-04	3.6E-04	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	44	1500	1	1.5E-03	1.5E-03	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	45	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	46	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	47	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	48	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	49	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	50	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	51	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	52	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	53	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	54	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	55	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	56	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	57	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	58	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	59	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	60	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	61	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	62	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	63	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	64	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	65	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	66	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	67	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	68	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	69	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	70	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	71	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	72	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	73	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	74	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	75	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	76	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	77	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	78	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	79	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	80	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	81	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	82	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1

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New Hampshire Department of Environmental Services

Conceptual Model (name)	Simulation Number	Soil Organic Carbon-Liquid Partition Coefficient (L/kg)	Freundlich Exponent (-)	Solid-Liquid Partition Coefficient (model layer 1) (m3/kg)	Solid-Liquid Partition Coefficient (model layers 2 to 4) (m3/kg)	Water Solubility (mg/L)	Water Diffusion Coefficient (cm2/s)	Water Diffusion Coefficient (m2/hr)	Air Diffusion Coefficient (cm2/s)	Henry's Law Constant (m3-atm/mol)	Molecular Weight (g/mol)	Volitilization Factor (-)
Sensitivity Analysis	83	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	84	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	85	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	86	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	87	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	88	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	89	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	90	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	91	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	92	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	93	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	94	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	95	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	96	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	97	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	98	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	99	64	1	6.4E-06	6.4E-06	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	100	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	101	64	1	6.4E-04	6.4E-04	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	102	64	1	6.4E-05	6.4E-05	9500	5.21E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	103	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	104	64	1	6.4E-05	6.4E-05	9500	6.37E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	105	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.03E-02	3.57E-06	410	1
Sensitivity Analysis	106	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	107	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.49E-02	3.57E-06	410	1
Sensitivity Analysis	108	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-03	410	1
Sensitivity Analysis	109	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	110	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-09	410	1
Sensitivity Analysis	111	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	112	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	0.5
Sensitivity Analysis	113	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	0
Sensitivity Analysis	114	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	115	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	116	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	117	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	118	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	119	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	120	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	121	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	122	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	123	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	124	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	125	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	126	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	127	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	128	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	129	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	130	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	131	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	132	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	133	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	134	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	135	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	136	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	137	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	138	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	139	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	140	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	141	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	142	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	143	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	144	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1
Sensitivity Analysis	145	64	1	6.4E-05	6.4E-05	9500	5.79E-06	2.08E-06	2.26E-02	3.57E-06	410	1

Table 4
Summary of SEVIEW Model Input Parameters and Simulation Results
Development of Leaching-Based Soil Values for PFAS
New Hampshire Department of Environmental Services

Conceptual Model (name)	Simulation Number	Point of Compliance Top Depth (m bWT)	Point of Compliance Bottom Depth (m bWT)	Distance to Point of Compliance (m)	Aquifer Horizontal Hydraulic Conductivity (AT123D) (m/hr)	Hydraulic Gradient (AT123D) (m/m)	Effective Porosity (AT123D) (-)	Bulk Density (AT123D) (g/cm3)	Longitudinal Dispersivity (AT123D) (m)	Transverse Dispersivity (AT123D) (m)	Vertical Dispersivity (AT123D) (m)	Aquifer Width (AT123D) (m)	Aquifer Thickness (AT123D) (m)
Subsurface Release CSM	1	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Subsurface Release CSM	2	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Subsurface Release CSM	3	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Subsurface Release CSM	4	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Surface Release CSM	5	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Surface Release CSM	6	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Surface Release CSM	7	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Surface Release CSM	8	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Surface Release CSM	9	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Surface Release CSM	10	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Surface Release CSM	11	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Surface Release CSM	12	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Surface Release CSM	13	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Surface Release CSM	14	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Surface Release CSM	15	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Surface Release CSM	16	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Surface Release CSM	17	0	0	0	0.36	0.005	0.30	1.30	0.83	0.083	8.30E-03	Inf	Inf
Surface Release CSM	18	0	0	0	0.36	0.005	0.30	1.30	0.83	0.083	8.30E-03	Inf	Inf
Surface Release CSM	19	0	0	0	0.36	0.005	0.30	1.30	0.83	0.083	8.30E-03	Inf	Inf
Surface Release CSM	20	0	0	0	0.36	0.005	0.30	1.30	0.83	0.083	8.30E-03	Inf	Inf
Sensitivity Analysis	21	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	22	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	23	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	24	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	25	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	26	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	27	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	28	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	29	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	30	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	31	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	32	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	33	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	34	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	35	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	36	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	37	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	38	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	39	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	40	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	41	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	42	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	43	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	44	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	45	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	46	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	47	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	48	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	49	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	50	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	51	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	52	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	53	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	54	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	55	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	56	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	57	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	58	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	59	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	60	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	61	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	62	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	63	0	0	0	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	64	0	0	0	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	65	0	0	0	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	66	0	0	0	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	67	0	0	0	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	68	0	0	0	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	69	0	0	0	0.36	0.005	0.30	1.30	0.83	0.083	8.30E-03	Inf	Inf
Sensitivity Analysis	70	0	0	0	0.36	0.005	0.30	1.30	0.83	0.083	8.30E-03	Inf	Inf
Sensitivity Analysis	71	0	0	0	0.36	0.005	0.30	1.30	0.83	0.083	8.30E-03	Inf	Inf
Sensitivity Analysis	72	0	0	0	0.36	0.005	0.30	1.30	0.83	0.083	8.30E-03	Inf	Inf
Sensitivity Analysis	73	0	0	0	0.36	0.005	0.30	1.30	0.83	0.083	8.30E-03	Inf	Inf
Sensitivity Analysis	74	0	0	0	0.36	0.005	0.30	1.30	0.83	0.083	8.30E-03	Inf	Inf
Sensitivity Analysis	75	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	76	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	77	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	78	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	79	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	80	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	81	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	82	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf

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New Hampshire Department of Environmental Services

Conceptual Model (name)	Simulation Number	Point of Compliance Top Depth (m bWT)	Point of Compliance Bottom Depth (m bWT)	Distance to Point of Compliance (m)	Aquifer Horizontal Hydraulic Conductivity (AT123D) (m/hr)	Hydraulic Gradient (AT123D) (m/m)	Effective Porosity (AT123D) (-)	Bulk Density (AT123D) (g/cm3)	Longitudinal Dispersivity (AT123D) (m)	Transverse Dispersivity (AT123D) (m)	Vertical Dispersivity (AT123D) (m)	Aquifer Width (AT123D) (m)	Aquifer Thickness (AT123D) (m)
Sensitivity Analysis	83	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	84	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	85	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	86	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	87	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	88	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	89	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	90	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	91	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	92	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	93	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	94	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	95	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	96	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	97	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	98	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	99	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	100	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	101	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	102	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	103	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	104	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	105	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	106	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	107	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	108	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	109	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	110	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	111	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	112	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	113	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	114	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	115	0	2	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	116	0	4	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	117	0	6	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	118	0	8	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	119	0	10	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	120	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	121	0	0	5	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	122	0	0	0	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	123	0	0	10	0.00036	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	124	0	0	10	0.0036	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	125	0	0	10	0.036	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	126	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	127	0	0	10	3.60	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	128	0	0	10	36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	129	0	0	10	0.36	0.010	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	130	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	131	0	0	10	0.36	0.003	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	132	0	0	10	0.36	0.001	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	133	0	0	10	0.36	0.005	0.40	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	134	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	135	0	0	10	0.36	0.005	0.20	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	136	0	0	10	0.36	0.005	0.10	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	137	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	138	0	0	10	0.36	0.005	0.30	1.50	20	2	2	Inf	Inf
Sensitivity Analysis	139	0	0	10	0.36	0.005	0.30	1.70	20	2	2	Inf	Inf
Sensitivity Analysis	140	0	0	10	0.36	0.005	0.30	1.30	20	2	2	Inf	Inf
Sensitivity Analysis	141	0	0	10	0.36	0.005	0.30	1.30	20	2	0.01	Inf	Inf
Sensitivity Analysis	142	0	0	10	0.36	0.005	0.30	1.30	20	0.1	0.01	Inf	Inf
Sensitivity Analysis	143	0	0	10	0.36	0.005	0.30	1.30	1	0.1	0.01	Inf	Inf
Sensitivity Analysis	144	0	0	10	0.36	0.005	0.30	1.30	0.83	0.083	8.30E-03	Inf	Inf
Sensitivity Analysis	145	0	0	10	0.36	0.005	0.30	1.30	1.00E-02	1.00E-09	1.00E-09	Inf	Inf

Table 4
Summary of SEVIEW Model Input Parameters and Simulation Results
Development of Leaching-Based Soil Values for PFAS
New Hampshire Department of Environmental Services

Conceptual Model	Simulation Number	Maximum Predicted Groundwater Concentration		Dilution-Attenuation Factor	Time to Max	AGQS		Leaching Based Soil Value		Layer 1 Calculated Retardation Factor	Layer 2-4 Calculated Retardation Factor
(name)		(mg/L)	(ug/L)	(-)	(years)	(ug/L)	(mg/L)	(mg/Kg)	(ng/g)	(-)	(-)
Subsurface Release CSM	1	7.35E-01	735.00	14	0.33	0.018	0.000018	0.000245	0.2449	1.3	1.3
Subsurface Release CSM	2	2.07E-01	207.00	48	1.33	0.011	0.000011	0.000531	0.5314	1.9	1.9
Subsurface Release CSM	3	1.68E-01	168.00	60	2.5	0.015	0.000015	0.000893	0.8929	4.5	4.5
Subsurface Release CSM	4	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Surface Release CSM	5	7.23E-01	723.00	14	0.33	0.018	0.000018	0.000249	0.2490	1.3	1.3
Surface Release CSM	6	2.07E-01	207.00	48	1.33	0.011	0.000011	0.000531	0.5314	1.9	1.9
Surface Release CSM	7	1.61E-01	161.00	62	2.5	0.015	0.000015	0.000932	0.9317	4.5	4.5
Surface Release CSM	8	7.52E-01	752.00	13	0.33	0.012	0.000012	0.000160	0.1596	1.3	1.3
Surface Release CSM	9	1.11E-01	111.00	90	0.83	0.018	0.000018	0.001622	1.6216	14.9	1.3
Surface Release CSM	10	3.29E-02	32.90	304	3.42	0.011	0.000011	0.003343	3.3435	45.0	1.9
Surface Release CSM	11	1.05E-02	10.50	952	9.17	0.015	0.000015	0.014286	14.286	175.2	4.5
Surface Release CSM	12	1.11E-01	111.00	90	0.83	0.012	0.000012	0.001081	1.0811	14.9	1.3
Surface Release CSM	13	1.65E-02	16.50	606	1.92	0.018	0.000018	0.010909	10.9091	14.9	1.3
Surface Release CSM	14	5.63E-04	0.56	17762	4.92	0.011	0.000011	0.195382	195.38	45.0	1.9
Surface Release CSM	15	1.51E-03	1.51	6623	19.92	0.015	0.000015	0.099338	99.34	175.2	4.5
Surface Release CSM	16	1.80E-02	18.00	556	1.92	0.012	0.000012	0.006667	6.6667	14.9	1.3
Surface Release CSM	17	1.80E+00	1800.00	6	1.58	0.018	0.000018	0.000100	0.1000	14.9	1.3
Surface Release CSM	18	8.59E-02	85.90	116	2.58	0.011	0.000011	0.001281	1.2806	45.0	1.9
Surface Release CSM	19	1.51E-01	151.00	66	14.58	0.015	0.000015	0.000993	0.9934	175.2	4.5
Surface Release CSM	20	1.95E+00	1950.00	5	1.58	0.012	0.000012	0.000062	0.0615	14.9	1.3
Sensitivity Analysis	21	7.48E-01	748.00	13	0.25	0.018	0.000018	0.000241	0.2406	1.2	1.2
Sensitivity Analysis	22	7.35E-01	735.00	14	0.33	0.018	0.000018	0.000245	0.2449	1.3	1.3
Sensitivity Analysis	23	5.98E-01	598.00	17	0.42	0.018	0.000018	0.000301	0.3010	1.4	1.4
Sensitivity Analysis	24	7.81E-01	781.00	13	0.25	0.018	0.000018	0.000230	0.2305	1.2	1.2
Sensitivity Analysis	25	7.00E-01	700.00	14	0.33	0.018	0.000018	0.000257	0.2571	1.3	1.3
Sensitivity Analysis	26	3.51E-01	351.00	28	1.17	0.018	0.000018	0.000513	0.5128	2.0	2.0
Sensitivity Analysis	27	2.19E-01	219.00	46	1.33	0.011	0.000011	0.000502	0.5023	1.6	1.6
Sensitivity Analysis	28	2.07E-01	207.00	48	1.33	0.011	0.000011	0.000531	0.5314	1.9	1.9
Sensitivity Analysis	29	1.04E-01	104.00	96	2.33	0.011	0.000011	0.001058	1.0577	3.5	3.5
Sensitivity Analysis	30	2.18E-01	218.00	46	1.33	0.011	0.000011	0.000505	0.5046	1.6	1.6
Sensitivity Analysis	31	1.72E-01	172.00	58	1.33	0.011	0.000011	0.000640	0.6395	2.4	2.4
Sensitivity Analysis	32	5.72E-02	57.20	175	3.5	0.011	0.000011	0.001923	1.9231	5.6	5.6
Sensitivity Analysis	33	2.70E-01	270.00	37	1.5	0.015	0.000015	0.000556	0.5556	3.0	3.0
Sensitivity Analysis	34	1.68E-01	168.00	60	2.5	0.015	0.000015	0.000893	0.8929	4.5	4.5
Sensitivity Analysis	35	1.25E-01	125.00	80	3.5	0.015	0.000015	0.001200	1.2000	5.8	5.8
Sensitivity Analysis	36	2.69E-01	269.00	37	1.5	0.015	0.000015	0.000558	0.5576	3.0	3.0
Sensitivity Analysis	37	1.28E-01	128.00	78	3.42	0.015	0.000015	0.001172	1.1719	5.7	5.7
Sensitivity Analysis	38	4.17E-02	41.70	240	10.67	0.015	0.000015	0.003597	3.5971	15.5	15.5
Sensitivity Analysis	39	7.42E-01	742.00	13	0.25	0.012	0.000012	0.000162	0.1617	1.2	1.2
Sensitivity Analysis	40	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	41	5.63E-01	563.00	18	0.5	0.012	0.000012	0.000213	0.2131	1.5	1.5
Sensitivity Analysis	42	7.09E-01	709.00	14	0.33	0.012	0.000012	0.000169	0.1693	1.4	1.4
Sensitivity Analysis	43	3.64E-01	364.00	27	1.33	0.012	0.000012	0.000330	0.3297	2.5	2.5
Sensitivity Analysis	44	9.06E-02	90.60	110	4.58	0.012	0.000012	0.001325	1.3245	7.5	7.5
Sensitivity Analysis	45	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	46	1.34E+00	1340.00	7	0.17	0.012	0.000012	0.000090	0.0896	1.3	1.3
Sensitivity Analysis	47	5.62E-01	562.00	18	1	0.012	0.000012	0.000214	0.2135	1.3	1.3
Sensitivity Analysis	48	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	49	6.51E-01	651.00	15	0.5	0.012	0.000012	0.000184	0.1843	1.3	1.3
Sensitivity Analysis	50	9.41E-01	941.00	11	0.17	0.012	0.000012	0.000128	0.1275	1.3	1.3
Sensitivity Analysis	51	3.42E-01	342.00	29	0.67	0.012	0.000012	0.000351	0.3509	1.3	1.3
Sensitivity Analysis	52	6.51E-01	651.00	15	0.5	0.012	0.000012	0.000184	0.1843	1.3	1.3
Sensitivity Analysis	53	9.38E-01	938.00	11	0.5	0.012	0.000012	0.000128	0.1279	1.3	1.3
Sensitivity Analysis	54	1.04E+00	1040.00	10	0.33	0.012	0.000012	0.000115	0.1154	1.3	1.3
Sensitivity Analysis	55	1.32E+00	1320.00	8	0.33	0.012	0.000012	0.000091	0.0909	1.3	1.3
Sensitivity Analysis	56	1.45E+00	1450.00	7	0.33	0.012	0.000012	0.000083	0.0828	1.3	1.3
Sensitivity Analysis	57	2.66E-01	266.00	38	0.33	0.012	0.000012	0.000451	0.4511	1.3	1.3
Sensitivity Analysis	58	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	59	1.57E+00	1570.00	6	0.42	0.012	0.000012	0.000076	0.0764	1.3	1.3
Sensitivity Analysis	60	1.86E+00	1860.00	5	0.42	0.012	0.000012	0.000065	0.0645	1.3	1.3
Sensitivity Analysis	61	1.89E+00	1890.00	5	0.5	0.012	0.000012	0.000063	0.0635	1.3	1.3
Sensitivity Analysis	62	1.89E+00	1890.00	5	0.5	0.012	0.000012	0.000063	0.0635	1.3	1.3
Sensitivity Analysis	63	3.33E-01	333.00	30	0.33	0.012	0.000012	0.000360	0.3604	1.3	1.3
Sensitivity Analysis	64	1.10E+00	1100.00	9	0.33	0.012	0.000012	0.000109	0.1091	1.3	1.3
Sensitivity Analysis	65	2.68E+00	2680.00	4	0.33	0.012	0.000012	0.000045	0.0448	1.3	1.3
Sensitivity Analysis	66	3.02E+00	3020.00	3	0.33	0.012	0.000012	0.000040	0.0397	1.3	1.3
Sensitivity Analysis	67	3.03E+00	3030.00	3	0.33	0.012	0.000012	0.000040	0.0396	1.3	1.3
Sensitivity Analysis	68	3.03E+00	3030.00	3	0.33	0.012	0.000012	0.000040	0.0396	1.3	1.3
Sensitivity Analysis	69	3.67E+01	36700.00	0.27	0.33	0.012	0.000012	0.000003	0.0033	1.3	1.3
Sensitivity Analysis	70	6.14E+01	61400.00	0.16	0.33	0.012	0.000012	0.000002	0.0020	1.3	1.3
Sensitivity Analysis	71	6.59E+01	65900.00	0.15	0.33	0.012	0.000012	0.000002	0.0018	1.3	1.3
Sensitivity Analysis	72	6.59E+01	65900.00	0.15	0.33	0.012	0.000012	0.000002	0.0018	1.3	1.3
Sensitivity Analysis	73	6.59E+01	65900.00	0.15	0.33	0.012	0.000012	0.000002	0.0018	1.3	1.3
Sensitivity Analysis	74	6.59E+01	65900.00	0.15	0.33	0.012	0.000012	0.000002	0.0018	1.3	1.3
Sensitivity Analysis	75	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	76	1.02E+00	1020.00	10	0.58	0.012	0.000012	0.000118	0.1176	1.3	1.3
Sensitivity Analysis	77	7.77E-01	777.00	13	0.33	0.012	0.000012	0.000154	0.1544	1.3	1.3
Sensitivity Analysis	78	6.51E-01	651.00	15	0.33	0.012	0.000012	0.000184	0.1843	1.3	1.3
Sensitivity Analysis	79	7.29E-01	729.00	14	0.33	0.012	0.000012	0.000165	0.1646	1.3	1.3
Sensitivity Analysis	80	7.92E-01	792.00	13	0.25	0.012	0.000012	0.000152	0.1515	1.3	1.3
Sensitivity Analysis	81	8.78E-01	878.00	11	0.25	0.012	0.000012	0.000137	0.1367	1.3	1.3
Sensitivity Analysis	82	1.15E+00	1150.00	9	0.17	0.012	0.000012	0.000104	0.1043	1.3	1.3

Table 4

Summary of SEVIEW Model Input Parameters and Simulation Results

Development of Leaching-Based Soil Values for PFAS

New Hampshire Department of Environmental Services

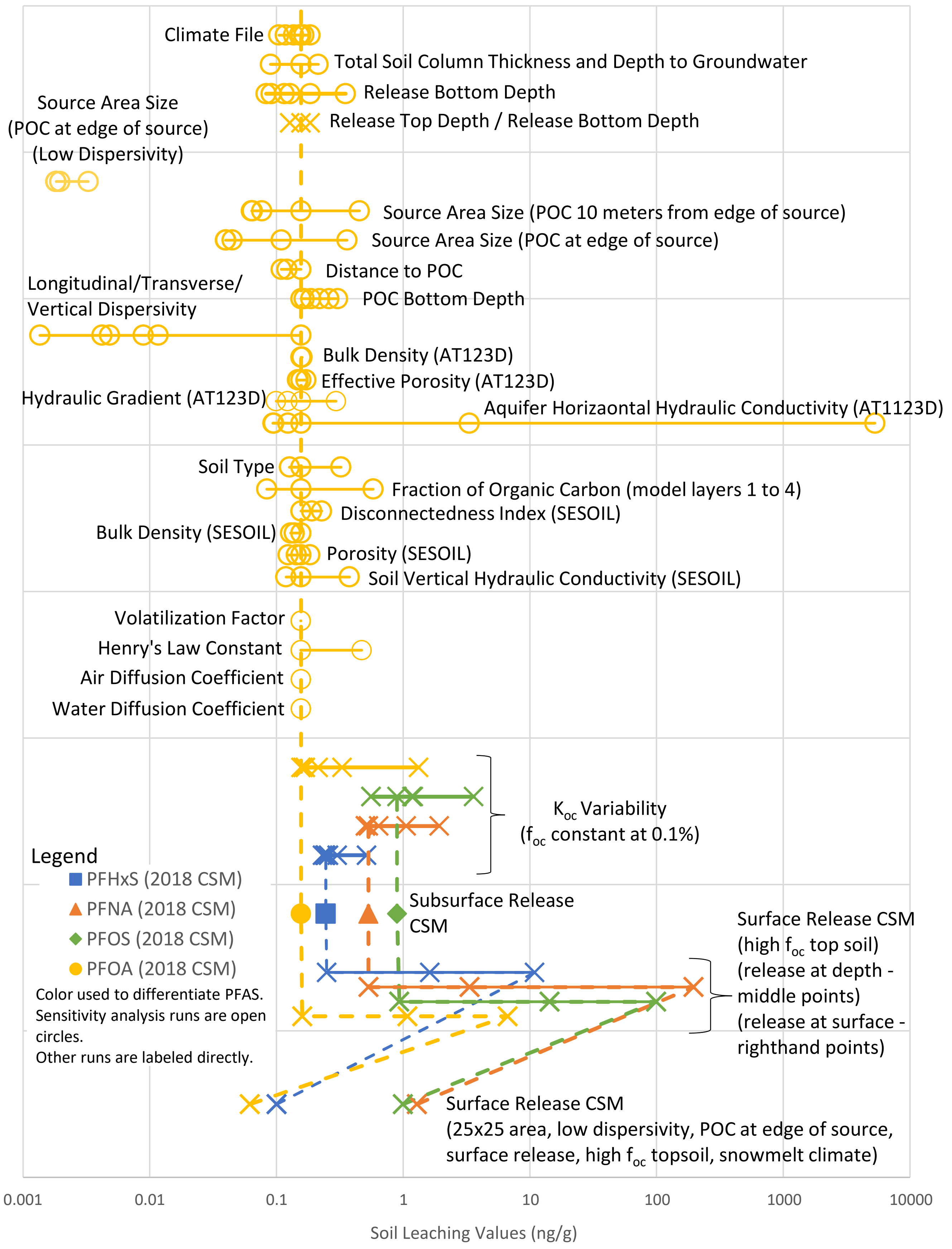
Conceptual Model	Simulation Number	Maximum Predicted Groundwater Concentration		Dilution-Attenuation Factor	Time to Max	AGQS		Leaching Based Soil Value		Layer 1 Calculated Retardation Factor	Layer 2-4 Calculated Retardation Factor
(name)		(mg/L)	(ug/L)	(-)	(years)	(ug/L)	(mg/L)	(mg/Kg)	(ng/g)	(-)	(-)
Sensitivity Analysis	83	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	84	9.47E-01	947.00	11	1.17	0.012	0.000012	0.000127	0.1267	1.5	1.5
Sensitivity Analysis	85	3.72E-01	372.00	27	1.83	0.012	0.000012	0.000323	0.3226	2.1	2.1
Sensitivity Analysis	86	1.01E+00	1010.00	10	0.17	0.012	0.000012	0.000119	0.1188	1.3	1.3
Sensitivity Analysis	87	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	88	3.19E-01	319.00	31	16.33	0.012	0.000012	0.000376	0.3762	1.3	1.3
Sensitivity Analysis	89	6.53E-01	653.00	15	0.33	0.012	0.000012	0.000184	0.1838	1.2	1.2
Sensitivity Analysis	90	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	91	8.36E-01	836.00	12	0.25	0.012	0.000012	0.000144	0.1435	1.4	1.4
Sensitivity Analysis	92	9.70E-01	970.00	10	0.17	0.012	0.000012	0.000124	0.1237	1.8	1.8
Sensitivity Analysis	93	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	94	8.66E-01	866.00	12	0.33	0.012	0.000012	0.000139	0.1386	1.3	1.3
Sensitivity Analysis	95	9.28E-01	928.00	11	0.33	0.012	0.000012	0.000129	0.1293	1.4	1.4
Sensitivity Analysis	96	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	97	6.32E-01	632.00	16	0.42	0.012	0.000012	0.000190	0.1899	1.3	1.3
Sensitivity Analysis	98	5.28E-01	528.00	19	0.67	0.012	0.000012	0.000227	0.2273	1.3	1.3
Sensitivity Analysis	99	1.43E+00	1430.00	7	0.17	0.012	0.000012	0.000084	0.0839	1.0	1.0
Sensitivity Analysis	100	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	101	2.07E-01	207.00	48	2.33	0.012	0.000012	0.000580	0.5797	3.8	3.8
Sensitivity Analysis	102	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	103	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	104	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	105	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	106	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	107	7.69E-01	769.00	13	0.33	0.012	0.000012	0.000156	0.1560	1.3	1.3
Sensitivity Analysis	108	2.55E-01	255.00	39	0.33	0.012	0.000012	0.000471	0.4706	1.3	1.3
Sensitivity Analysis	109	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	110	7.72E-01	772.00	13	0.33	0.012	0.000012	0.000155	0.1554	1.3	1.3
Sensitivity Analysis	111	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	112	7.71E-01	771.00	13	0.33	0.012	0.000012	0.000156	0.1556	1.3	1.3
Sensitivity Analysis	113	7.72E-01	772.00	13	0.33	0.012	0.000012	0.000155	0.1554	1.3	1.3
Sensitivity Analysis	114	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	115	7.26E-01	725.50	14	0.33	0.012	0.000012	0.000165	0.1654	1.3	1.3
Sensitivity Analysis	116	6.42E-01	641.60	16	0.33	0.012	0.000012	0.000187	0.1870	1.3	1.3
Sensitivity Analysis	117	5.48E-01	547.70	18	0.33	0.012	0.000012	0.000219	0.2191	1.3	1.3
Sensitivity Analysis	118	4.63E-01	463.40	22	0.33	0.012	0.000012	0.000259	0.2590	1.3	1.3
Sensitivity Analysis	119	3.95E-01	394.80	25	0.33	0.012	0.000012	0.000304	0.3040	1.3	1.3
Sensitivity Analysis	120	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	121	9.90E-01	990.00	10	0.33	0.012	0.000012	0.000121	0.1212	1.3	1.3
Sensitivity Analysis	122	1.10E+00	1100.00	9	0.33	0.012	0.000012	0.000109	0.1091	1.3	1.3
Sensitivity Analysis	123	9.75E-01	975.00	10	44.17	0.012	0.000012	0.000123	0.1231	1.3	1.3
Sensitivity Analysis	124	1.26E+00	1260.00	8	4.75	0.012	0.000012	0.000095	0.0952	1.3	1.3
Sensitivity Analysis	125	1.28E+00	1280.00	8	0.75	0.012	0.000012	0.000094	0.0938	1.3	1.3
Sensitivity Analysis	126	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	127	3.62E-02	36.20	276	0.33	0.012	0.000012	0.003315	3.3149	1.3	1.3
Sensitivity Analysis	128	2.27E-05	0.02	440529	0.33	0.012	0.000012	5.286344	5286.3	1.3	1.3
Sensitivity Analysis	129	4.07E-01	407.00	25	0.33	0.012	0.000012	0.000295	0.2948	1.3	1.3
Sensitivity Analysis	130	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	131	9.82E-01	982.00	10	0.33	0.012	0.000012	0.000122	0.1222	1.3	1.3
Sensitivity Analysis	132	1.21E+00	1210.00	8	0.5	0.012	0.000012	0.000099	0.0992	1.3	1.3
Sensitivity Analysis	133	7.01E-01	701.00	14	0.33	0.012	0.000012	0.000171	0.1712	1.3	1.3
Sensitivity Analysis	134	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	135	8.19E-01	819.00	12	0.33	0.012	0.000012	0.000147	0.1465	1.3	1.3
Sensitivity Analysis	136	8.09E-01	809.00	12	0.33	0.012	0.000012	0.000148	0.1483	1.3	1.3
Sensitivity Analysis	137	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	138	7.61E-01	761.00	13	0.33	0.012	0.000012	0.000158	0.1577	1.3	1.3
Sensitivity Analysis	139	7.53E-01	753.00	13	0.33	0.012	0.000012	0.000159	0.1594	1.3	1.3
Sensitivity Analysis	140	7.70E-01	770.00	13	0.33	0.012	0.000012	0.000156	0.1558	1.3	1.3
Sensitivity Analysis	141	1.03E+01	10300.00	1.0	0.33	0.012	0.000012	0.000012	0.0117	1.3	1.3
Sensitivity Analysis	142	1.35E+01	13500.00	0.7	0.33	0.012	0.000012	0.000009	0.0089	1.3	1.3
Sensitivity Analysis	143	2.49E+01	24900.00	0.4	0.58	0.012	0.000012	0.000005	0.0048	1.3	1.3
Sensitivity Analysis	144	2.86E+01	28600.00	0.3	0.58	0.012	0.000012	0.000004	0.0042	1.3	1.3
Sensitivity Analysis	145	8.84E+01	88400.00	0.1	0.58	0.012	0.000012	0.000001	0.0014	1.3	1.3

Table 5
Summary of MODFLOW USG Transport Input Parameters and Simulation Results for PFOA
Development of Leaching-Based Soil Values for PFAS
New Hampshire Department of Environmental Services

Model Scenario	Model Grid Dimensions				Grid Layer Setup	Release Area/Depth	Soil Types Simulated	Model Parameters						Vadose Zone Soil Parameters				Calculated PFOA Soil Leaching Values		
	Width	Length	Bottom	Top				Horizontal Hydraulic Conductivity (x-axis and y-axis)	Vertical Hydraulic Conductivity (z-axis)	Horizontal Dispersivity (x-axis)	Horizontal Dispersivity (y-axis)	Vertical Dispersivity (z-axis)	PFOA Soil-Water Partition Coefficient	Alpha	Beta	Brooks-Corey exponent	Residual Saturation	Well Average	Water Table	Plume Center
	(meters)							(meters/day)		(meters)			(m^3/kg)	(1/cm)	(-)	(-)	(-)	(ng/g)		
1	90	100	0	23	Equivalent to Subsurface Release CSM in SEVIEW Simulations	10x10 meter Subsurface (1-2m)	Homogeneous Sand	8.64	0.864	20	2	2	6.40E-05	0.147	2.67	4.198	0.0466	0.75	0.72	0.64
2	90	100	10	23		10x10 meter Subsurface (1-2m)	Homogeneous Sand	8.64	0.864	0.83	0.083	0.0083	6.40E-05	0.147	2.67	4.198	0.0466	0.41	0.55	0.20
3	90	100	10	23	Equivalent to Surface Release CSM in SEVIEW simulations	10x10 meter Surface (0-20cm)	Homogeneous Sand	8.64	0.864	0.83	0.083	0.0083	0.0032 (surface soil 0-20 cm) 0.000064 (sub-surface soil)	0.147	2.67	4.198	0.0466	0.35	0.54	0.18
4	90	100	10	23		10x10 meter Surface (0-20cm)	Heterogeneous Sand	Geomean 10, Log-normal (2.3,0.5) Rand()	10 to 1 ratio of Horizontal to Vertical Hydraulic Conductivity	0.83	0.083	0.0083	0.0032 (surface soil 0-20 cm) 0.000064 (sub-surface soil)	0.147	2.67	4.198	0.0466	0.37	0.61	0.19
5	90	100	10	23		10x10 meter Surface (0-20cm)	Heterogeneous Layered sand/silt	Geomean 0.1, Log-normal (-2.3,0.5) Rand() Geomean 1, Log-normal (0,0.8) Rand() Geomean 10, Log-normal (2.3,0.5) Rand()		0.83	0.083	0.0083	0.0032 (surface soil 0-20 cm) 0.000064 (sub-surface soil)	0.0757	1.89	5.247	0.0644	0.41	0.31	0.21
6	90	100	10	23		10x10 meter Surface (0-20 cm)	Heterogeneous Sandy Loam overlying Sandy Clay	Geomean 1, Log-normal (0,0.8) Rand() Geomean 1E-5, Log-normal (-11.5,1.2) Rand()		0.83	0.083	0.0083	0.0032 (surface soil 0-20 cm) 0.000064 (sub-surface soil)	0.0757 0.027	1.89 1.28	5.247 10.143	0.0644 0.0993	2.04	0.20	0.20

Figure

Figure 1
Summary of Leaching-based Soil Values by Input Parameter



"POC" is Point of Compliance or Compliance Point.
"K_{oc}" is Soil Organic Carbon-Liquid Partition Coefficient.
"CSM" is Conceptual Site Model.
"f_{oc}" is Fraction of of Organic Carbon.

Appendix A

Organic Carbon-Liquid Partition Coefficient (K_{oc}) Selection Approach

Appendix A
Organic Carbon-Liquid Partition Coefficient (K_{oc}) Selection Approach

A.1 2023 USGS NH STUDY

Given the variables and unknowns influencing partitioning and leaching of per- and polyfluoroalkyl substances (PFAS) as described in Section 1.3 of the report, the New Hampshire Department of Environmental Services (NHDES) partnered with the U.S. Geological Survey (USGS) to study occurrence and leachability of PFAS in shallow soils in New Hampshire (hereafter referred to as the 2023 USGS NH Study). A stated purpose of the 2023 USGS NH Study was to investigate partitioning for New Hampshire soils.

The 2023 USGS NH Study included laboratory testing of soils to derive sample-specific solid-liquid partition coefficient (K_d) values, and the data and documentation were accessed via the USGS data release webpage (Tokranov et al., 2023). A summary of the soil K_d isotherm, or batch equilibrium, experimental structure is provided in Exhibit A-1. These were 10-day batch equilibrium samples based on contact times confirmed by the USGS in kinetic tests included in the study.

Exhibit A-1: Summary of Soil K_d Isotherm Experimental Structure

Sample Location	Sample Type	Spike Levels	Number of K_d Samples
BTW-C-1	Contaminated Soil	0	3
BTW-C-2	Contaminated Soil	0	3
BTW-U-1	Uncontaminated Soil	0, L1-L5	18
BTW-U-2	Uncontaminated Soil	0, L1-L5	18
NHF-C-1	Contaminated Soil	0	3
NHF-U-1	Uncontaminated Soil	0, L1-L5	18
SGB-C-1	Contaminated Soil	0, L1-L5	20
WND-C-1	Contaminated Soil	0	3
WND-U-1	Uncontaminated Soil	0, L1-L5	18

Notes:

1. Contaminated soil and uncontaminated soil designations were assigned as part of the 2023 USGS NH Study. Contaminated designation indicates sample locations that were collected from areas with a known PFAS release.
2. Spike levels include “0” for samples that are not spiked and spiked PFAS levels L1, L2, L3, L4, and L5, in order of increasing spiked mass. The spiked masses associated with each level are reported with the USGS data release (Tokranov et al., 2023).
3. K_d samples include at least three samples per spike level.

A.2 SOIL ISOTHERM SAMPLE SELECTION

The soil isotherm K_d values, and associated K_{oc} values, were screened by Sanborn Head to select samples that were (i) representative of the soils and conditions included in the conceptual site models (CSMs) used for the soil leaching model scenarios, and (ii) provided relatively stable partitioning values. The rationale for the sample selection approach is outlined below.

- Samples with no spiked PFAS were selected because they were considered more representative of desorption (leaching) of PFAS introduced under field conditions. The spiked PFAS samples were spiked under laboratory conditions and are more representative of adsorption. As shown below in Exhibit A-2, the K_{OC} values tended to decrease with increased spiked level. Sufficient concentrations of perfluorooctanoic acid (PFOA), perfluorononanoic acid (PFNA), perfluorohexane sulfonic acid (PFHxS), and perfluorooctane sulfonic acid (PFOS) were present for most zero-spike samples to calculate partitioning values without needing the laboratory spike.

- Uncontaminated samples were selected because of the greater, unexplained variability in the K_{oc} values associated with contaminated samples. Contaminated designation was assigned in the study for sample locations that were collected from areas with a known PFAS release. A plot of K_{oc} by sample type (contaminated and uncontaminated) is shown in Exhibit A-3. The narrower range of uncontaminated sample K_{oc} values suggests the uncontaminated K_{oc} values are more broadly applicable, whereas the contaminated sample K_{oc} values include unusually high and unusually low values that may not be representative of typical soils. For example, site-specific factors that are not broadly applicable to other soils, such as co-contaminants and release history, may have affected the contaminated sample K_{oc} values.

A.3 SELECTION OF K_{OC} APPROACH

As discussed in the report Section 1.3.1, chemical-specific, solid-phase partitioning is typically represented by a K_d (i.e., solid-liquid partition coefficient). Non-linear sorption can be described using the form $K_d = C_S / C_L^n$,, where C_S is solid-phase concentration, C_L is liquid-phase concentration, and n is the Freundlich exponent. A common adaptation of the K_d approach is to use K_{oc} (organic carbon-liquid partition coefficient) to normalize to soil organic carbon using the relationship represented by the formula $K_d = K_{oc} \times f_{oc}$, where f_{oc} is the fraction of organic carbon in soil. This section discusses the rationale for selecting a linear K_{oc} approach for specifying the solid-liquid partitioning parameters in modeling.

A.3.1 Linearity

The K_{oc} values were calculated by Sanborn Head using the sample K_d and sample location f_{oc} values reported in the 2023 USGS NH Study. The 2023 USGS NH Study also reported the experimental water and solids results associated with the K_d values. An initial soil concentration reported for each sample location was shared by the replicate K_d samples. Even for uncontaminated samples, PFOA, PFNA, PFHxS, and PFOS were detected at most of the sample locations. As an example, the BTW-U-1 location had an initial soil concentration of 0.395 nanograms per gram PFOA that was associated with three replicate K_d samples for BTW-U-1, and each of those BTW-U-1 K_d samples had different isotherm water concentrations, isotherm solid concentrations, and calculated K_d and K_{oc} values for PFOA. Some of the differences between replicates may be from variability introduced by splitting samples and laboratory measurement variability.

The Exhibit A-4 K_{oc} Freundlich isotherm plots were used to assess non-linearity and estimate the Freundlich exponent (n) for the equation $K_{oc} = C_{oc} / C_L^n$, where C_{oc} is the solid-phase concentration normalized to soil organic carbon content. The Freundlich plots use axes of $y = \log10(C_{oc})$ and $x = \log10(C_L)$, and two best fit lines are plotted:

- The red, non-linear sorption best fit line uses the equation $\log10(C_{oc}) = n \times \log10(C_L) + \log10(K_{oc})$, which is a reorganization of $K_{oc} = C_{oc} / C_L^n$ using logarithm rules. The slope of the best fit line is n and the intercept is $\log10(K_{oc})$.
- The green, linear sorption best fit line has a slope (n) of 1, so the equation is $\log10(C_{oc}) = \log10(C_L) + \log10(K_{oc})$. The intercept is $\log10(K_{oc})$.

Visually, there is similar goodness of fit for both the red non-linear sorption lines and the green linear sorption lines for PFOA, PFNA, and PFOS. The non-linear fit for PFHxS appears to have somewhat better fit, but the linear fit for PFHxS is also fine. Because the goodness of fit is generally comparable for the linear and non-liner approaches, the linear approach is preferred because it is a less complex approach that avoids overfitting to the variable data.

Linearity was further visualized in Exhibit A-5, which shows K_d and K_{oc} values plotted against initial soil concentration, isotherm water concentration, and isotherm solid concentration. If there were consistent increasing or decreasing trends in K_d or K_{oc} with concentration, then that trend would indicate a potential non-linear sorption. Because there are not consistent increasing or decreasing trends in K_d and K_{oc} with concentration, sorption can be assumed to be linear.

A.3.2 Organic Carbon and Other Soil Parameters

Various soil parameters were also reported for each sample location, including initial soil PFAS concentrations, fraction of organic carbon (f_{oc}), clay and silt content, protein content, soil pH, cation exchange capacity (CEC), and anion exchange capacity (AEC).

Exhibit A-6 shows the linear relationship between f_{oc} and K_d for uncontaminated soil isotherm samples with no spiked PFAS. The linear fit is based on $K_d = K_{oc} \times f_{oc}$ such that the slope of the line is an estimate of K_{oc} and the y-intercept is zero. In the title for each plot, an estimated slope (K_{oc}) and associated p-value are provided. The p-values, which were all very significant (<0.001), indicate that $K_{oc} \times f_{oc}$ is a better predictor of K_d than just using the mean K_d. For instance, the mean PFOA K_d was about 1.4 liter per kilogram (L/kg). The NHF-U-1 sample had relatively high f_{oc} (>0.04 kilograms organic carbon per kilogram solid [kg-oc/kg-solid]) and relatively high PFOA K_d values (>2 L/kg). If the K_d values were not already known, then it could be estimated that the NHF-U-1 sample would tend to have higher than average K_d values because it had higher than average f_{oc} values.

Exhibit A-7 shows K_d and K_{oc} values plotted against soil parameters for uncontaminated soil isotherm samples with no spiked PFAS. Some apparent trends between K_d and soil parameters are present, such as increasing K_d with f_{oc} and protein; and decreasing K_d with clay and silt content, soil pH, and AEC. Some of these trends are consistent with the solid-phase partitioning literature discussed in Section 1.3 of the report, and we understand there is ongoing work by the USGS that further analyzes trends of K_d with soil parameters and water chemistry in the 2023 USGS NH Study data. There were not consistent increasing or decreasing trends of soil parameters with K_{oc}, which suggests these other soil parameters do not provide additional information for estimating solid-phase partitioning using these data.

A.4 SELECTED K_{OC} VALUES

The K_{oc} values for the selected samples are summarized in Table 2. Table 2 also includes tabular and dot plot comparisons of selected 2023 USGS NH Study data and literature values. The first and second columns of plots with mini tables in Table 2 compare literature K_d and K_{oc} values obtained from Rovero et al. (2021), which is a review of published literature that reported PFAS partitioning values. The literature included a wide range of studies, such as laboratory studies, field studies, adsorption studies, and desorption studies. Laboratory studies and adsorption studies tend to report lower K_d values for PFAS (Rovero et al., 2021). The selected isotherm samples with no spiked PFAS from the 2023 USGS NH Study were laboratory desorption values, and the selected 2023 USGS NH Study K_d and K_{oc} values largely fall around the first quartile or median of values compiled by Rovero et al. (2021). Specifically, the selected PFOA K_{oc} values fall around the literature first quartile, and the selected PFNA, PFHxS, and PFOS K_{oc} values mostly fall between the literature first quartile and median. Because these New Hampshire-specific K_{oc} values tend to fall below median literature K_{oc} values, use of the New Hampshire-specific values would tend to predict faster leaching and result in the calculation of more protective leaching-based soil values, as compared to using median literature values.

To derive a single, representative K_{oc} for PFOA, PFNA, PFHxS, and PFOS to be used in modeling, the median value for each PFAS was selected from the 2023 USGS NH Study. The third column of plots with mini tables in Table 2 includes other summary statistics for comparison, such as the mean and geometric mean. The calculated K_{oc} values based on the linear Freundlich plots (Exhibit A-4) and K_d-f_{oc} linear correlation (Exhibit A-6) are also included in the third column mini tables in Table 2. These values are generally similar for a given PFAS, especially considering the variable methods for calculating the K_{oc} values and order-of-magnitude variability observed in literature values. The 2023 USGS NH Study median value was selected because it is a measure of the central tendency of the data that is robust to outlying values. For example, a high outlying value could result in a large increase of the mean and geometric mean, or a low outlying value could result in a large decrease of the mean and geometric mean.

The third column of plots with mini tables in Table 2 also includes K_{oc} values obtained from the United States Environmental Protection Agency (USEPA) Regional Screening Levels (RSLs) chemical specific parameters generic table (USEPA, 2023). The selected median K_{oc} values for PFOA, PFNA, and PFHxS are less than the K_{oc} values included in the USEPA RSLs table, and the selected median PFOS K_{oc} is greater than the value included in the USEPA RSLs table. The K_{oc} values selected by the USEPA for calculation of RSLs are from laboratory studies by Higgins and Luthy (2023) and Guelfo and Higgins (2013). These were batch adsorption isotherm studies that were not specific to New Hampshire soils. The lower 2023 USGS NH Study K_{oc} values for PFOA, PFNA, and PFHxS would tend to result in calculation of more protective leaching-based soil values, while the higher 2023 USGS NH Study K_{oc} value for PFOS would tend to result in calculation of a less protective leaching-based soil value. Because the 2023 USGS NH Study data were generated for the purpose of investigating partitioning in New Hampshire soils, the use of these New Hampshire-specific values likely results in a more representative leaching-based soil value than the use of other literature-based values.

A.5 APPLICATION OF SELECTED K_{OC} VALUES

Modeling described in Report Section 5 used solid-liquid partitioning based on the equation $K_{d,model} = f_{oc,model} \times K_{oc,USGS,median}$. The selection process for f_{oc} values used in modeling is presented in the Conceptual Site Model Section (Report Section 4). A table of the selected K_{oc} values and example calculated model K_d values is provided below in Exhibit A-8. Model layer K_d values for each model simulation are included in Report Table 2.

In Exhibit A-8, medians of the 2023 USGS NH Study select K_{oc} values are provided in two columns. The first column provides median K_{oc} values based on f_{oc} values that were adjusted for soil moisture; the adjustment for soil moisture compensates for the original soil organic content data being reported on a wet-weight basis. These “adjusted” K_{oc} values are the values presented in this Appendix A as well as the primary data presented in Report Table 2. The second column provides median K_{oc} values based on f_{oc} values that were not adjusted for soil moisture; these “unadjusted” K_{oc} values were calculated for and used in the modeling prior to Sanborn Head being aware that soil organic content data were reported on a wet-weight basis. The adjusted K_{oc} values were typically about 20 to 22 percent lower than the unadjusted values, and if they were used in the modeling, then they would tend to result in the calculation of more protective leaching-based soil values. As shown on Report Table 2, the unadjusted K_{oc} values fell well within the range of the adjusted USGS K_{oc} values, and the modeling results using the unadjusted K_{oc} are considered sufficiently representative for the purposes of the modeling results presented in the Report. We understand that the NHDES is aware of the need to use soil moisture adjusted values in subsequent modeling to calculate proposed leaching-based soil values.

Some of the calculated model layer K_d values fell within the range of the selected 2023 USGS NH Study data, and some of the calculated model layer K_d values fell outside the range of the selected 2023 USGS NH Study data. The selected 2023 USGS NH Study data f_{oc} values range from 0.0096 to 0.047 kilogram-organic carbon per kilogram-dry soil (kg-oc/kg), and the $K_d = K_{oc} \times f_{oc}$ function was used to extrapolate K_d values for model layers with f_{oc} values outside the range of the selected 2023 USGS NH Study data. For model layers where soil f_{oc} was assumed to be relatively low (for example, 0.001 and 0.0001 kg-oc/kg), the calculated K_d values were well below the range of K_d values measured in the 2023 USGS NH Study uncontaminated isotherm samples with no spiked PFAS. Extrapolating the study-specific K_d/K_{oc} relationship to those low f_{oc} soils may tend to over predict leachability because there could be some solid-phase partitioning, such as hydrophobic or electrostatic adsorption to inorganics, that may not be accounted for.

Based on the available information, the K_{oc} approach using the selected 2023 USGS NH Study data helps to estimate more realistic solid-phase partitioning than other approaches, such as not adjusting for soil organic carbon content or using literature values that may not be representative of typical New Hampshire soils. As compared to a model that includes inorganic adsorption in low f_{oc} soils that the selected K_{oc} approach does not account for, the selected K_{oc} approach tends to result in the calculation of more protective leaching-based soil values.

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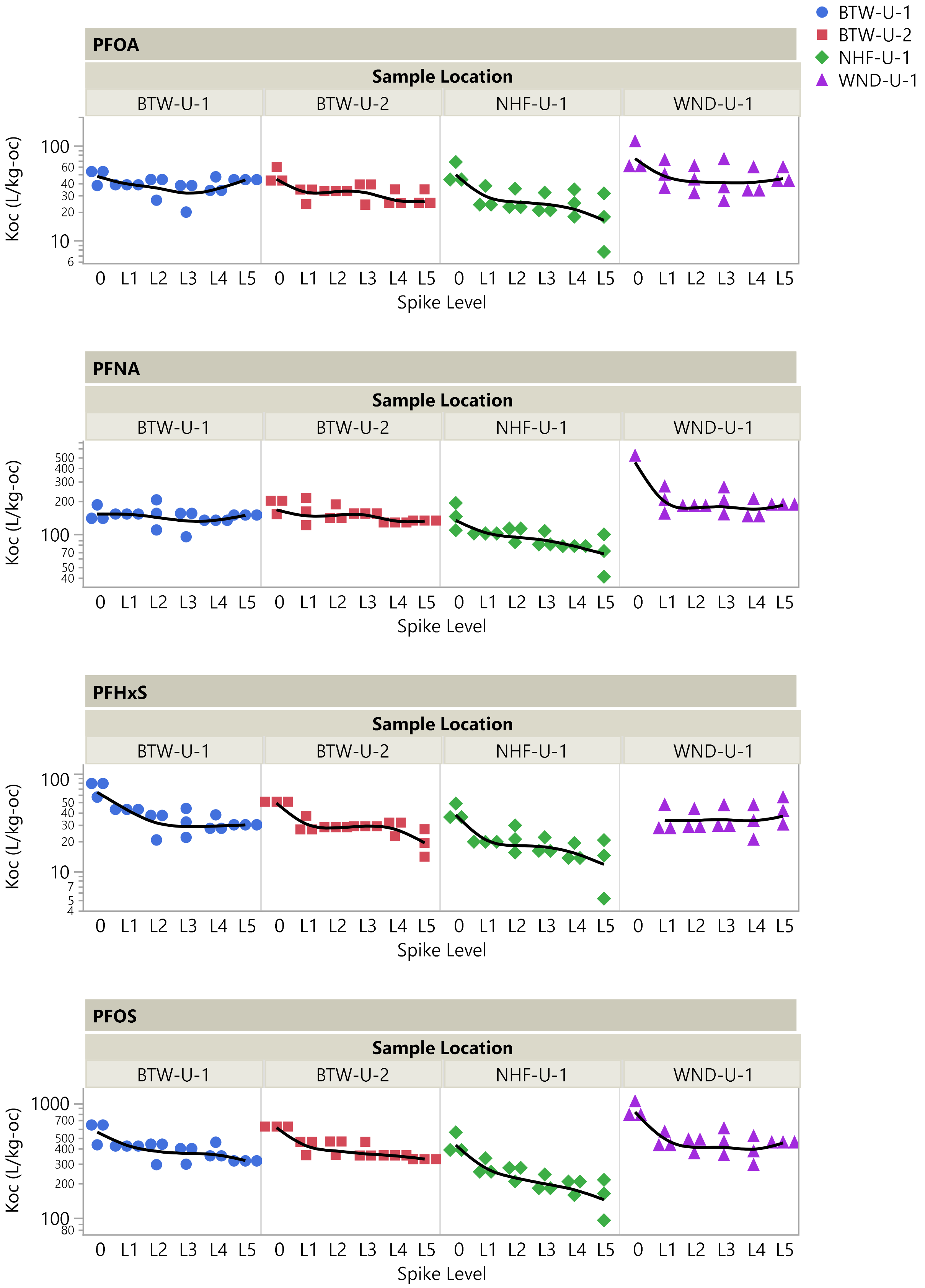
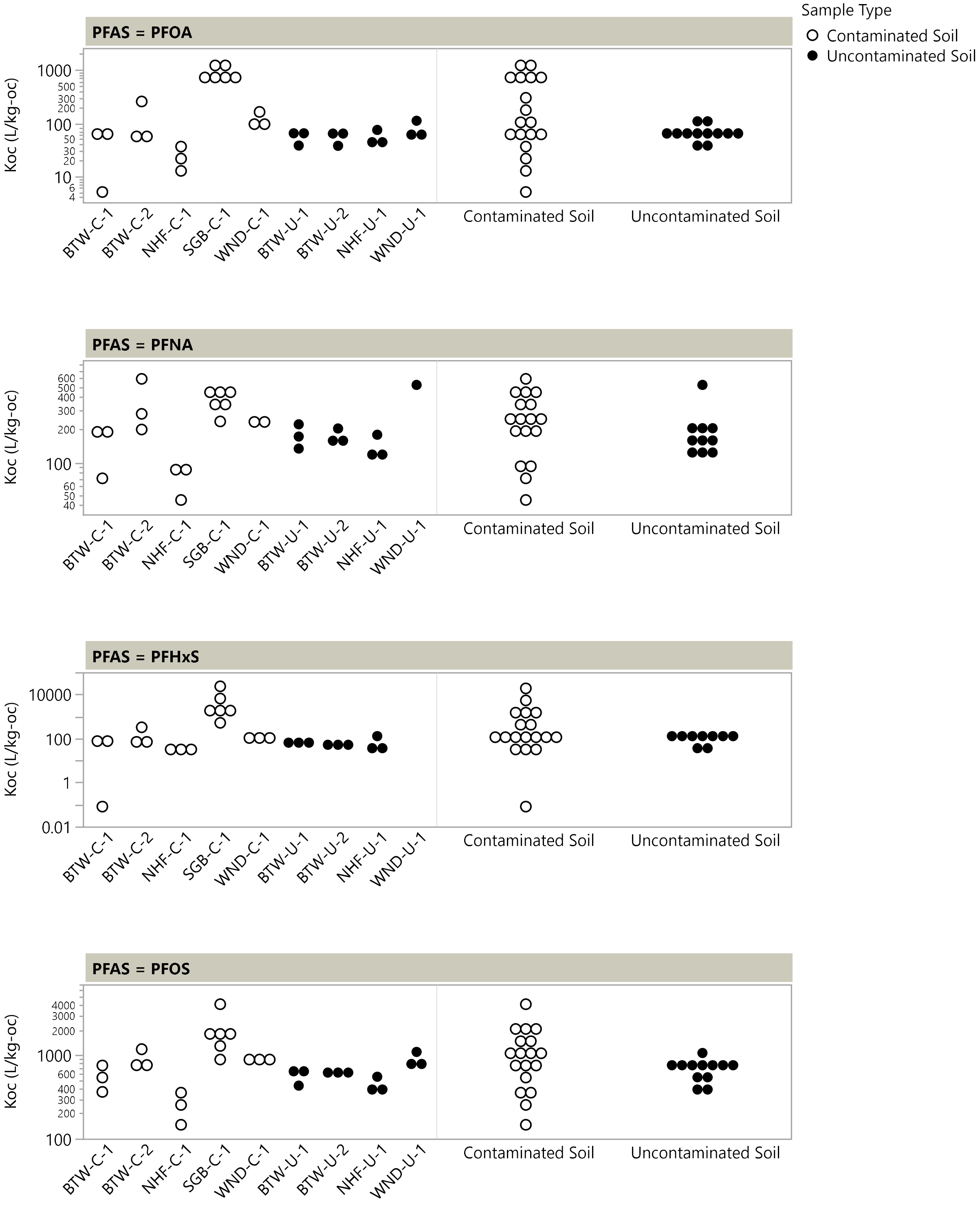
USEPA. 2023. Regional Screening Level (RSL) Chemical-specific Parameters Supporting Table. <web page> Located at: https://www.epa.gov/risk/regional-screening-levels-rsls-generic-tables. Accessed: March 2023

Exhibit A-2 - K_{oc} by Spike Levels



Note: Plotted samples are uncontaminated soil isotherm samples.

Exhibit A-3 – K_{oc} by Contaminated and Uncontaminated Soils



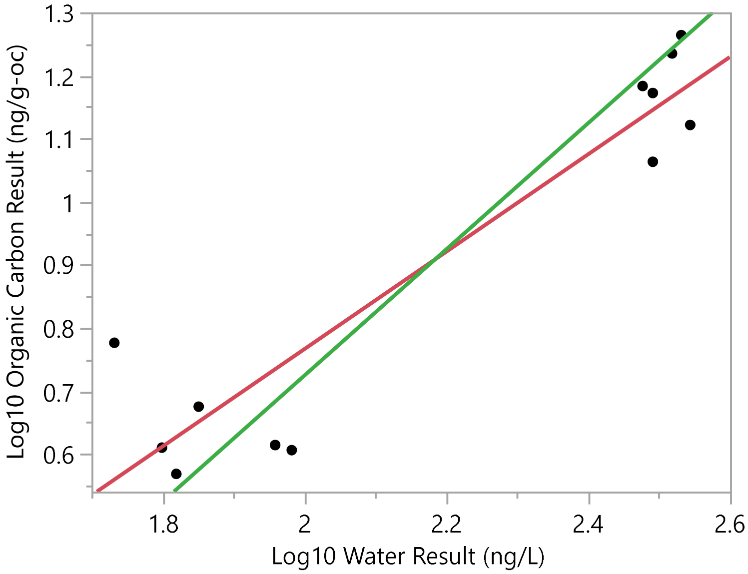
Note: Plotted samples are soil isotherm samples with no spiked PFAS.

Exhibit A-4 – K_{oc} Freundlich Isotherms

PFOA:

$$\log\left(C_{oc}\left[\frac{ng}{g-oc}\right]\right) = 0.772 \times \log\left(C_w\left[\frac{ng}{L}\right]\right) - 0.777,\ p_{slope} = <0.0001,\ p_{intercept} = 0.0034$$

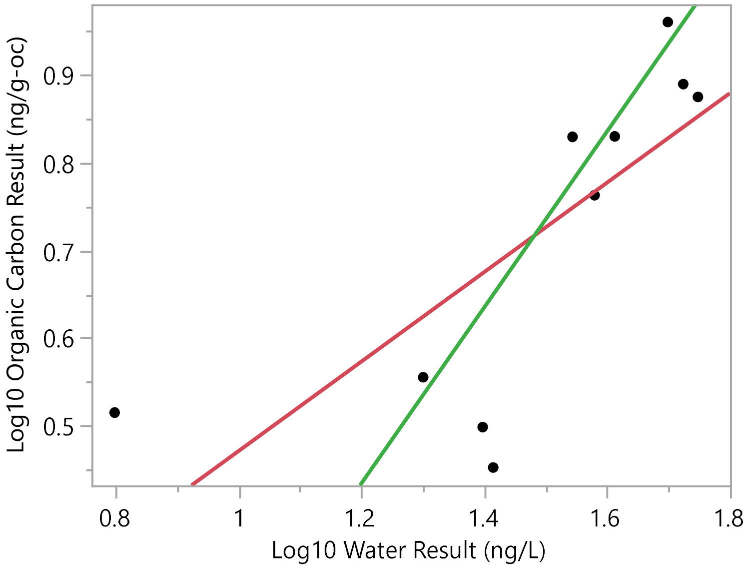
$$\log\left(C_{oc}\left[\frac{ng}{g-oc}\right]\right) = \log\left(C_w\left[\frac{ng}{L}\right]\right) - 1.28,\ p_{intercept} = <0.0001$$



PFNA:

$$\log\left(C_{oc}\left[\frac{ng}{g-oc}\right]\right) = 0.508 \times \log\left(C_w\left[\frac{ng}{L}\right]\right) - 0.0368,\ p_{slope} = 0.0113,\ p_{intercept} = 0.8788$$

$$\log\left(C_{oc}\left[\frac{ng}{g-oc}\right]\right) = \log\left(C_w\left[\frac{ng}{L}\right]\right) - 0.766,\ p_{intercept} = <0.0001$$



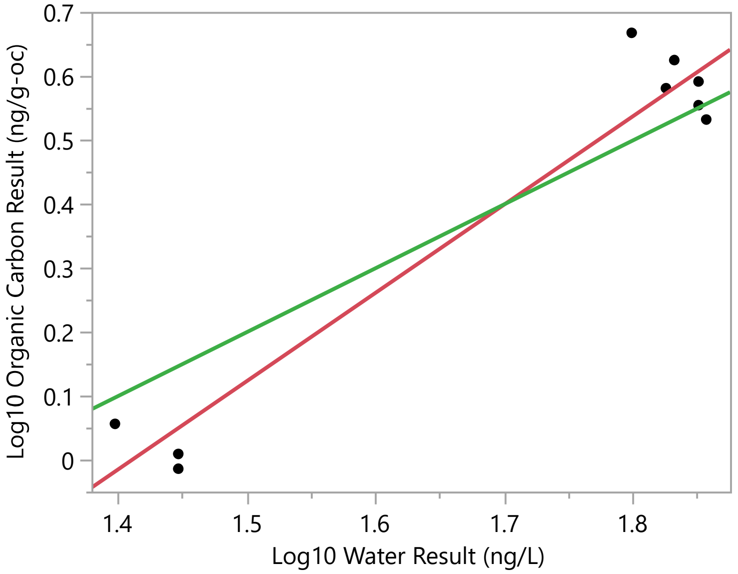
Note: Plotted samples are uncontaminated soil isotherm samples with no spiked PFAS.
The red line shows the non-linear sorption K_{oc} Freundlich isotherm fit (best-fit slope).
The green line shows the linear sorption K_{oc} Freundlich isotherm fit (slope of 1).

Exhibit A-4 continued

PFHxS:

$$\log\left(C_{oc}\left[\frac{ng}{g-oc}\right]\right) = 1.38 \times \log\left(C_{w}\left[\frac{ng}{L}\right]\right) - 1.95\text{ , } p_{slope} = <0.0001\text{, } p_{intercept} = <0.0001$$

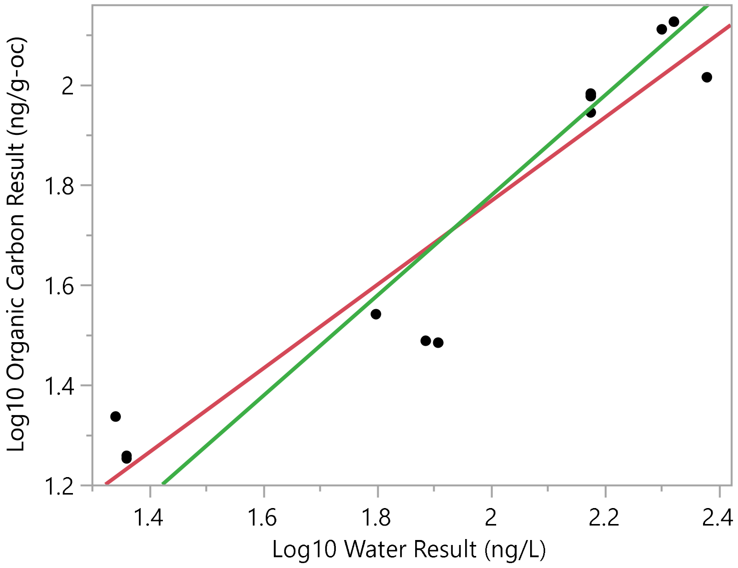
$$\log\left(C_{oc}\left[\frac{ng}{g-oc}\right]\right) = \log\left(C_{w}\left[\frac{ng}{L}\right]\right) - 1.30\text{ , } p_{intercept} = <0.0001$$



PFOS:

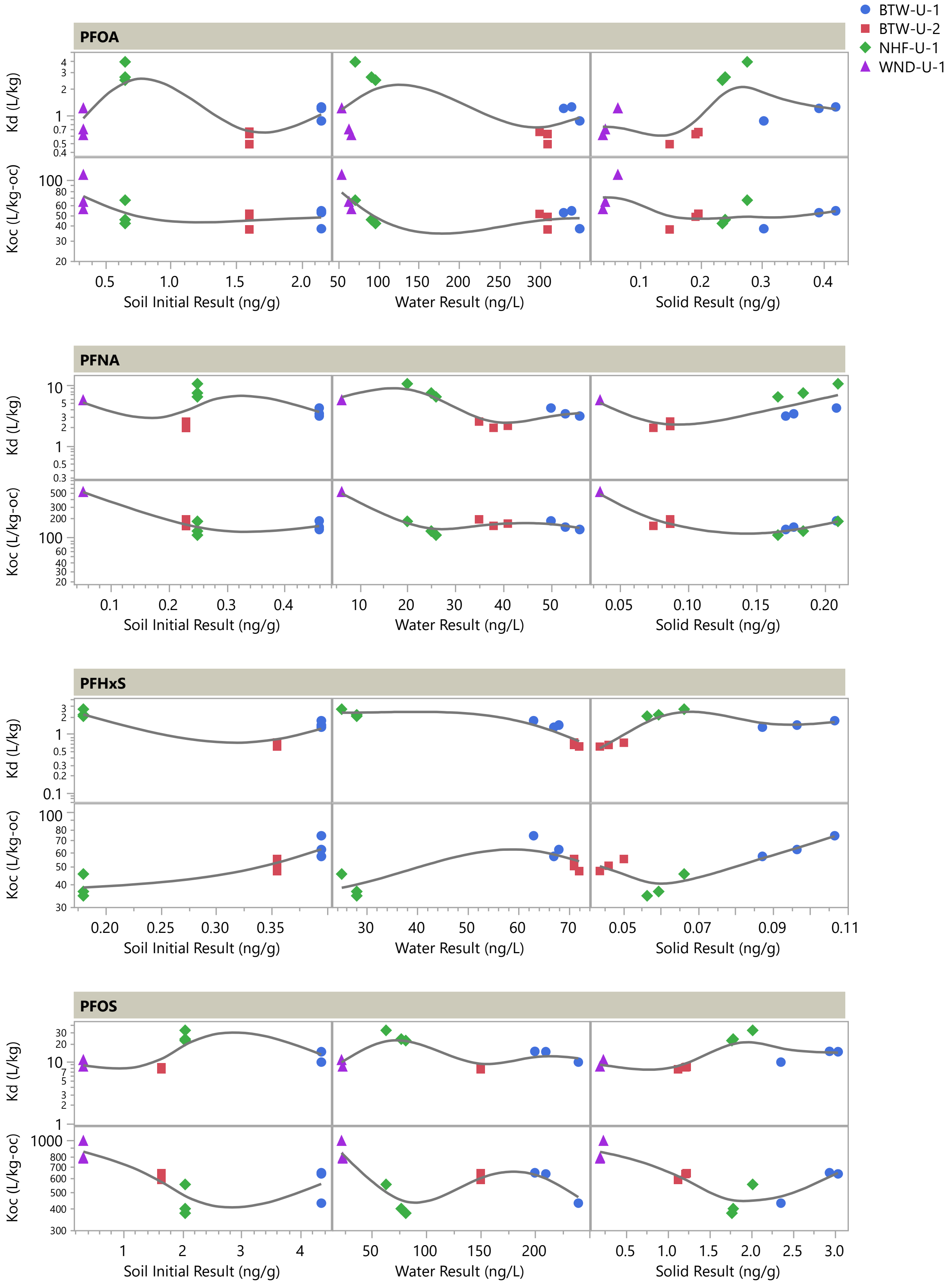
$$\log\left(C_{oc}\left[\frac{ng}{g-oc}\right]\right) = 0.836 \times \log\left(C_{w}\left[\frac{ng}{L}\right]\right) + 0.0926\text{ , } p_{slope} = <0.0001\text{, } p_{intercept} = 0.597$$

$$\log\left(C_{oc}\left[\frac{ng}{g-oc}\right]\right) = \log\left(C_{w}\left[\frac{ng}{L}\right]\right) - 0.225\text{ , } p_{intercept} = <0.0001$$



Note: Plotted samples are uncontaminated soil isotherm samples with no spiked PFAS.
The red line shows the non-linear sorption K_{oc} Freundlich isotherm fit (best-fit slope).
The green line shows the linear sorption K_{oc} Freundlich isotherm fit (slope of 1).

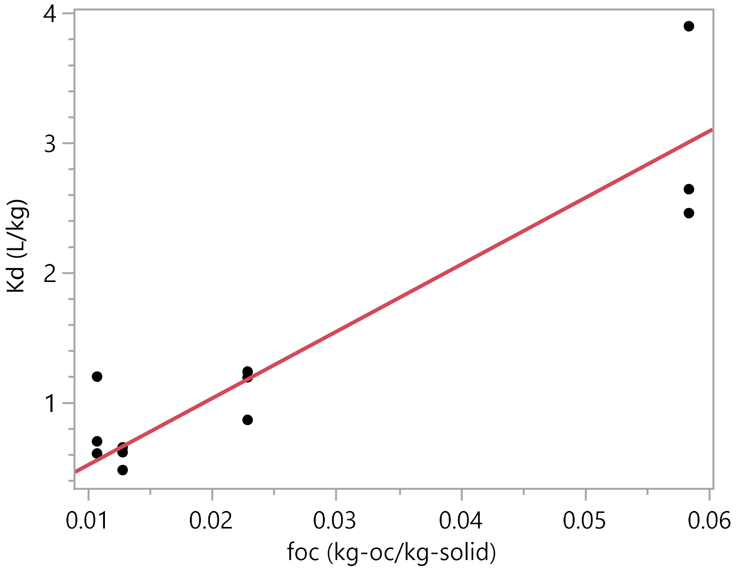
Exhibit A-5 - K_d and K_{oc} by Sample Concentrations



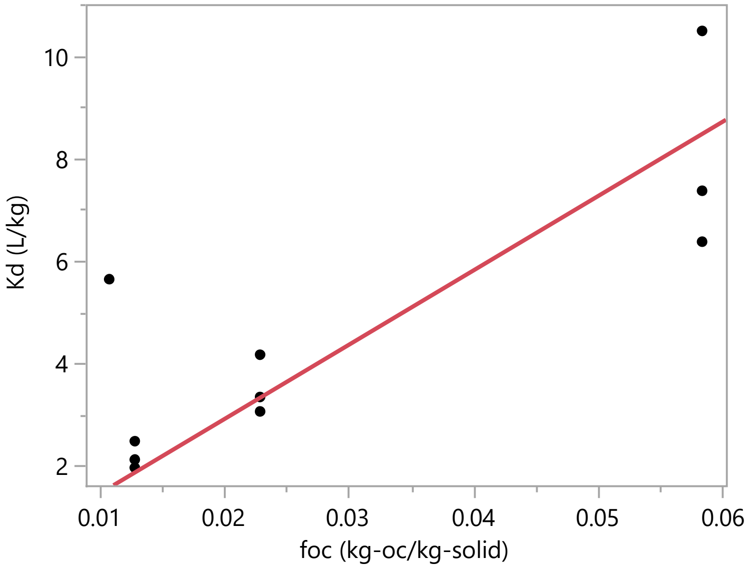
Note: Plotted samples are uncontaminated soil isotherm samples with no spiked PFAS.

Exhibit A-6 – Linear Correlations of K_d and f_{oc}

PFOA: $K_d = 51.4 \frac{L}{kg-oc} \times f_{oc}$ **, p = <0.0001**



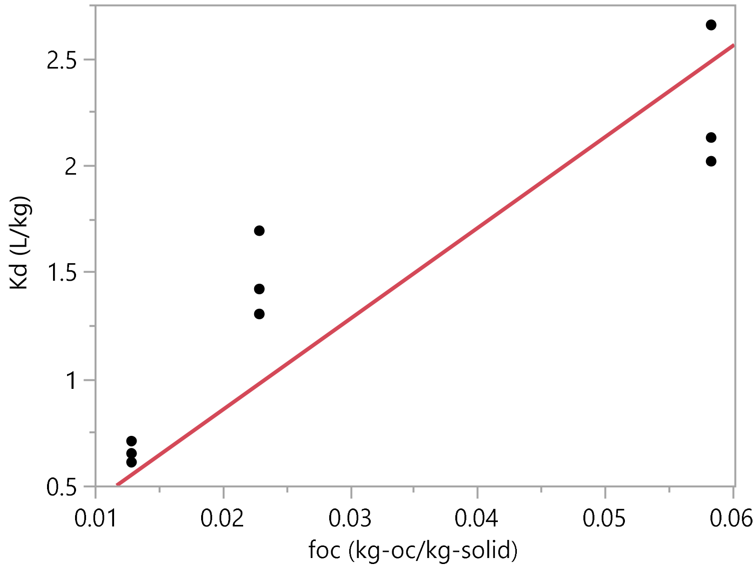
PFNA: $K_d = 145 \frac{L}{kg-oc} \times f_{oc}$ **, p = <0.0001**



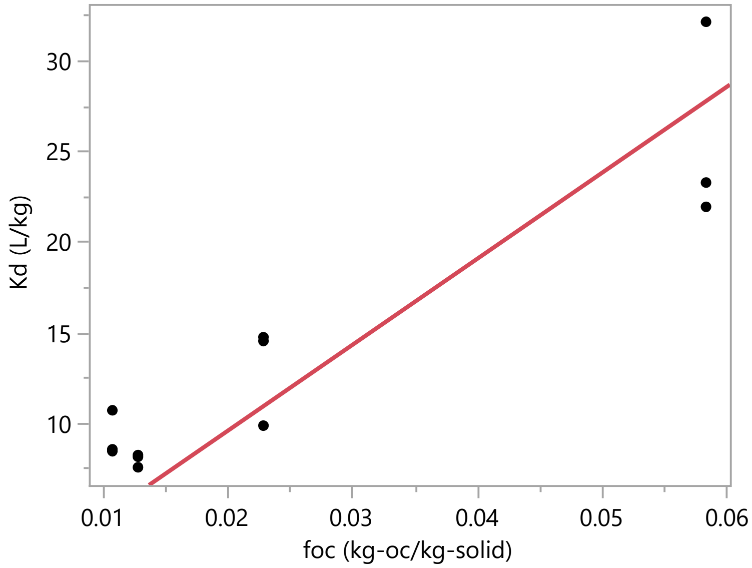
Note: Plotted samples are uncontaminated soil isotherm samples with no spiked PFAS.

Exhibit A-6 continued

PFHxS: $K_d = 42.6\ \frac{L}{kg-oc} \times f_{oc}$ **, p = <0.0001**

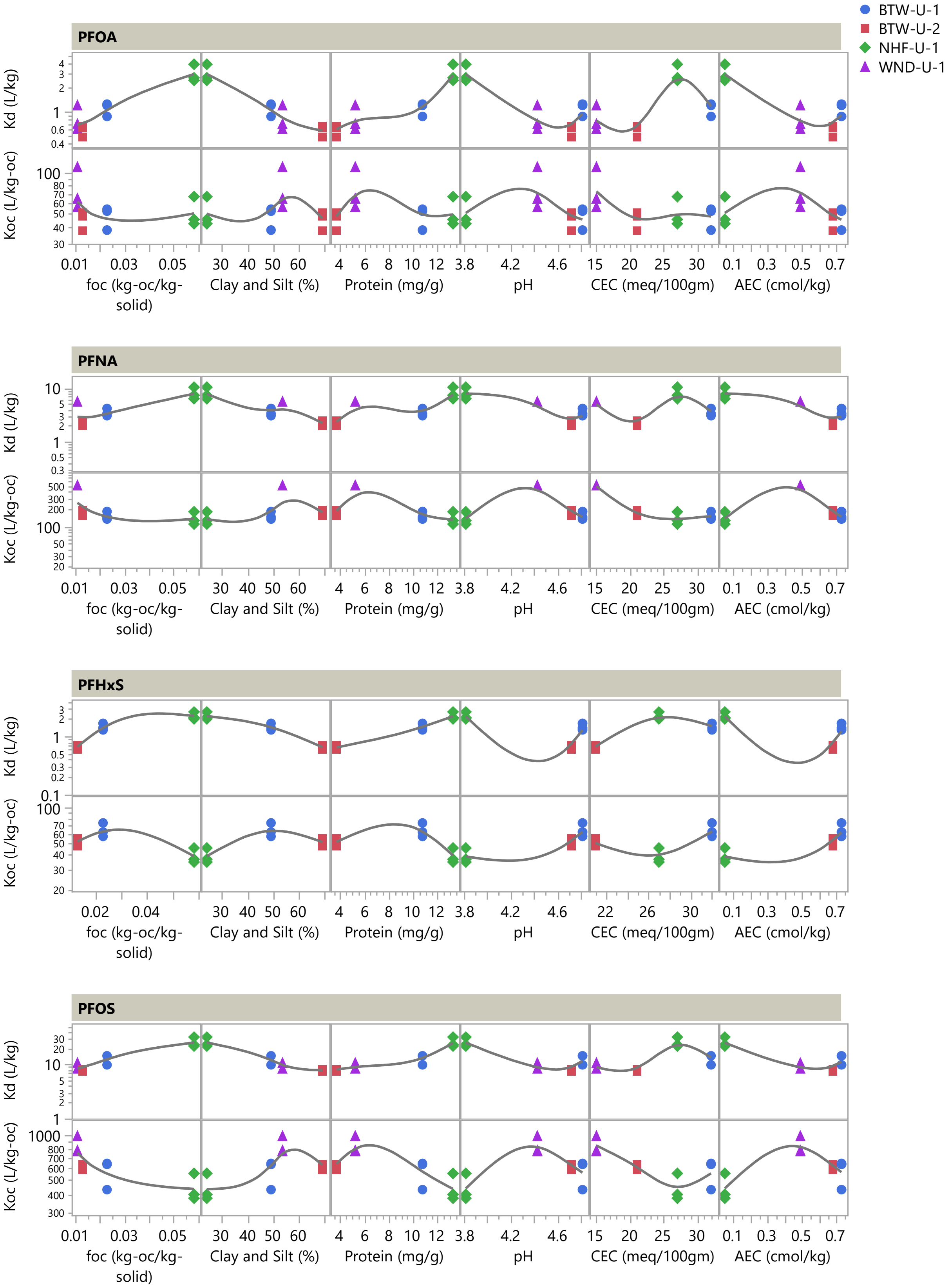


PFOS: $K_d = 475\ \frac{L}{kg-oc} \times f_{oc}$ **, p = <0.0001**



Note: Plotted samples are uncontaminated soil isotherm samples with no spiked PFAS.

Exhibit A-7 - K_d and K_{oc} by Soil Parameters



Note: Plotted samples are uncontaminated soil isotherm samples with no spiked PFAS.

Exhibit A-8 – Selected Median K_{oc} Values and Example Calculated Model K_d Values

PFAS	**Selected Median K_{oc} (L/kg-oc)** ***f_{oc} adjusted for soil moisture***	**Selected Median K_{oc} (L/kg-oc, unadjusted)** ***f_{oc} not adjusted for soil moisture***	**Model Layer f_{oc} (kg-oc/kg)**	**Model Layer K_d (L/kg)** ***Using K_{oc} unadjusted***	**Range of Select 2023 USGS NH Study K_d Values (L/kg)**
PFOA	51	64	0.05	3.2	0.48 to 3.9
			0.01	0.64	
			0.001	0.064	
			0.0001	0.0064	
PFNA	160	200	0.05	10.15	2.0 to 10
			0.01	2.03	
			0.001	0.203	
			0.0001	0.0203	
PFHxS	50	64	0.05	3.2	0.61 to 2.7
			0.01	0.64	
			0.001	0.064	
			0.0001	0.0064	
PFOS	630	800	0.05	40.2	7.5 to 32
			0.01	8.04	
			0.001	0.804	
			0.0001	0.0804	

Notes:
Range of select 2023 USGS NH Study K_d values base on uncontaminated soil isotherm samples with no spiked PFAS. Values rounded to two significant figures.

The table includes median K_{oc} values based on f_{oc} values that were not adjusted for soil moisture. These "unadjusted" K_{oc} values were calculated for and used in the modeling prior to Sanborn Head being aware that soil organic content data were reported on a wet-weight basis. See Appendix A Section A.5 for additional information.

Appendix B

MODFLOW Input Parameter Values

Appendix B
MODFLOW-USG Transport Model
Model Grid Setup and Selection of Input Parameter Values

Grid Setup

The MODFLOW-USG Transport model is setup as a five-layer model, with layers 1 to 4 being representative of vadose zone soils (analogous to SESOIL component of the SEVIEW model), and layer 5 being representative of fully saturated groundwater conditions (analogous to the AT123D component of the SEVIEW model). As summarized in Exhibit B-1, to replicate the model grid setup used in the SEVIEW model simulations, a three meters thick vadose zone is assigned to model layers 1 to 4 (model elevation of 20 to 23 meters), and the underlying aquifer (model layer 5) has a thickness of 20 meters for scenario 1 (elevation of 0 to 20 meters), or reduced thickness of 10 meters for scenarios 2 to 6 (elevation of 10 to 20 meters). Using the MODFLOW USG Transport unstructured grid function, each parent layer was divided into sublayers having a thickness of 10 centimeters (cm).

Exhibit B.1 Summary of MODFLOW-USG Transport Model Grid Setup

Parent Layer #	No. of USG Sublayers	Layer Top Elevation (meters)	Layer Bottom Elevation (meters)	Subsurface Zone
1	2	23	22.8	Vadose Zone Soil
2	8	22.8	22	
3	10	22	21	
4	10	21	20	
5	10 or 20	20	10 or 0	Aquifer

In the horizontal dimension, the MODFLOW-USG Transport model is assigned a parent grid with model cells that are 10-by-10 meters with 10 grid cells in the east-west direction (x-axis) and 9 grid cells in the north-south directions (y-axis), such that the full grid has dimensions of 100-by-90 meters. Each model cell in the parent grid was subsequently refined using the MODFLOW USG Transport unstructured grid function to have sub-cells with dimensions of 1-by-1 meters.

Stress Periods and Time-Steps for Transient Models

Transient flow and transport simulations were performed for each scenario. Time was divided into 120 monthly stress periods (for a total simulation duration of 10 years). Each stress period was 30.4 days in length and was divided into 10 time-steps with a 1.2 time-step multiplier.

MODFLOW-USG Transport Model Input Parameters

Hydraulic Conductivity

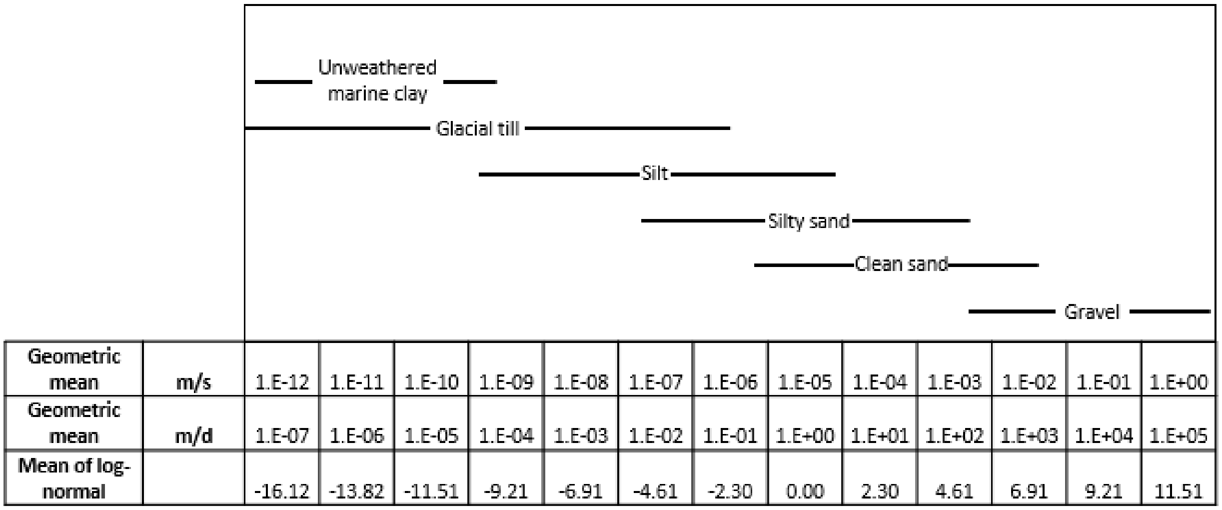
For model simulations with homogeneous (i.e., a constant value in an area and by depth in a layer) soil properties (Scenarios 1 to 3) a value of 8.64 meters per day was assigned to the horizontal hydraulic conductivity (i.e., equivalent to the 0.36 meters per hour applied in the AT123D simulations). Each simulation uses a 10 to 1 horizontal to vertical anisotropy (e.g., with a horizontal hydraulic conductivity of 8.64 meters per day) resulting in the vertical hydraulic conductivity being set to 0.864 meters per day. Models that included simulation of heterogeneous soils (Scenarios 4 to 6), which are further described below, also assumed a 10 to 1 anisotropy ratio.

Statistical Approximation of Hydraulic Conductivity for Heterogeneous Soils
When simulating groundwater flow in a model, one approach is to use a simplified representation of soil hydraulic conductivity by applying a single uniform value as described above for homogeneous soil. In the environment, soil properties do not conform to a single value, but can be defined by a range of values (i.e., a heterogenous soil). Heterogeneous soil can be defined as a soil that has physical properties (e.g., hydraulic conductivity) that are variable across an area and/or by depth in a soil profile. Some models (including MODFLOW-USG Transport) have the ability to represent the variable properties of a heterogeneous soil. According to Groundwater (Freeze and Cherry, 1979), one approach that can be used to define the properties of a heterogenous soil is described as follows:

> *Many hydrogeologists and petroleum geologists have used statistical distributions to provide a quantitative description of the degree of heterogeneity in a geological formation. There is now a large body of direct evidence to support the statement that the probability density function for hydraulic conductivity is log-normal. Warren and Price (1961) and Bennion and Griffiths (1966) found this to be the case in oilfield reservoir rocks, and Willardson and Hurst (1965) and Davis (1969) support the conclusion for unconsolidated water-bearing formations. A log-normal distribution for K is one for which a parameter Y, defined as Y = log K, shows a normal distribution. Freeze (1975) provides a table, based on the references above, that shows the standard deviation on Y (which is independent of the units of measurement) is usually in the range 0.5–1.5. This means that K values in most geological formations show internal heterogeneous variations of 1–2 orders of magnitude. Trending heterogeneity within a geological formation can be thought of as a trend in the mean value of the probability distribution. The same standard deviation may be evident in measurements at different positions in the formation, but the trending means lead to an increase in the overall observed range for the formation.*

The arithmetic mean of the log-normal data is equivalent to the natural logarithm of the geometric mean of the original data. For example, soil that has a geometric mean of 10 meters/day has a value of 2.30 for the arithmetic mean of the logs.

Exhibit B-2: Summary of the relationship between geometric mean and log-normal mean hydraulic conductivity values, with typical ranges of hydraulic conductivity values for different soil types provided for reference (adapted from Freeze and Cherry, 1979).



Geometric mean	m/s	1.E-12	1.E-11	1.E-10	1.E-09	1.E-08	1.E-07	1.E-06	1.E-05	1.E-04	1.E-03	1.E-02	1.E-01	1.E+00
Geometric mean	m/d	1.E-07	1.E-06	1.E-05	1.E-04	1.E-03	1.E-02	1.E-01	1.E+00	1.E+01	1.E+02	1.E+03	1.E+04	1.E+05
Mean of log-normal		-16.12	-13.82	-11.51	-9.21	-6.91	-4.61	-2.30	0.00	2.30	4.61	6.91	9.21	11.51

As summarized in Exhibit B-3, we identified a series of values for standard deviation of the log-normal distribution, which when applied can be used to generate datasets with approximate order-of-magnitude ranges.

Exhibit B-3: Summary of Standard Deviation Values for Log-Normal Dataset and Resulting Order of Magnitude Ranges

Order of Magnitude	Zero	One	Two	Three
Standard Deviation of the Log-Normal Dataset	0.1	0.5	0.8	1.2

For each model simulation with a heterogeneous soil, we created log-normal datasets using Excel's log-normal distribution function and Excel's function for generation of random numbers. The mean and standard deviation of the log-normal distribution is defined for each dataset using the approach described above. Specific values selected for each model scenario are summarized in the following exhibits.

Exhibit B-4: Scenario 4 - Heterogeneous Sand

Soil Type	Geometric mean (meters/day)	Parameters of Log-Normal Distribution		Calculated Statistics for Dataset of Randomly Generated Values of Log-Normal Distribution			
		Mean	Standard Deviation	Lower value	Mean	Geometric Mean	Upper value
Sand	10	2.3	0.5	2.7	11	10	41

Exhibit B-5: Scenario 5 - Heterogeneous Layered Silt and Sand

Soil Type	Geometric mean (meters/day)	Parameters of Log-Normal Distribution		Calculated Summary Statistics for Dataset of Randomly Generated Values of Log-Normal Distribution			
		Mean	Standard Deviation	Lower value	Mean	Geometric Mean	Upper value
Silt	0.1	-2.3	0.5	0.018	0.11	0.10	0.74
Fine Sand	1	0	0.8	0.079	1.4	1.0	8.4

Coarse Sand	10	2.3	0.5	2.7	11	10	41

Exhibit B-6: Scenario 6 - Heterogeneous Sand over Till

Soil Type	Geometric mean (meters/day)	Parameters of Log-Normal Distribution		Calculated Statistics for Dataset of Randomly Generated Values of Log-Normal Distribution			
		Mean	Standard Deviation	Lower value	Mean	Geometric Mean	Upper value
Sand	1	0	0.8	0.024	1.4	1.0	33
Till	1E-5	-11.5	1.2	3.6E-8	2.1E-5	1.0E-5	0.0029

Dispersivity Values

Dispersivity values are applied in the model simulations for horizontal (longitudinal and transverse) and vertical dispersivity. To replicate the Subsurface Release CSM simulated in SEVIEW, model scenario 1 uses dispersivity values of 20 meters, 2 meters, and 2 meters. To replicate the Surface Release CSM simulated in SEVIEW, each of the subsequent scenarios 2 to 6 applies a commonly used empirical method to define horizontal (longitudinal) dispersivity based on length of contaminant flow path (X), which was established by Xu & Eckstein (1995) where:

Longitudinal Dispersivity (D_L) = $0.83 \times \log_{10}(X)^{2.414}$
And X is in units of meters.

Transverse Dispersivity (D_T) is commonly assigned a value of one tenth of the longitudinal dispersivity (Gelhar et al., 1992 in BIOSCREEN, 1996), and the vertical dispersivity a value of one hundredth of the longitudinal dispersivity.

Using the above method, for a groundwater transport length (X) of 10 meters (i.e., distance between edge of source area and the downgradient point of compliance), the longitudinal dispersivity is 0.83 meters; transverse dispersivity of 0.083 meters; and vertical dispersivity of 0.0083 meters.

Water-solid distribution coefficient (K_d) values

MODFLOW-USG Transport model simulations used a soil-water partition coefficient (K_d) value based on an organic carbon adsorption coefficient (K_{oc}) value for PFOA of 64 L/kg, and a soil fraction organic carbon (f_{oc}) of either 0.1% or 5%, i.e., the same values used for PFOA and f_{oc} in the Subsurface Release CSM and Surface Release CSM in the SEVIEW model simulations. Model scenario 1 assumes a constant f_{oc} of 0.1% with resulting K_d value of 6.4E-5 m^3/kg. Model scenarios 2 to 6 simulate a higher f_{oc} soil of 5% in model layer 1 (K_d value of 0.0032 m^3/kg), and lower f_{oc} soil of 0.1% in model layers 2 to 5 (K_d value of 6.4E-5 m^3/kg).

Vadose Zone Parameters

Simulation of vadose zone flow in MODFLOW-USG Transport implements the Richards Equation with the van Genuchten function for moisture retention and the Brooks Corey function for relative permeability. In Groundwater Vistas, the parameters required to implement vadose zone flow include the van Genuchten parameters (Alpha, Beta), the Brooks-Corey exponent, and residual saturation. We note that the van Genuchten parameters defined as alpha (α) and beta (β) in MODFLOW-USG Transport are often defined with alpha (α) having the same symbol, but with beta defined by the symbol "n". In addition, the Brooks-Corey exponent in MODFLOW-USG Transport is often defined in literature by the symbol "*p*".

Tabulated parameter values are provided below for a range of USDA soil types. The van Genuchten parameters (α and *n*), and residual saturation values are based on recommended mean values selected from probability distributions for vadose zone soil hydraulic parameters provided in the U.S. Nuclear Regulatory Commission report titled Uncertainty Analyses of Infiltration and Subsurface Flow and Transport for SDMP Sites (U.S. Nuclear Regulatory Commission, 1997). We note that the Brooks Corey exponent is often defined in literature using the relationship developed by Corey (1977) for conversion of van Genuchten parameters to Brooks-Corey parameters and vice-versa. To obtain the Brooks-Corey exponent (*p*), the van Genuchten "*m*" parameter is first defined by the relationship m = 1 – (1/*n*), and subsequently, the Brooks-Corey exponent (*p*) is defined by the relationship *p* = 1 + (2/*m*).

Exhibit B-7: Summary of Representative Vadose Zone Soil Hydraulic Parameters [adapted from U.S. Nuclear Regulatory Commission (1997)]

USDA Soil Type	Van Genuchten			Brooks Corey	Residual Saturation
	α	n	m	p	θ_r
	1/cm	(-)	(-)	(-)	(-)
Sand	0.147	2.67	0.625	4.198	0.0466
Loamy Sand	0.125	2.27	0.559	4.575	0.0569
Sandy Loam	0.0757	1.89	0.471	5.247	0.0644
Sandy Clay Loam	0.0572	1.48	0.324	7.167	0.101
Loam	0.0367	1.56	0.359	6.571	0.0776
Silt Loam	0.0193	1.41	0.291	7.878	0.067
Silt	0.0178	1.38	0.275	8.263	0.0352
Clay Loam	0.019	1.32	0.242	9.250	0.0954
Silty Clay Loam	0.0104	1.23	0.187	11.696	0.088
Sandy Clay	0.027	1.28	0.219	10.143	0.0993
Silty Clay	0.00413	1.16	0.138	15.500	0.0706
Clay	0.00618	1.13	0.115	18.385	0.0685

Saturated Zone - Bulk Density/Porosity/Specific Yield/Specific Storage

Each model simulation performed with MODFLOW-USG Transport used a constant set of values for the bulk density, porosity, specific yield, and specific storage parameters. Consistent with the SEVIEW model simulations, a porosity fraction of 0.3, and a bulk density of 1,300 kg/m^3, was assigned for each model simulation. A specific yield (Sy) value of 0.2, and a specific storage (Ss) value of 5E-5 was assigned based on typical literature values for a sand soil (Freeze and Cherry, 1979).

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