# MODIFIED SESOIL MODEL FOR SIMULATING PFAS TRANSPORT IN THE VADOSE ZONE

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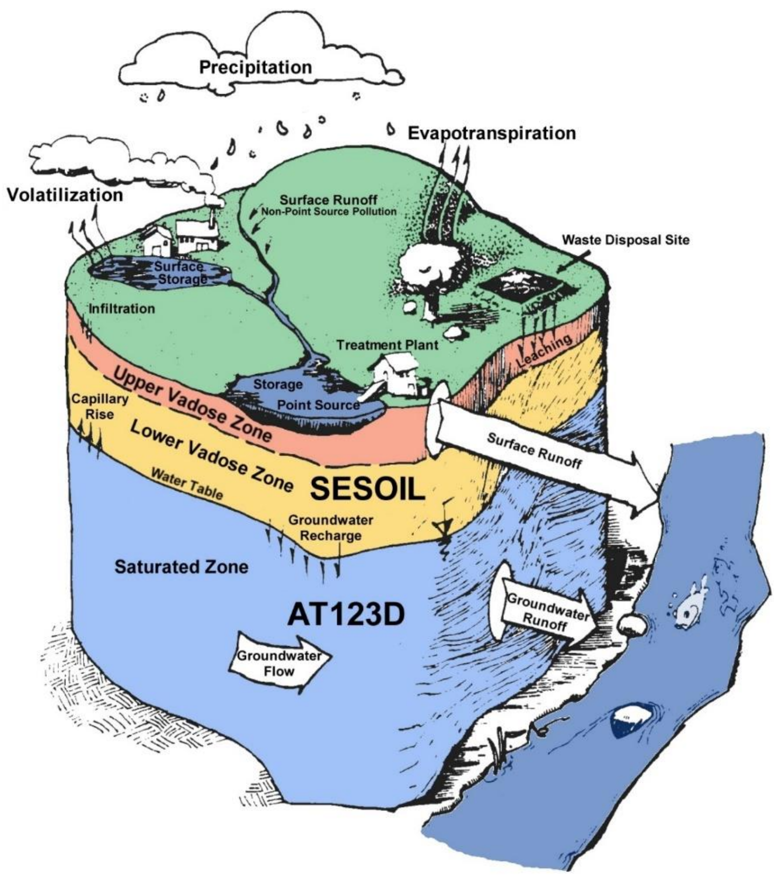
September 23, 2024

# SESOIL
## Vadose Zone




**SE**asonal **SOIL** model (1981)

**Marcos Bounazountas**
**Janet Wagner**
Arthur D. Little, Inc.

For the
U.S. EPA Office of Toxic Substances

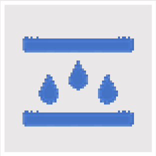
**Used by state agencies to establish soil leaching standards protective of groundwater quality**

# SESOIL Hydrologic Cycle

**Surface Water Runoff**

**Infiltration**

**Evapotranspiration**



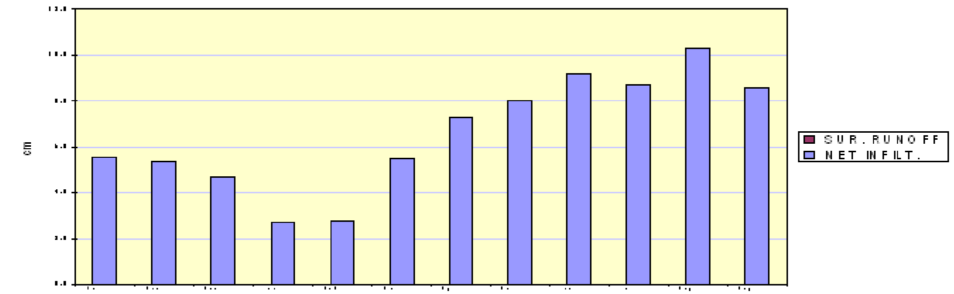
**Soil Moisture**

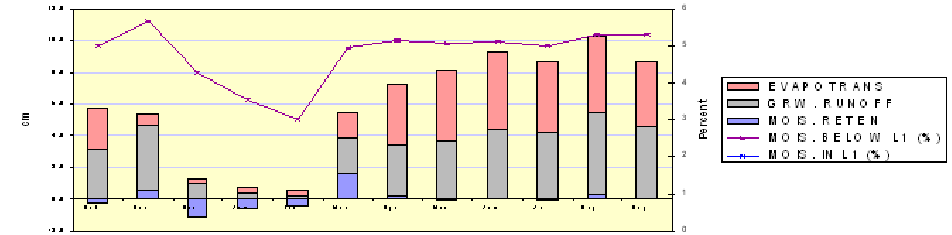
**Groundwater Recharge**

## SESOIL Hydrologic Cycle Report

**Scenario Description:** Benzene with default data

**SESOIL Output File:** C:\SEATPRG7\BENZ01.OUT




| | Surface Water Runoff | | Net Infiltration | | Evapotranspiration | | Soil Moisture Retention | | Groundwater Runoff (Recharge) | | Soil Moisture Layer 1 | Soil Moisture Below Layer 1 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Units | cm | Inches | cm | Inches | cm | Inches | cm | Inches | cm | Inches | Percent | Percent |
| **October** | 0.00 | 0.00 | 5.52 | 2.17 | 2.59 | 1.02 | -0.04 | -0.02 | 2.97 | 1.17 | 4.95 | 4.95 |
| **November** | 0.00 | 0.00 | 5.27 | 2.07 | 0.71 | 0.28 | 0.58 | 0.23 | 3.98 | 1.57 | 5.65 | 5.65 |
| **December** | 0.00 | 0.00 | 0.11 | 0.04 | 0.30 | 0.12 | -1.17 | -0.46 | 0.97 | 0.38 | 4.25 | 4.25 |
| **January** | 0.00 | 0.00 | 0.10 | 0.04 | 0.30 | 0.12 | -0.60 | -0.24 | 0.41 | 0.16 | 3.53 | 3.53 |
| **February** | 0.00 | 0.00 | 0.13 | 0.05 | 0.30 | 0.12 | -0.42 | -0.17 | 0.24 | 0.09 | 3.03 | 3.03 |
| **March** | 0.00 | 0.00 | 5.47 | 2.15 | 1.65 | 0.65 | 1.60 | 0.63 | 2.22 | 0.87 | 4.95 | 4.95 |
| **April** | 0.00 | 0.00 | 7.28 | 2.87 | 3.83 | 1.51 | 0.17 | 0.07 | 3.28 | 1.29 | 5.15 | 5.15 |
| **May** | 0.00 | 0.00 | 8.04 | 3.17 | 4.43 | 1.74 | -0.06 | -0.02 | 3.68 | 1.45 | 5.08 | 5.08 |
| **June** | 0.00 | 0.00 | 9.24 | 3.64 | 4.81 | 1.89 | 0.04 | 0.02 | 4.39 | 1.73 | 5.13 | 5.13 |
| **July** | 0.00 | 0.00 | 8.55 | 3.37 | 4.41 | 1.74 | -0.10 | -0.04 | 4.24 | 1.67 | 5.00 | 5.00 |
| **August** | 0.00 | 0.00 | 10.30 | 4.06 | 4.87 | 1.92 | 0.25 | 0.10 | 5.17 | 2.04 | 5.30 | 5.30 |
| **September** | 0.00 | 0.00 | 8.62 | 3.39 | 4.03 | 1.59 | 0.00 | 0.00 | 4.59 | 1.81 | 5.30 | 5.30 |
| **Total** | 0.00 | 0.00 | 68.62 | 27.01 | 32.23 | 12.69 | 0.25 | 0.10 | 36.14 | 14.23 | | |

# SESOIL Pollutant Cycle

**Mass Balance**

**Leachate Concentration**

**Migration Depth**

## SESOIL Pollutant Cycle Report

**Scenario Description:** Benzene with default data

**SESOIL Output File:** C:\SEATPRG7\BENZ01.OUT

| SESOIL Process | Pollutant Mass (µg) | Percent of Total |
|---|---|---|
| Volatilized | 3.206E+07 | 94.30 |
| In Soil Air | 3.025E+01 | 0.00 |
| Sur. Runoff | 0.000E+00 | 0.00 |
| In Washld | 0.000E+00 | 0.00 |
| Ads On Soil | 6.161E+01 | 0.00 |
| Hydrol Soil | 0.000E+00 | 0.00 |
| Degrad Soil | 0.000E+00 | 0.00 |
| Pure Phase | 0.000E+00 | 0.00 |
| Complexed | 0.000E+00 | 0.00 |
| Immobile CEC | 0.000E+00 | 0.00 |
| Hydrol CEC | 0.000E+00 | 0.00 |
| In Soil Moi | 3.510E+01 | 0.00 |
| Hydrol Mois | 0.000E+00 | 0.00 |
| Degrad Mois | 0.000E+00 | 0.00 |
| Other Trans | 0.000E+00 | 0.00 |
| Other Sinks | 0.000E+00 | 0.00 |
| Gwr. Runoff | 1.934E+06 | 5.69 |
| Total Output | 3.399E+07 | 99.99 |
| Total Input | 3.400E+07 | |
| Input - Output | 2.160E+03 | |

**Maximum leachate concentration:** 3.421E-01 **mg/l**

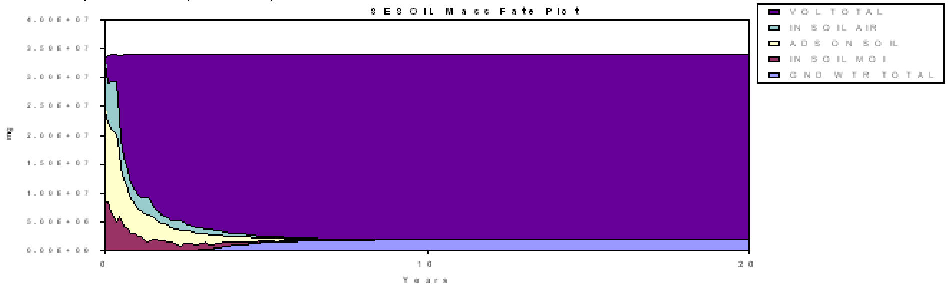
**Climate File:** MADISON, DANE COUNTY AIRPORT
C:\SEATPRG7\MADISON.CLM

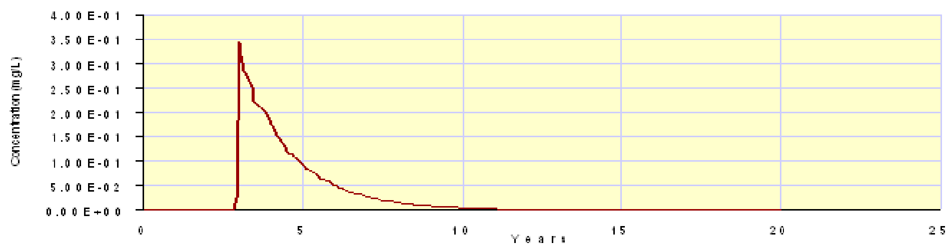
**Chemical File:** Benzene
C:\SEATPRG7\BENZENE.CHM

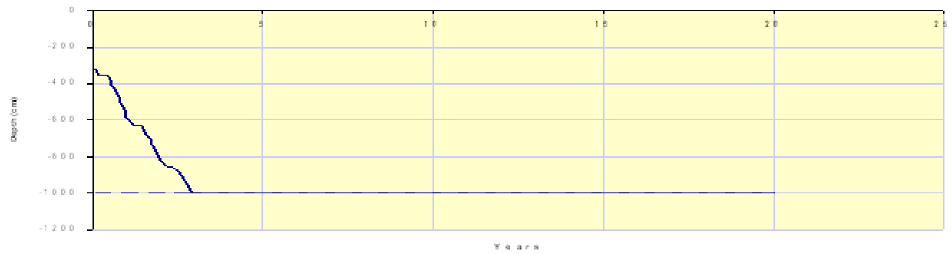
**Soil File:** Sand, Perm = 1.00E-3 cm/sec
C:\SEATPRG7\SAND.SOI

**Application File:** SEVIEW Default Application Parameters
C:\SEATPRG7\DEFAULT.APL

**Starting Depth:** 324.90 **cm**
**Ending Depth:** 1000.00 **cm**
**Total Depth:** 1000.00 **cm**

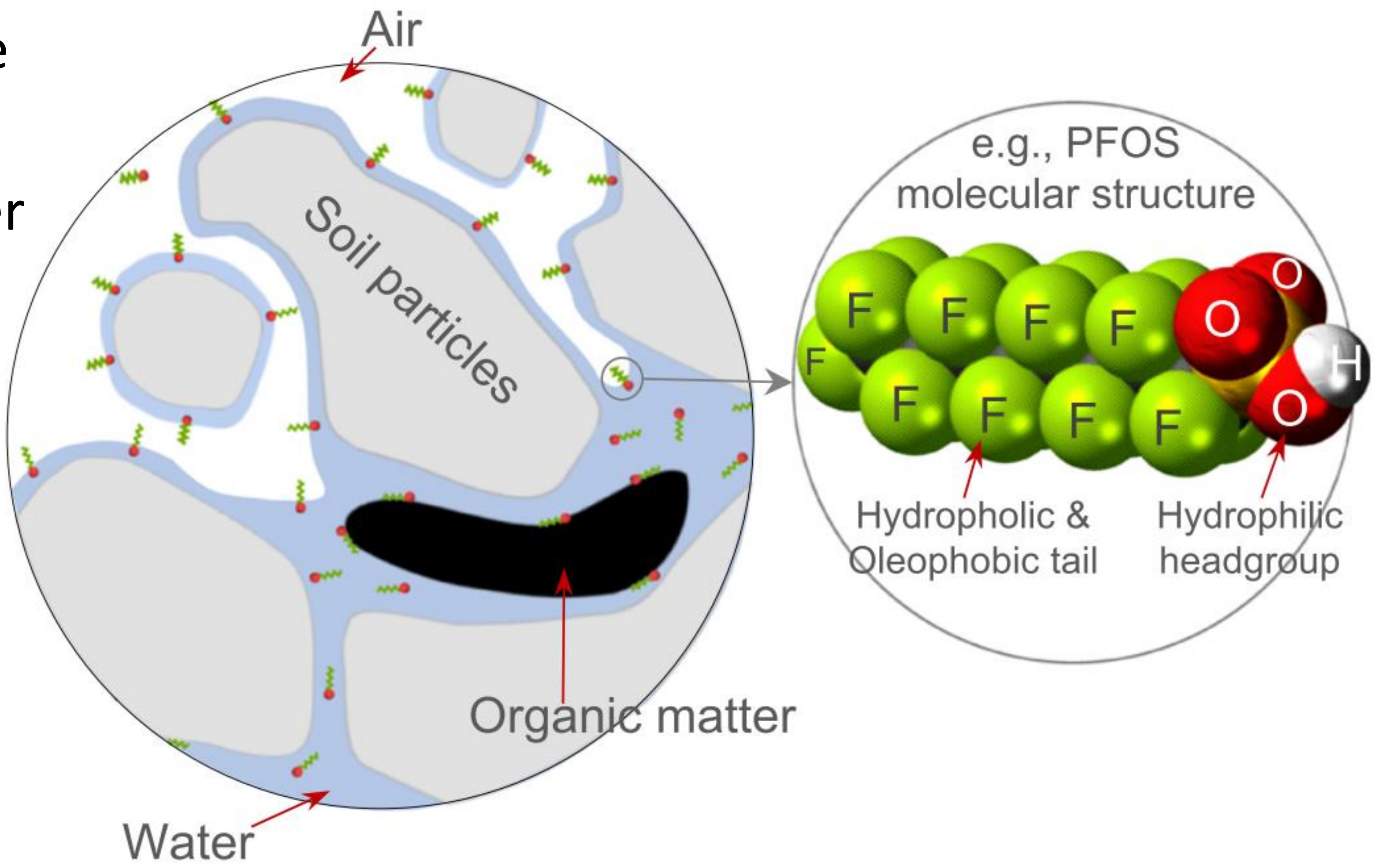


# PFAS in the Vadose Zone

- Adsorption of PFAS in the vadose zone is complex
- Can occur at the air-water interfacial areas
- Existing models may not be appropriate




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

# PFAS leaching standards using SESOIL

**Massachusetts Department of Environmental Protection**

**Maine Department of Environmental Protection**

**New Hampshire Department of Environmental Services**

- SESOIL was modified to simulate the transport of PFAS in the vadose zone
- Suggested by Nihar Mohanty at the Mass DEP

# PFAS concentration adsorbed at the air-water interfacial areas

$$C_{aw} = A_{aw} K_{aw} C^{\frac{1}{f_{aw}}}$$

| Parameter | Description |
|---|---|
| $C_{aw}$ | Contaminant concentration adsorbed at the air-water interfacial areas (μg/g), |
| $A_{aw}$ | Air-water interfacial areas ($cm^2/cm^3$), |
| $K_{aw}$ | Contaminant air-water interfacial adsorption coefficient ($cm^3/cm^2$), |
| $C$ | Contaminant concentration in soil water (μg/ml), |
| $f_{aw}$ | $K_{aw}$ Freundlich exponent. |

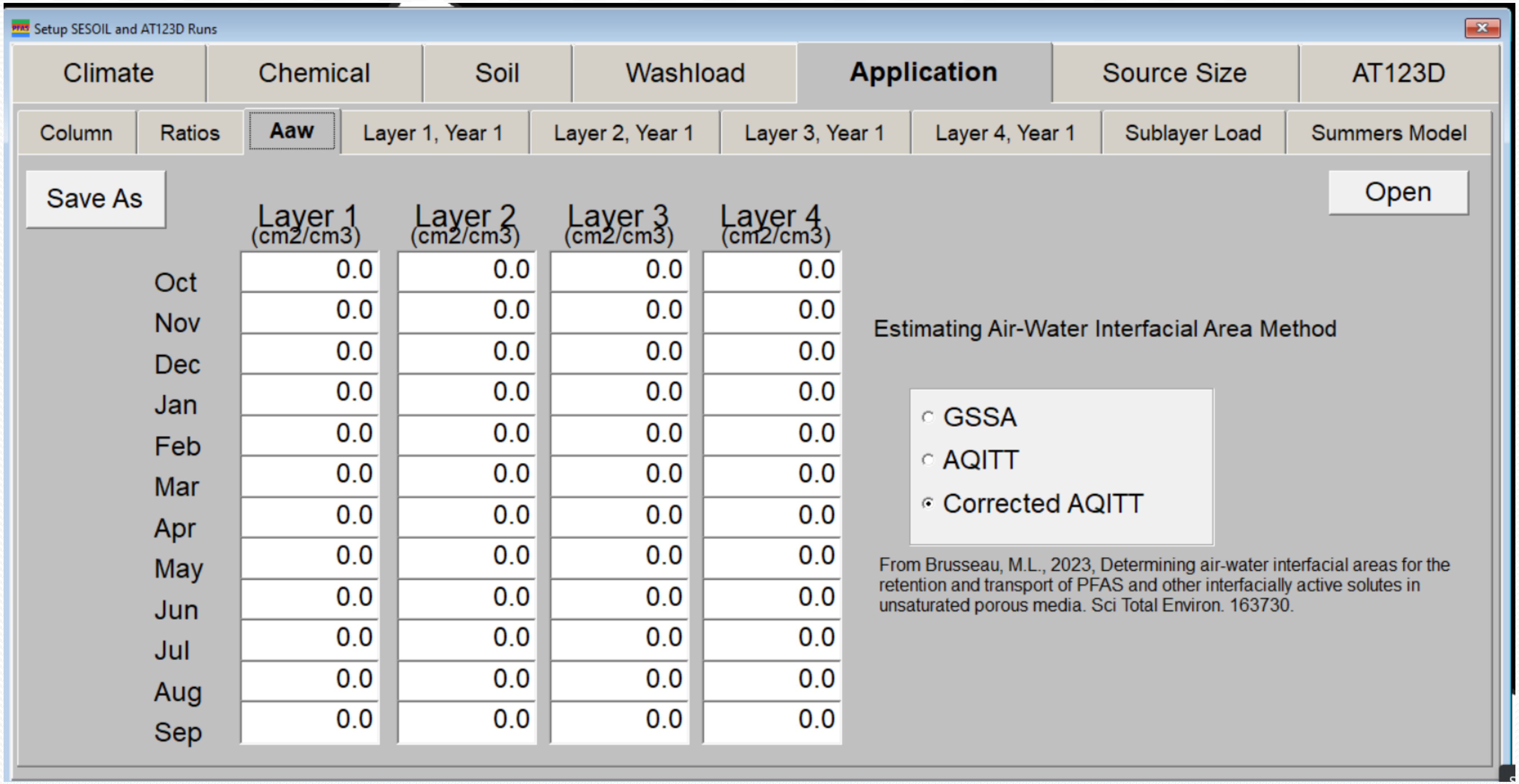
Guo, B., J. Zeng, M. L. Brusseau, A mathematical model for the release, transport, and retention of per- and polyfluoroalkyl substances (PFAS) in the vadose zone. Water Resour. Res. 57, 2020.

# Contaminant Migration Depth

$$D = \frac{J_w t_c}{\theta + \rho_b K_d + A_{aw} K_{aw} + \frac{f_a H}{R(T + 273)}}$$

| Parameter | Description |
|---|---|
| $D$ | Contaminant depth (cm) |
| $J_w$ | Water velocity (cm/s) |
| $t_c$ | Advection time (s) |
| $\theta$ | Soil water content ($cm^3/cm^3$) |
| $\rho_b$ | Soil bulk density ($g/cm^3$) |
| $K_d$ | Chemical distribution coefficient (μg/g)/(μg/ml) |
| $K_{aw}$ | Air-water interfacial adsorption coefficient ($cm^3/cm^2$) |
| $f_a$ | $f - \theta$ = the air-filled porosity (ml/ml) |
| $H$ | Henry's law constant ($m^3$ atm/mol) |
| $R$ | Gas constant [8.2 X $10^{-5}$ $m^3$ atm/(mol °K)] |
| $T$ | Soil temperature (°C) |

# Monthly Air-Water Interfacial Areas Values




**Separate monthly $A_{aw}$, values for each of the 4 SESOIL layers**

# Geometric Smooth-Surface Area

$$A_{aw} = (1 - \theta_w)\left(\frac{6(1 - n_t)}{d_{50}}\right)$$

where:

| Parameter | Description |
|---|---|
| $A_{aw}$ | Air-water interfacial areas ($cm^2/cm^3$) |
| $\theta_w$ | Monthly volumetric soil moisture content of the SESOIL soil column ($cm^3/cm^3$) |
| $n_t$ | Total soil porosity ($cm^3/cm^3$) |
| $d_{50}$ | Median soil particle diameter (cm) |

**Separate total porosity and $d_{50}$ values for each of the 4 SESOIL layers**

**Brusseau, M.L., 2023, Determining air-water interfacial areas for the retention and transport of PFAS and other interfacially active solutes in unsaturated porous media. Sci Total Environ. 163730.**

# Aqueous Interfacial Tracer Tests

$$A_{aw} = (1 - \theta_w) * 3.9 * {d_{50}}^{-1.2}$$

where:

| Parameter | Description |
| --- | --- |
| $A_{aw}$ | Air-water interfacial areas ($cm^2/cm^3$) |
| $\theta_w$ | Monthly volumetric soil moisture content of the SESOIL soil column ($cm^3/cm^3$) |
| $d_{50}$ | Median soil particle diameter (cm) |

**Separate $d_{50}$ values for each of the 4 SESOIL layers**

Brusseau, M.L., 2023, Determining air-water interfacial areas for the retention and transport of PFAS and other interfacially active solutes in unsaturated porous media. Sci Total Environ. 163730.

# Corrected Aqueous Interfacial Tracer Tests

$$A_{aw} = [-2.85 * \theta_w + 3.6] * \left[(1-\theta_w) * 3.9 * {d_{50}}^{-1.2}\right]$$

where:

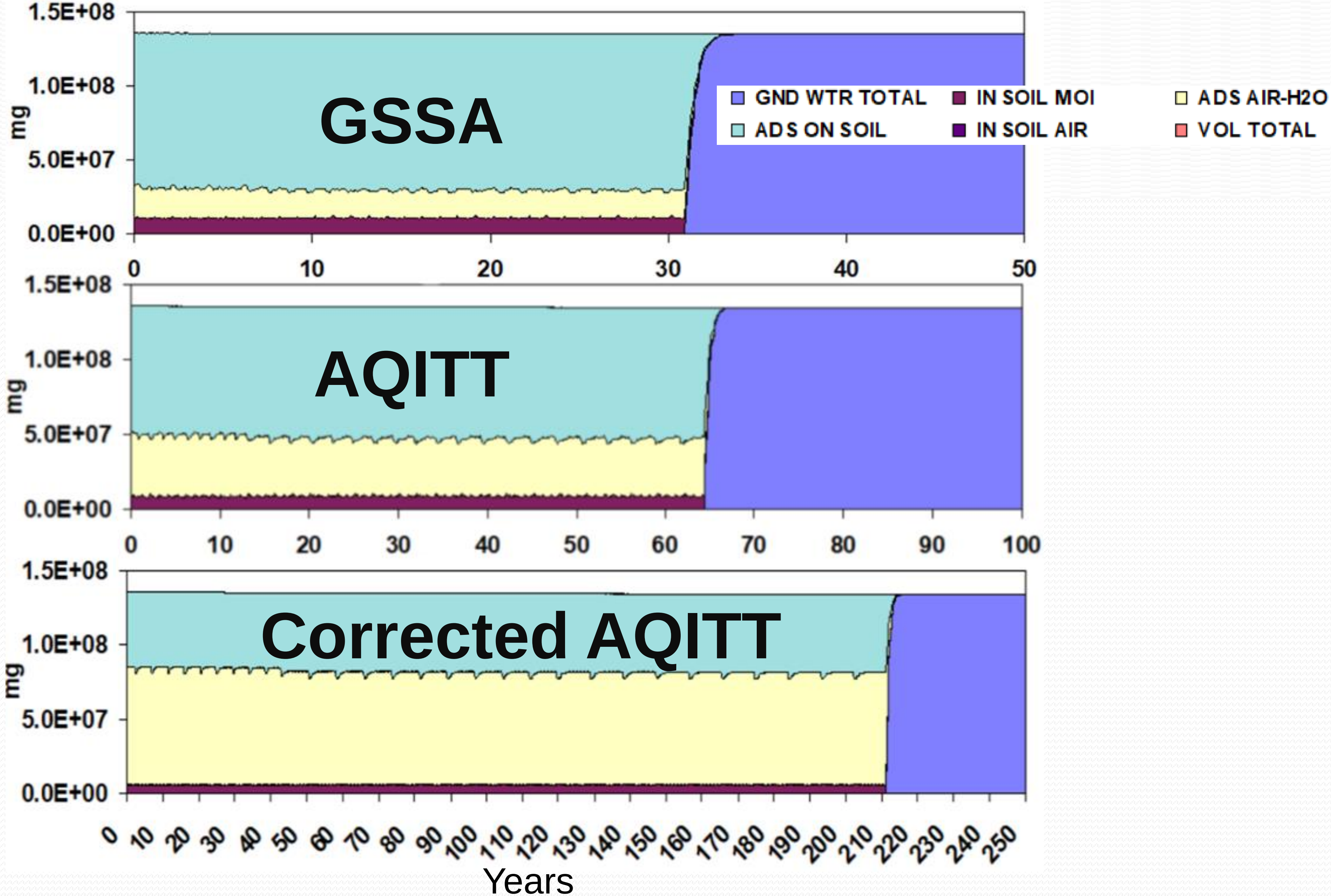
| Parameter | Description |
|---|---|
| $A_{aw}$ | Air-water interfacial areas ($cm^2/cm^3$) |
| $\theta_w$ | Monthly volumetric soil moisture content of the SESOIL soil column ($cm^3/cm^3$) |
| $d_{50}$ | Median soil particle diameter (cm) |

**Separate $d_{50}$ values for each of the 4 SESOIL layers**

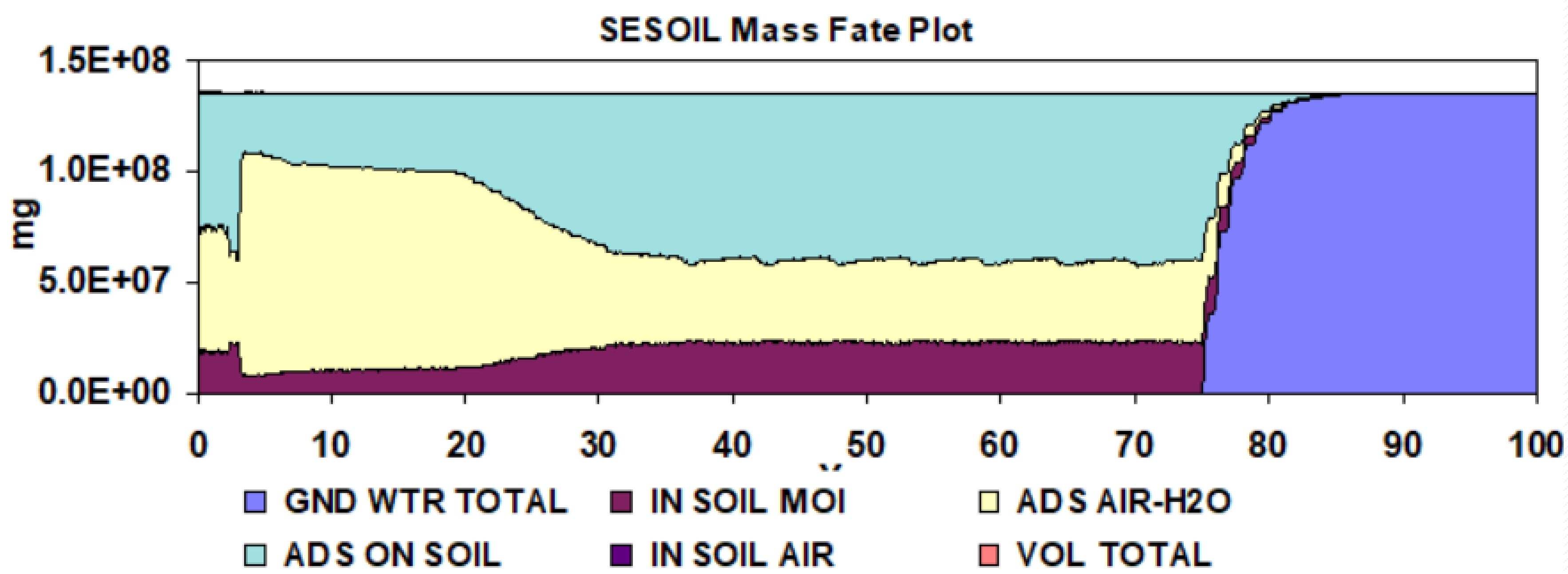
**Brusseau, M.L., 2023, Determining air-water interfacial areas for the retention and transport of PFAS and other interfacially active solutes in unsaturated porous media. Sci Total Environ. 163730.**

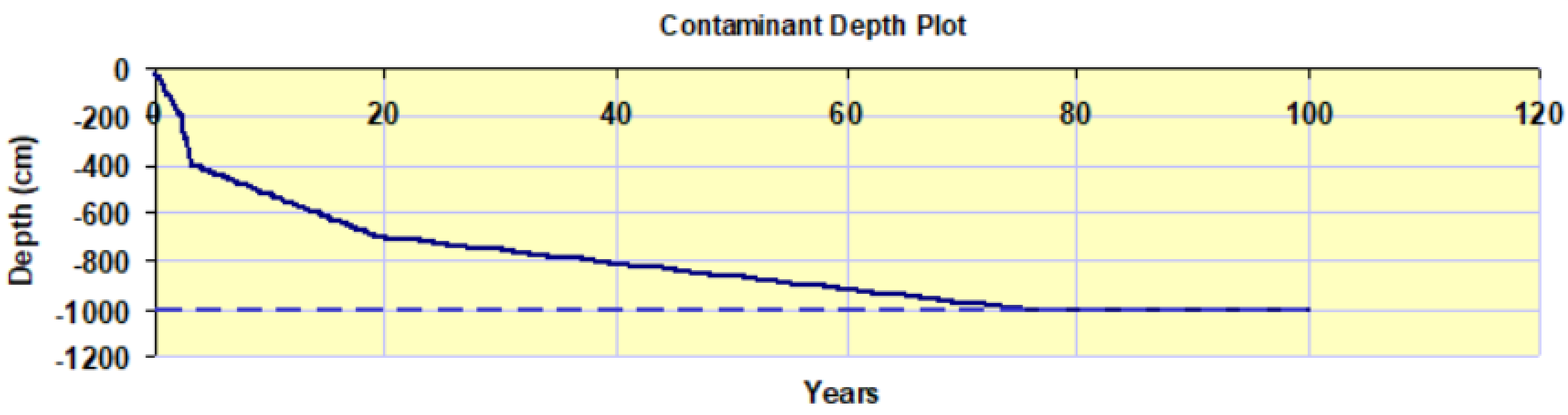
# Results

# SESOIL Mass Fate Plot



# Soil Heterogeneity



# Testing and Validation

- Very high and very low loads produced a mass balance error
- Expanded SESOIL range
- Likely enough for most cases
- But not all
- Scaling factor slides range up/down

| SESOIL Process | Pollutant Mass (ug) | Percent of Total |
|---|---|---|
| Volatilized | 3.376E+04 | 0.02 |
| In Soil Air | 2.132E+03 | 0.00 |
| Sur. Runoff | 0.000E+00 | 0.00 |
| In Washload | 0.000E+00 | 0.00 |
| Ads On Soil | 7.322E+07 | 53.84 |
| Hydrol Soil | 0.000E+00 | 0.00 |
| Degrad Soil | 0.000E+00 | 0.00 |
| Pure Phase | 0.000E+00 | 0.00 |
| Complexed | 0.000E+00 | 0.00 |
| Immobile CEC | 0.000E+00 | 0.00 |
| Hydrol CEC | 0.000E+00 | 0.00 |
| In Soil Moi | 2.193E+07 | 16.13 |
| Ads Air-H2O | 4.039E+07 | 29.70 |
| Hydrol Mois | 0.000E+00 | 0.00 |
| Degrad Mois | 0.000E+00 | 0.00 |
| Other Trans | 0.000E+00 | 0.00 |
| Other Sinks | 0.000E+00 | 0.00 |
| Gwr. Runoff | 0.000E+00 | 0.00 |
| Total Output | 1.355E+08 | 99.69 |
| Total Input | 1.360E+08 | |
| Input - Output | 4.196E+05 | |

# Testing and Validation

**Massachusetts Department of Environmental Protection**

**Maine Department of Environmental Protection**

**New Hampshire Department of Environmental Services**

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# Summary

- SESOIL was enhanced to simulate PFAS migration
- Robust and comprehensive PFAS modeling
- Needs further testing and validation

# Conflict of Interest

The author has developed the SEVIEW contaminant transport and fate modeling software referred to in this research. The author receives compensation for the sale, support, and training of the software.

# Questions?