

VLX: A Convenient Spreadsheet for Modeling Vadose Zone Contaminant Leaching to Groundwater

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VLX Introduction

ABSTRACT VLX is a spreadsheet with a Visual Basic script that computes vadose zone leaching of organic compounds. VLX was designed to incorporate the functions of the old VLEACH program on a convenient to use spreadsheet, and to increase its versatility. VLX supports the modeling of a soil column with heterogeneous physical properties (porosity, water content, organic carbon). VLX models a one-dimensional soil column discretized into cells. The VLX user inputs the physical properties of the soil at each cell, the chemical properties of the subject compound, and the initial concentration of the subject compound at each cell in the soil.

VLX computes the partitioning of the initial concentrations of the compound between dissolved, vapor, and adsorbed phases. VLX then computes, by the explicit finite difference method, the fluxes of the subject compound resulting from vapor phase diffusion, aqueous phase diffusion, and aqueous phase advection into and out from each cell for a limited time step. Then VLX re-equilibrates the distribution of the subject compound between dissolved, vapor, and adsorbed phases. Following the re-equilibration, fluxes are computed for the next time step.

Results are displayed in tabular and graphical forms. Results include the changes in the concentration profile at specified time during the run, and mass balances through the time of the run, and the mass fluxes between the surface and the water table. Examples are shown of vapor migration in a uniform soil type, a uniform soil type with a variable moisture column, and a column with soils of greatly varying properties. Finally, an application of VLX to compute the effective recharge concentration for input to an MT3D groundwater contaminant transport model is illustrated.

Objectives

This poster describes VLX, an Excel-based workbook that duplicates most of the capabilities of USEPA's model VLEACH (Ravi and Johnson 1992). The developer wanted to preserve the desirable features of the original VLEACH:

- Simplicity: A relatively small input list was needed;
- Flexibility: Soil properties and chemical properties completely controlled by the user.

And to overcome some of the limitations of currently available VLEACH software:

- Age: Must be piggybacked onto a modern user interface.
- Homogeneous Soil Column: While VLEACH supports a variable initial concentration in the cells of the soil column, the relevant physical properties of the soil (porosity, moisture, density, organic carbon) cannot be changed from ground surface to water table.

This spreadsheet was developed to gain

- Convenience: spreadsheet, rather than a stand-alone program.
- Versatility: Supports heterogeneity of soil properties.

Computational Approach

The computational algorithms in VLX are migration-centered. Therefore VLX computes VOC flux from each migration process explicitly in each time step, then resultant contaminant masses in each cell are computed, and finally vapor, dissolved, and adsorbed fractions each cell are computed from the new mass results to give the resulting concentrations.

Mass Migration Calculation

Migration within the Vadose zone

Diffusive flux of VOC Vapor from overlying cell

$$J_{vt}(i) = \{2[D_v(i) D_v(i-1)/(D_v(i) + D_v(i-1))]\} (C_g(i-1) - C_g(i))/dz \} Adt$$

Diffusive flux of VOC Vapor to underlying cell

$$J_{vb}(i) = \{2[D_v(i) D_v(i+1)/(D_v(i) + D_v(i+1))]\} (C_g(i) - C_g(i+1))/dz \} Adt$$

Diffusive flux of dissolved VOC from overlying cell

$$J_{wt}(i) = \{2[D_l(i) D_l(i-1)/(D_l(i) + D_l(i-1))]\} (C_w(i-1) - C_w(i))/dz \} Adt$$

Diffusive flux of dissolved VOC to underlying cell

$$J_{wb}(i) = \{2[D_l(i) D_l(i+1)/(D_l(i) + D_l(i+1))]\} (C_w(i) - C_w(i+1))/dz \} Adt$$

Dissolved VOC advection from overlying cell

$$P_{wt}(i) = \{Q C_w(i-1)\} Adt$$

Dissolved VOC advection to underlying cell

$$P_{wb}(i) = \{Q C_w(i)\} Adt$$

And after each time step

$$M_i(i,t) = M_i(i, t-dt) + (J_{vt}(i) - J_{vb}(i)) + (J_{wt}(i) - J_{wb}(i)) + (P_{wt}(i) - P_{wb}(i))$$

Migration at the upper boundary

At the upper boundary (ground surface, cell 1) The mass fluxes are

$$J_{vt}(1) = \{2[D_v(1)]\} (C_{atm} - C_g(1))/dz \} Adt$$

$$J_{wt}(1) = 0$$

$$P_{wt}(1) = \{Q C_{inf}\} Adt$$

An option exists to let the ground surface be impervious to vapor phase diffusion. In that case

$$J_{vt}(1) = 0$$

Migration at the lower boundary

At the lower boundary, ground water table, cell n, the mass fluxes are

$$J_{vb}(n) = \{2[D_v(n)]\} (C_g(n) - K_h C_{gw})/dz \} Adt$$

$$J_{wb}(n) = \{2[D_l(n)]\} (C_w(n) - C_{gw})/dz \} Adt$$

$$P_{wb}(n) = \{Q C_w(n)\} Adt$$

An option exists to let the water table be impervious to vapor phase diffusion. In that case

$$J_{vb}(n) = 0$$

Computation of Diffusion Coefficient

Effective diffusion coefficients for VOC in soil vapor $D_v(i)$ at cell I, and in pore water $D_l(i)$ are computed against Millington and Quirk's formula

$$D_v(i) = D_a * (\phi(i)^{10/3}) \div p(i)^2 \text{ and}$$

$$D_l(i) = D_w * (\theta(i)^{10/3}) \div p(i)^2$$

Conceptual Approach

In VLX we model the transport of a volatile or semi volatile organic compound present in the unsaturated zone.

It is present in the vadose zone in one of three fractions,

- adsorbed onto soil organic carbon,
- dissolved in soil pore water, or
- vaporized into soil air.

It migrates within the vadose zone by

- vapor phase diffusion,
- liquid phase diffusion and dispersion,
- and liquid phase advection

The properties of the soil column which control fractionation and migration, (organic carbon content, porosity, and moisture content) may be heterogeneous, but they may not change with time during the course of a simulation. Sorption and vaporization isotherms are linear, and no separate phase is present.

The initial concentration of the VOC typically is variable in space. During a simulation, VOC can enter the system.

- Infiltration of water from the ground surface may add VOC dissolved in the infiltrant.
- Diffusion of vapor from the atmosphere may introduce VOC into the soil gas of the vadose zone.
- VOC dissolved in the groundwater may diffuse into the vadose zone in either water of the capillary fringe and enter the soil gas.

During a simulation, VOC can leave the system:

- At the ground surface, VOC can volatilize into the atmosphere,
 - Or the ground surface can be made impervious to volatilization
- At the water table, VOC will leach to the ground water by dissolved phase advection
- Diffusion to the ground water can occur
 - Into or out from the water table where the ground water concentration is specified.
 - Into the water table where the migration rate is unconstrained by the concentration ground water.
 - Alternatively, the water table can be made impervious to vapor phase diffusion.

Basis for Re-equilibration and computation of concentrations

Once the new mass has been determined, the distribution among the dissolved, adsorbed, and vapor fractions is calculated. This is done according to the following relationships between contaminant mass and concentrations

$$M_w(i) = V C_w(i) * \theta(i) \quad M_g(i) = V C_g(i) * \phi(i) \quad M_s(i) = V C_s(i) * \rho(i)$$

$$M_t(i) = V \{ C_w(i) * \theta(i) + C_g(i) * \phi(i) + C_s(i) * \rho(i) \}$$

The relations between the concentrations in each fraction are

$$C_g(i) = K_h * C_w(i) \quad C_s(i) = k_d(i) * C_w(i)$$

Incorporating the concentration relationships into the mass fraction equations we get

$$M_t(i) = V * \{ C_w(i) * \theta(i) + C_w(i) * K_h * \phi(i) + C_w(i) * k_d(i) * \rho(i) \}$$

And solving for $C_w(i)$

$$C_w(i) = M_t(i) \div \{ V * [\theta(i) + K_h * \phi(i) + k_d(i) * \rho(i)] \}$$

Using this equation, the equilibrated $C_w(i)$ is computed from the new $M_t(i)$. Then the equilibrated $C_g(i)$ and $C_s(i)$ are computed from $C_w(i)$, and the VOC mass in each fraction is computed from the new concentrations each fraction. Total concentration $C_t(i)$ is not used for in the computational steps, but its computed for display according to the formula

$$C_t(i) = M_t(i) \div \{ V * [\theta(i) + \rho(i)] \}$$

Computation of Time Step

The length of the time step must not exceed a certain value to prevent instability in the computations that produces divergent results. The primary cause of divergent results in an explicit finite difference model is a time step long enough for the mass transport from one cell to cross over two cells. According von Neumann, the stability criterion for diffusive flux is

$$D_v(i) * \phi(i) * dt \div \{ [\theta(i) + K_h * \phi(i) + k_d(i) * \rho(i)] * dx^2 \} < 1$$

$$dt_v < \{ [\theta(i) + K_h * \phi(i) + k_d(i) * \rho(i)] * dx^2 \} \div [D_v(i) * \phi(i)]$$

Similarly the stability criterion for advective flux is

$$Q * \theta(i) * dt \div \{ [\theta(i) + K_h * \phi(i) + k_d(i) * \rho(i)] * dx \} < 1 \text{ and}$$
$$dt_w < \{ [\theta(i) + K_h * \phi(i) + k_d(i) * \rho(i)] * dx \} \div Q * \theta(i)$$

The advective and diffusive transport processes are additive, so the stability criterion must reflect that. Accordingly the following time step is computed for this model

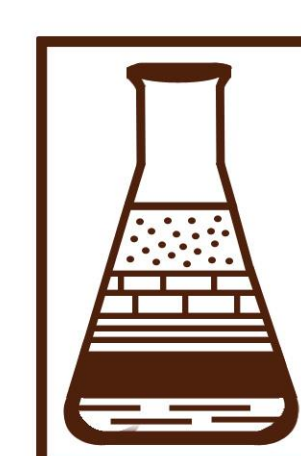
$$dt = dt_v * dt_w \div (dt_v + dt_w)$$

References:

Jury WA, Spencer WF, Farmer WJ. "Behavior assessment model for trace organics in soil: I. Model description." *Journal of Environmental Quality* 1983;12(4):558-564.

Millington RJ, Quirk JM. "Permeability of porous solids." *Transactions of the Faraday Society* 1961;57:1200-1207.

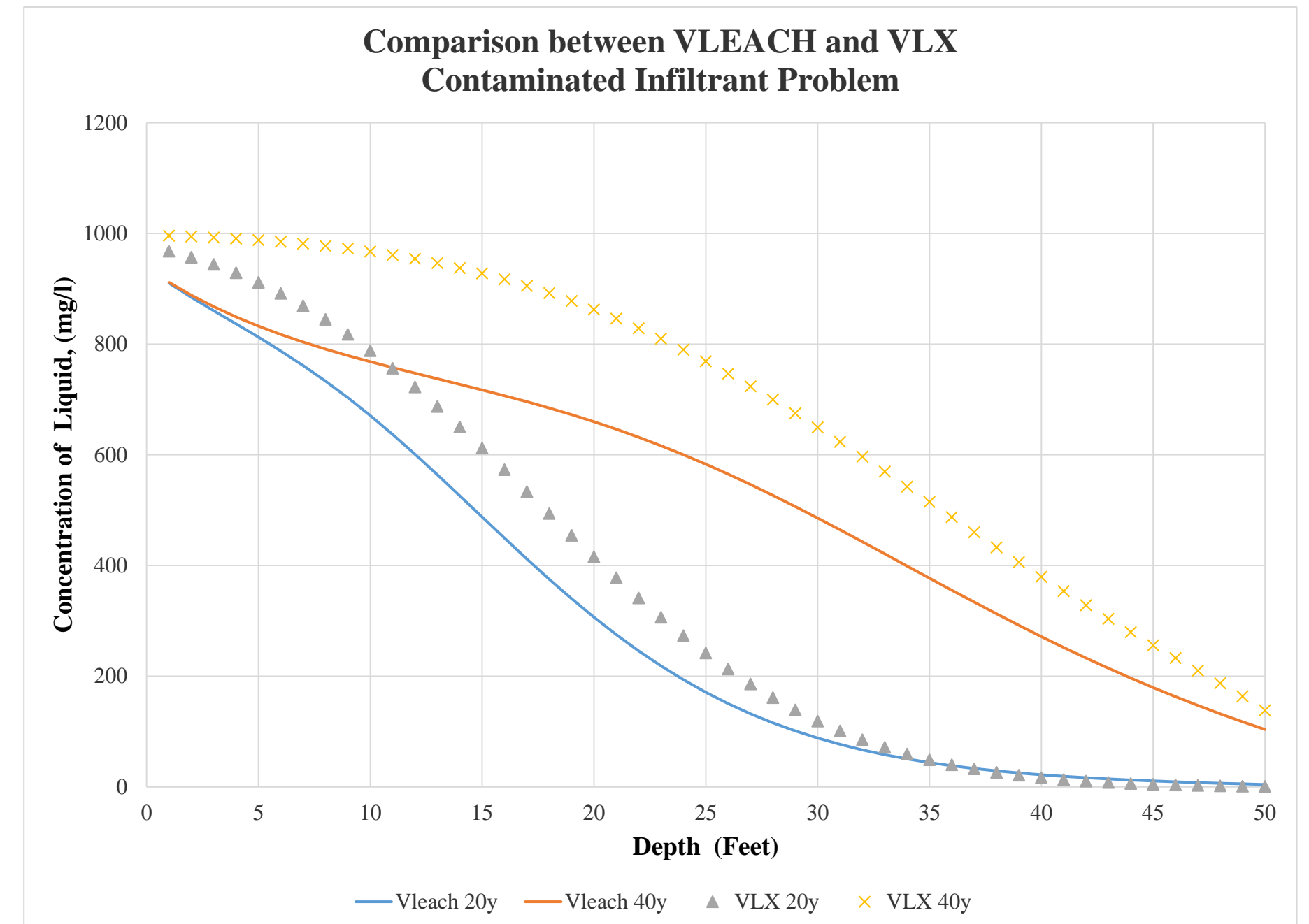
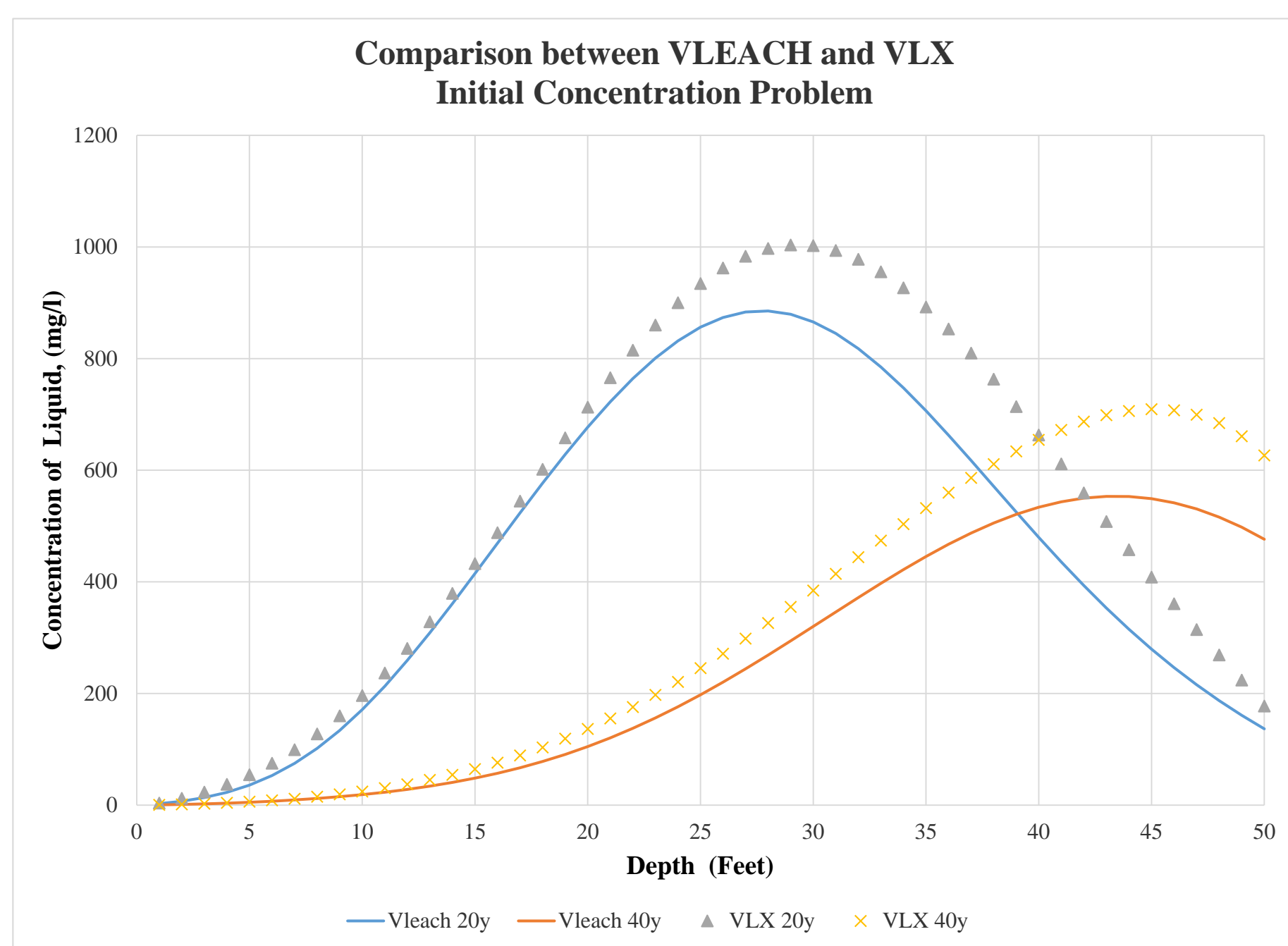
Ravi, Varadhan and Johnson, Jeffrey A. *VLEACH A One-Dimensional Finite Difference Vadose Zone Leaching Model Version 2.2 - 1997* USEPA Office of Research and Development Robert S. Kerr Environmental Research Laboratory Center for Subsurface Modeling Support Ada, Oklahoma



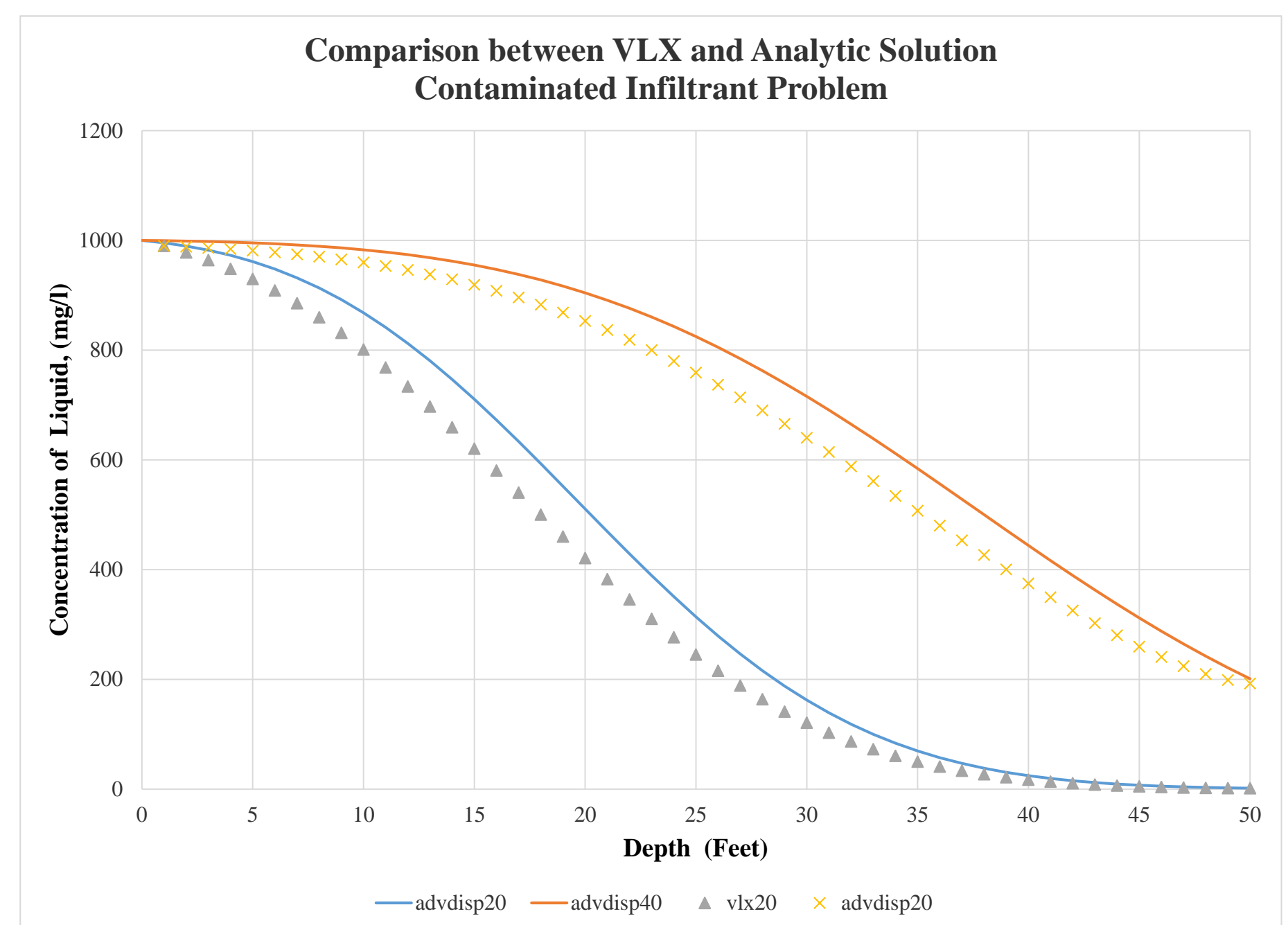
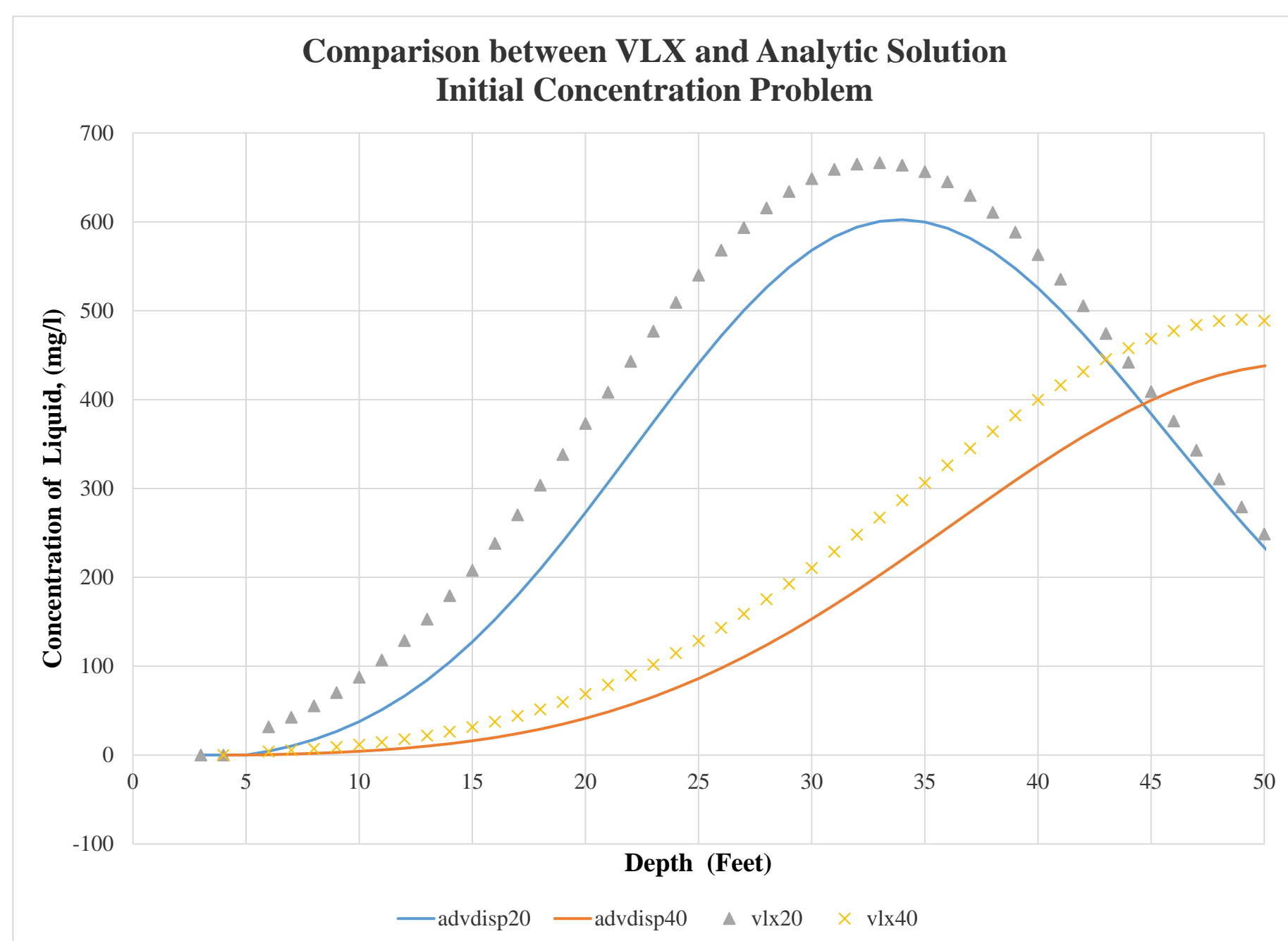
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VLX Validation

Comparison between VLX and VLEACH example problems



Comparison between VLX and Analytic Solution of Example Problems



VLX Operation

User input worksheet for VLX

One worksheet is devoted to user input. The user inputs include the time controls, (computational time step, simulation time and output time steps), compound name and properties, site wide properties and cell size. For each cell they include soil properties and initial concentrations. It is the User's responsibility to chose soil properties, and to ensure that they plausibly represent real soils. Cell specific diffusivities and partition coefficients are then computed. One worksheet is devoted to printing out these intermediate calculations.

Initial concentrations are input in practical units (mg/kg). They are then converted to mass in each cell, then distributed among the three fractions. Once the initial equilibrium status is determined, the migration time steps are followed. The user can specify a computational time step is user input, which will be overridden if any stability criterion is exceeded.

Output is provided in separate worksheets, one sheet for mass flux results to groundwater and atmosphere, and four sheets for concentration profiles at each cell.

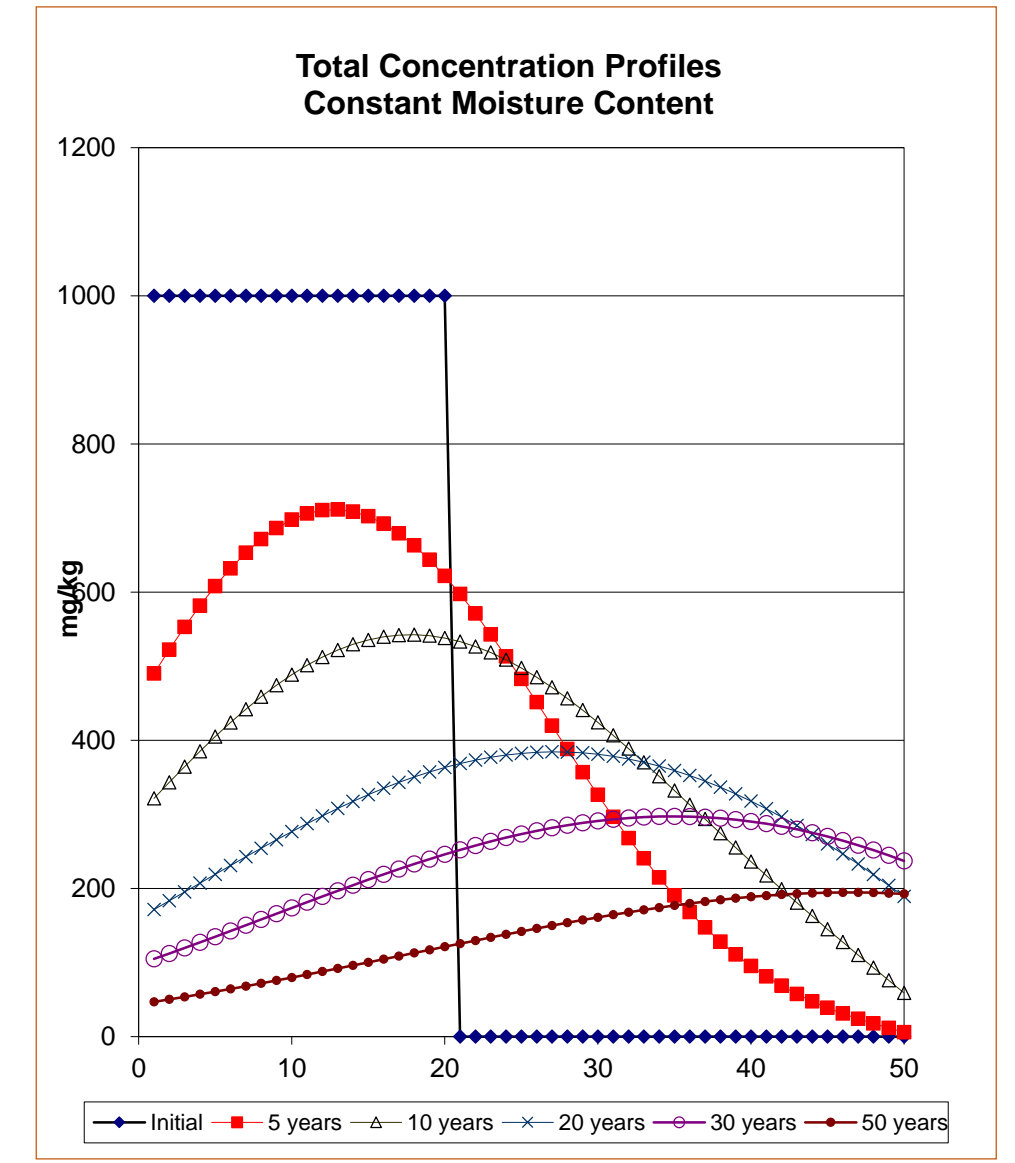
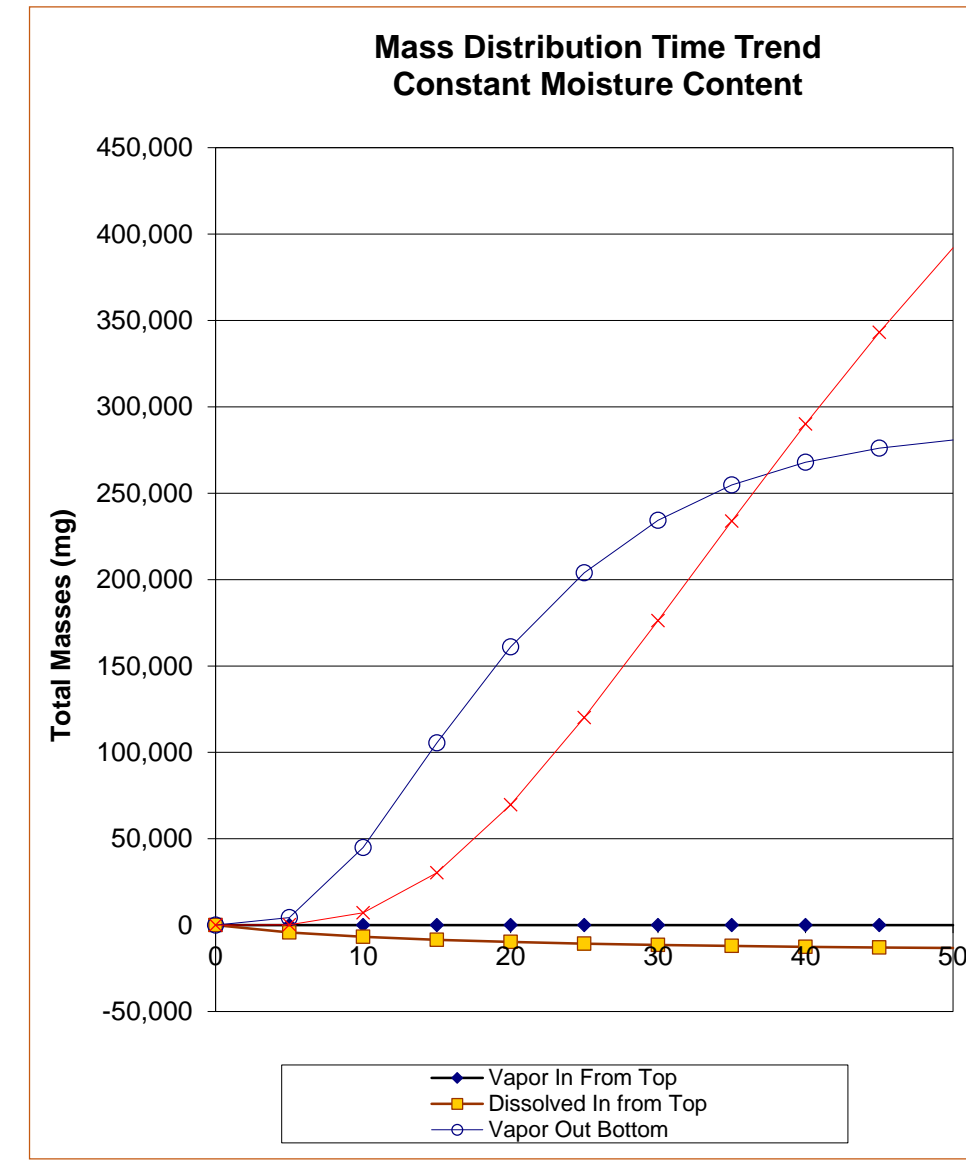
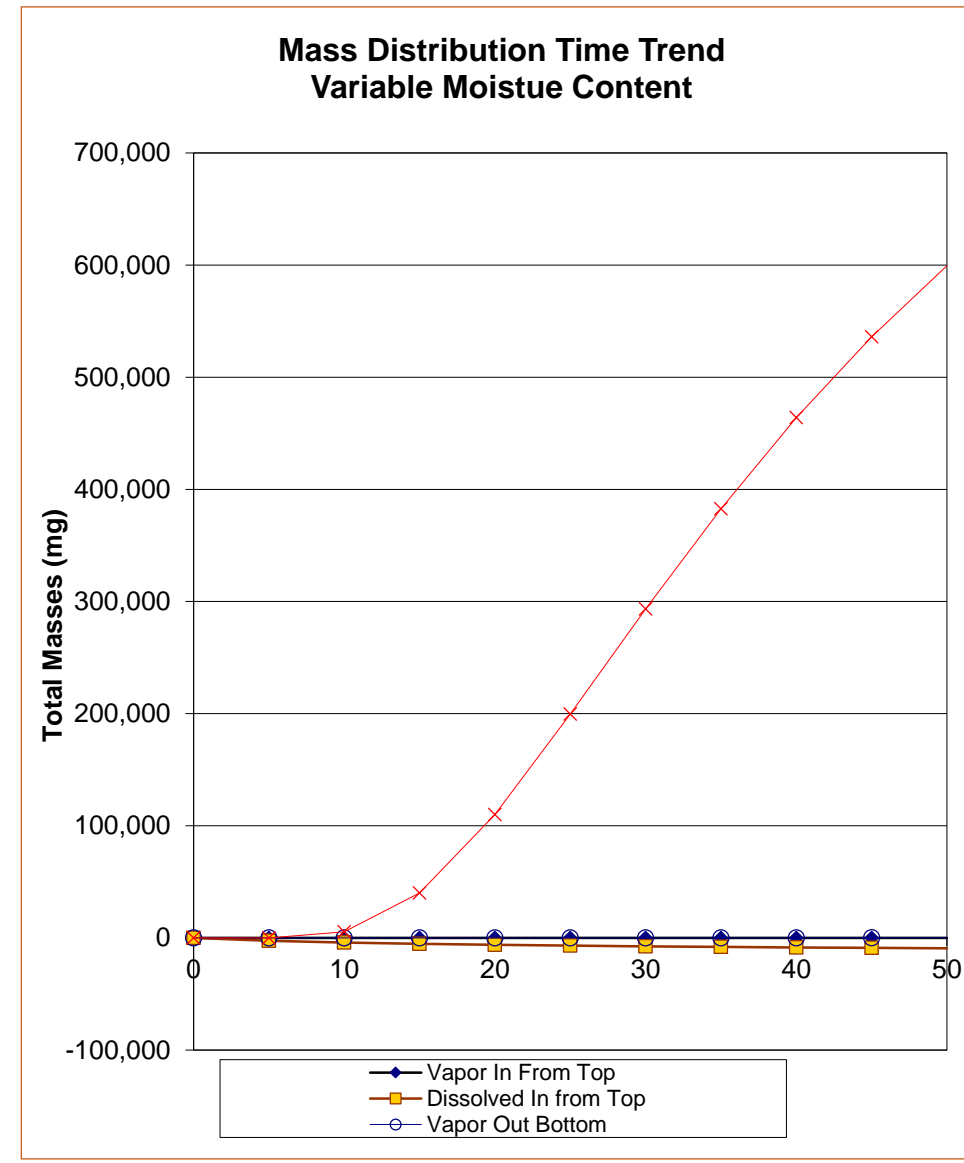
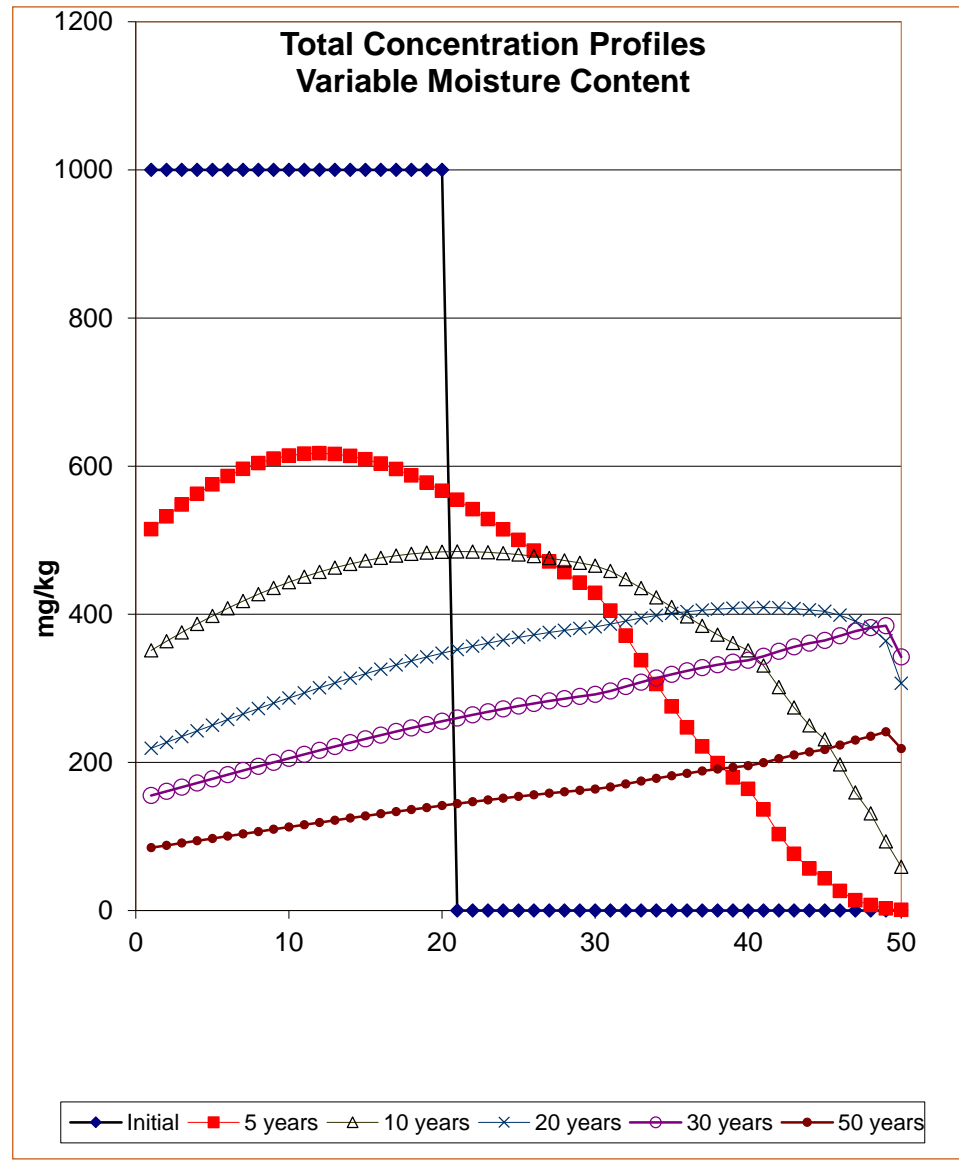
Graphical output consist of seven charts. Four charts show the concentration profiles of each fraction (dissolved, adsorbed, vapor, and total) at selected times. One chart shows the migration totals of the contaminant to atmosphere or groundwater, one shows the total movement of contaminant through the system, and one shows the effective concentration of the liquid that recharges the groundwater.

Vadose Zone Leaching Model General Conditions				Vadose Zone Leaching Model Soil Properties						Vadose Zone Leaching Model Initial Concentrations in Soils		
Title of Run	Demonstration Problem 3			from cell	to cell	Bulk Dry Density	Total Porosity	Moisture Content	Organic Carbon Content	from cell	to cell	Concentration (mg/kg)
Site ID	Location with High Carbon Layer			1	1	1.6	0.25	0.2	0.005	1	15	0
Length of Time steps	0.1	0.000176	= ACTUAL TIME STE	2	15	1.6	0.4	0.2	0.005	16	25	0
Length of Simulation Time	30 years			16	25	1.6	0.4	0.2	0.05	26	46	0
Length of Interval for Migration Output	3 years			26	44	1.6	0.4	0.2	0.005	47	50	0
Length of Interval for Profile Output	3 years			45	48	1.6	0.4	0.25	0.005			
Constituent of Concern	TCE			49	50	1.6	0.4	0.35	0.005			
Koc	100 mg/kg in soil per mg/l in water											
Henry's Law Constant	0.4 mg/l in vapor per mg/l in water											
Solubility	1100 mg/l											
Diffusivity (in air)	0.683 m ² per day											
Diffusivity (in water)	0.0000786 m ² per day											
Site Area	1000 square feet											
Cell Thickness	1 feet											
Number of Cells	50											
Recharge Rate	1											
Concentration In Recharge Water (mg/l)	1000											
Concentration in Overlying Air (mg/l)	0 Minus if impervious to volatilization											
Concentration in Groundwater (mg/l)	0											
Water Table Diffusion Control Flag	0 Plus for fixed conc, 0 for free boundary, minus for impervious											
Hydraulic Conductivity of Underlying G	40.0 feet per day											
Undelying Groundwater Gradient	0.0020 feet per foot											



VLX Application

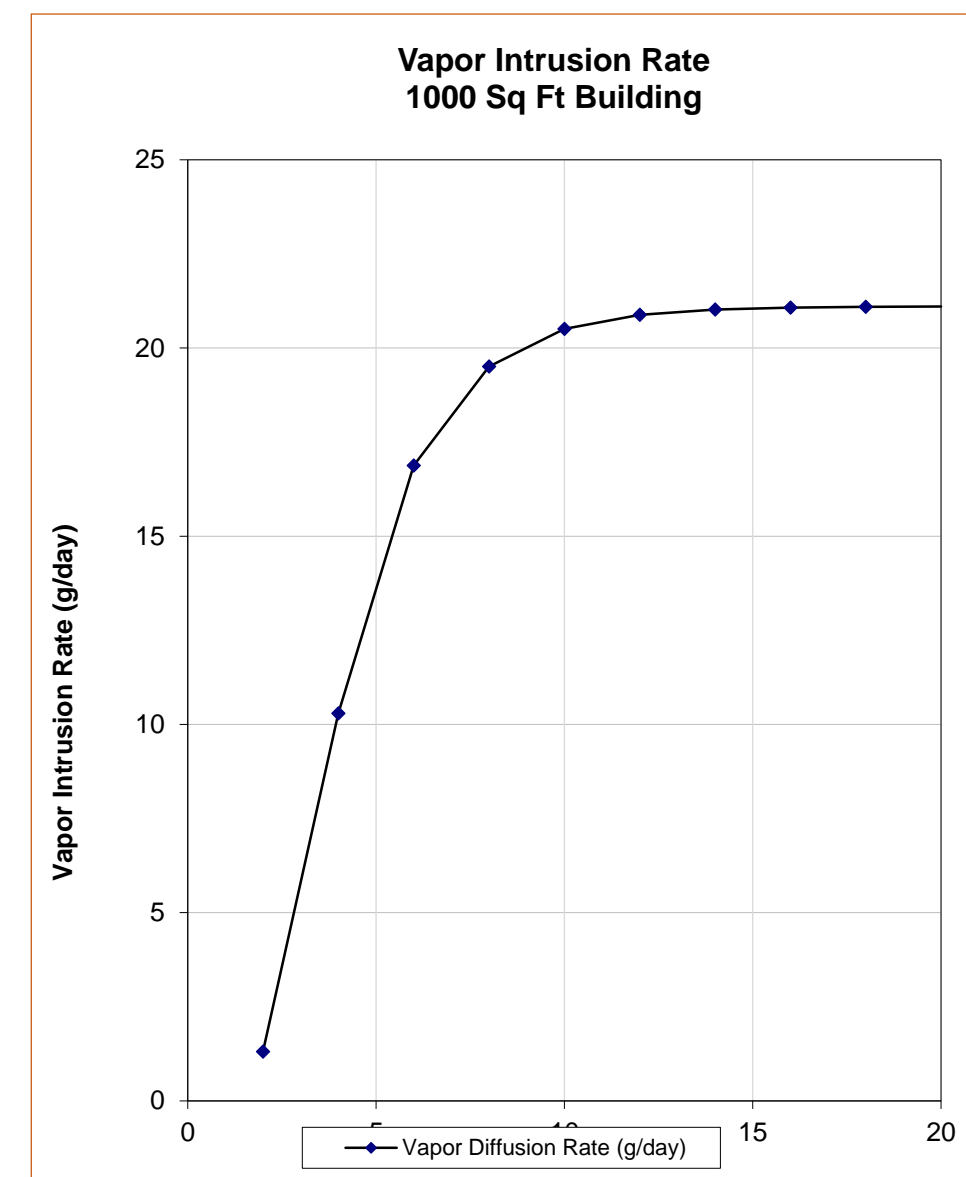
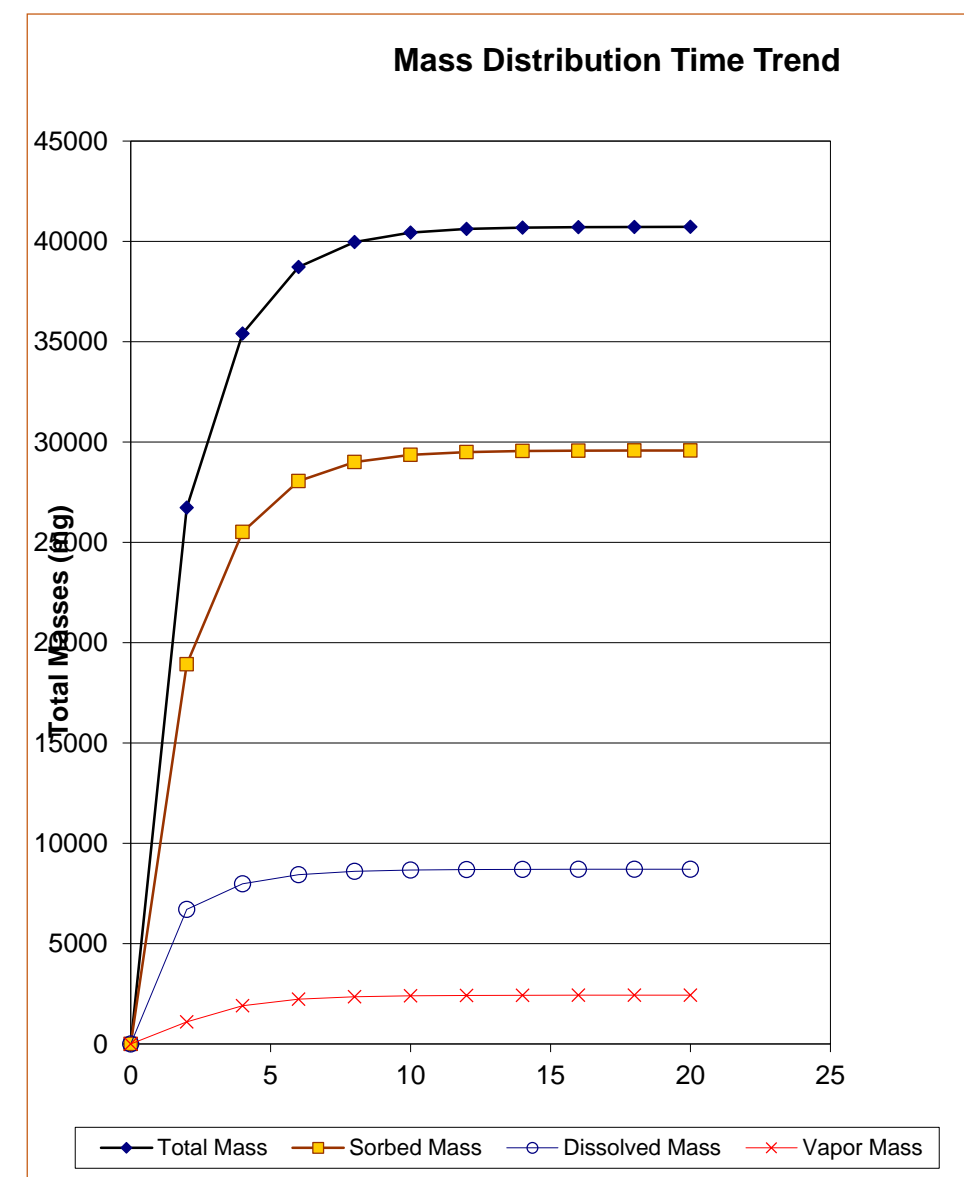
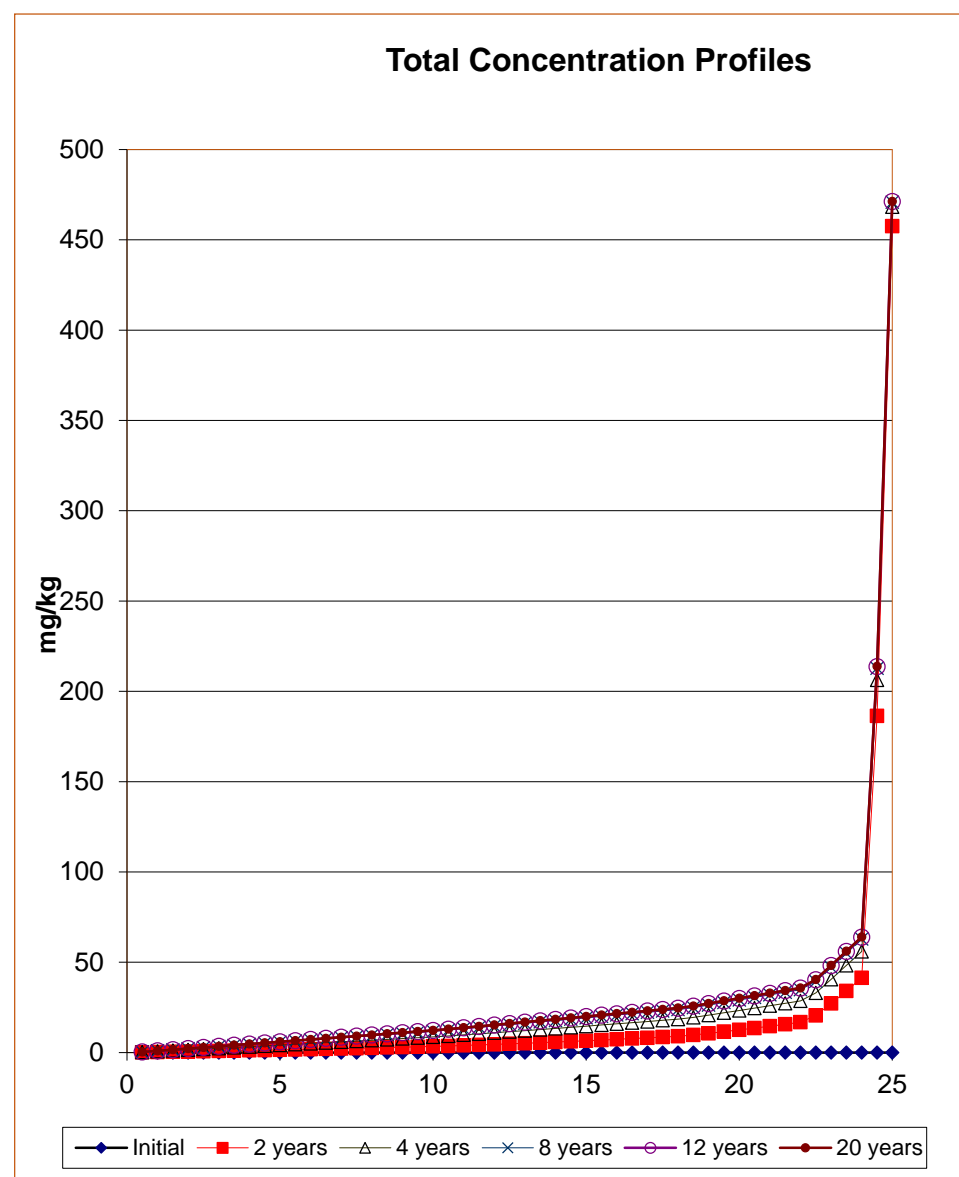
Effect of Variable Soil Moisture



On these four charts, the effects of variable moisture content and air-filled porosity are illustrated. The charts on the left show concentration profiles, and mass transfer histories for the soil column with a variable moisture, and the charts on the right show the concentration profile and mass transfer histories for a soil column with a averaged and constant moisture content. The average moisture permitted more rapid dissipation of the initial TCE, because the capillary fringe retards vapor migration.

Vadose Zone Leaching Model Soil Properties					
from cell	to cell	Bulk Dry Density	Total Porosity	Moisture Content	Organic Carbon Content
1	30	1.6	0.4	0.2	0.005
31	40	1.6	0.4	0.25	0.005
41	45	1.6	0.4	0.3	0.005
46	48	1.6	0.4	0.34	0.005
49	50	1.6	0.4	0.39	0.005

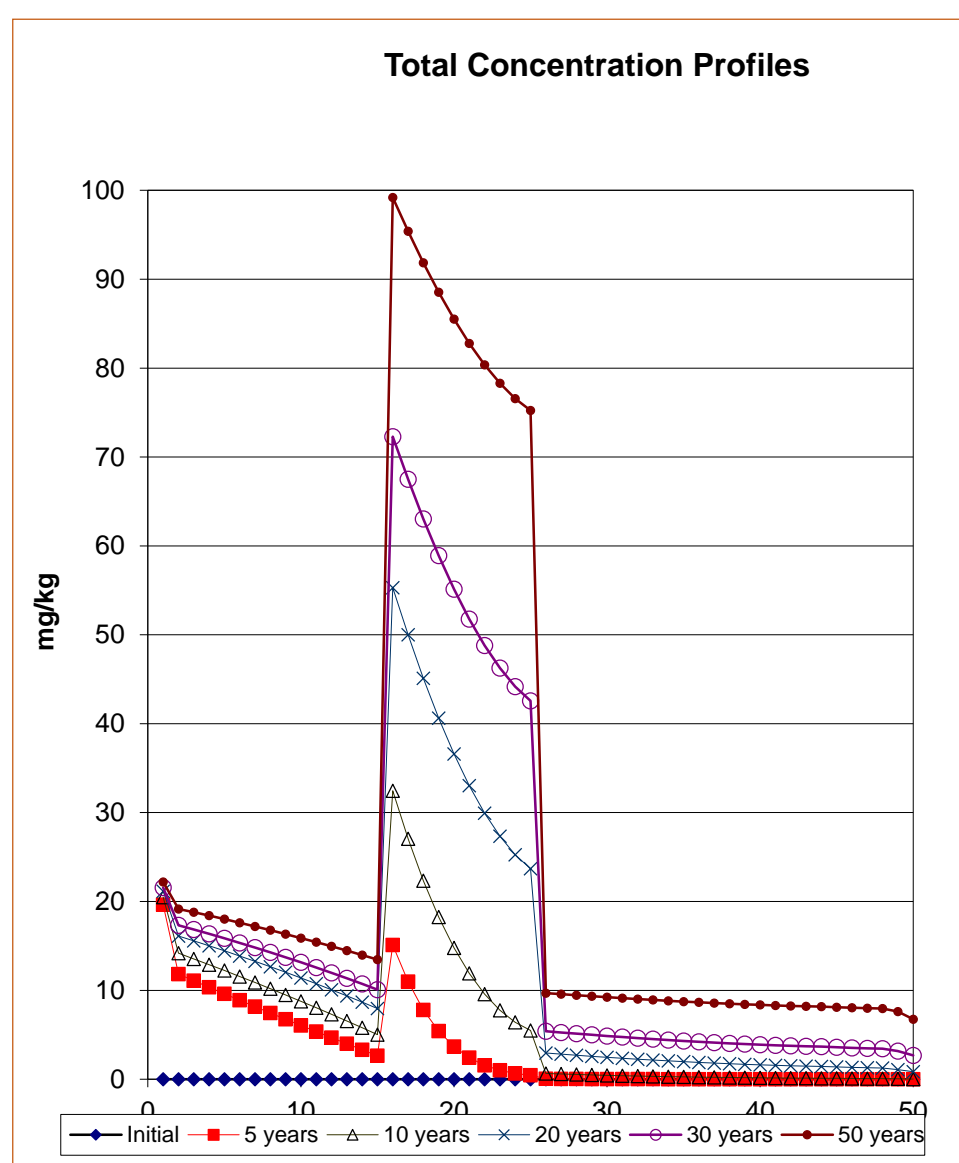
Vadose Zone Leaching Model Soil Properties					
from cell	to cell	Bulk Dry Density	Total Porosity	Moisture Content	Organic Carbon Content
1	30	1.6	0.4	0.236	0.005
31	40	1.6	0.4	0.236	0.005
41	45	1.6	0.4	0.236	0.005
46	48	1.6	0.4	0.236	0.005
49	50	1.6	0.4	0.236	0.005



Vapor Intrusion Problem

Normal capillary fringe in soil
Groundwater contains 1000 mg/l trichloroethene, Ground surface is 25 feet above water table. Within 4 years vapor intrusion rate is half of maximum, 90% of maximum within 8 years. 21 grams per day to enter 1000 square foot building.

Effect of Organic Rich Layer

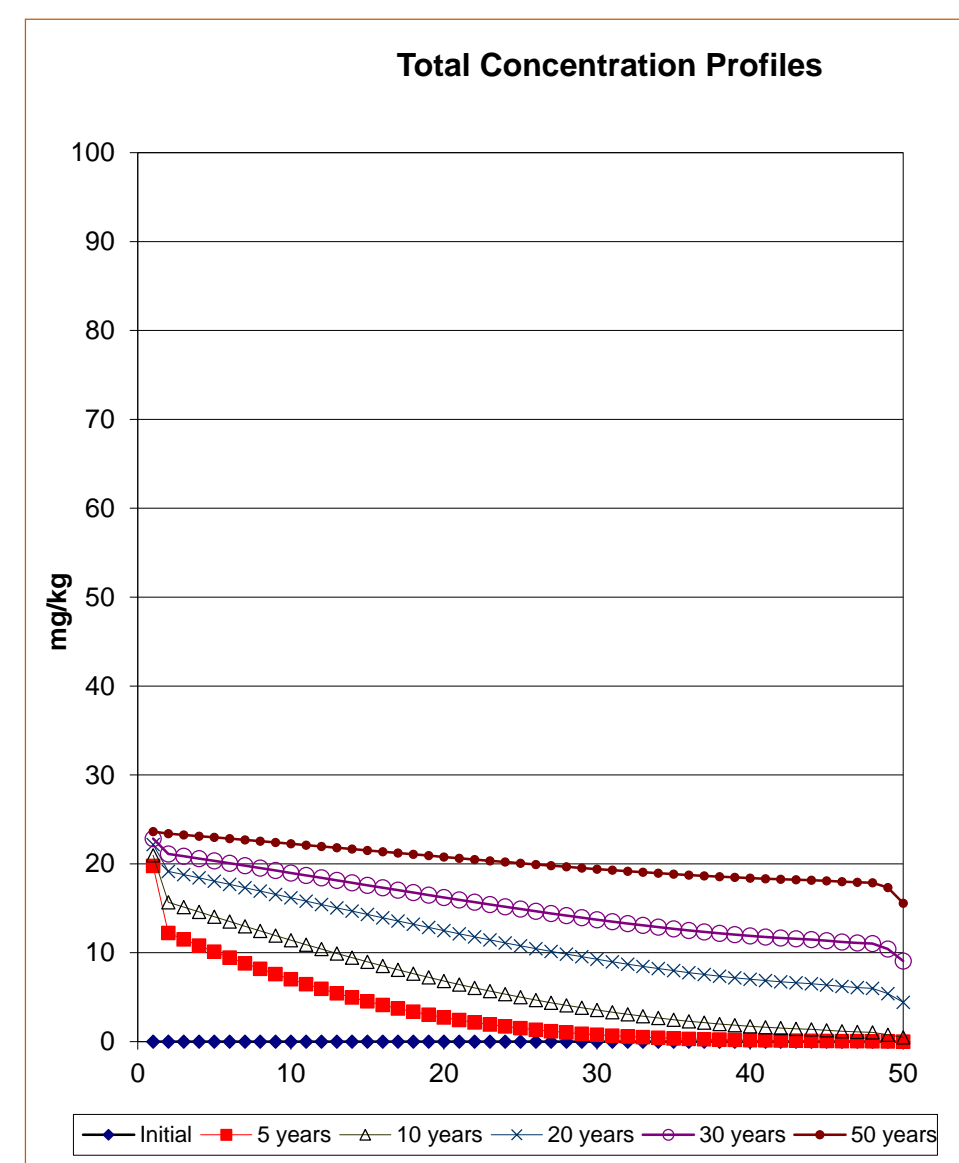


Vadose Zone Leaching Model Soil Properties					
from cell	to cell	Bulk Dry Density	Total Porosity	Moisture Content	Organic Carbon Content
1	1	1.6	0.25	0.2	0.005
2	15	1.6	0.4	0.2	0.005
16	25	1.6	0.4	0.2	0.05
26	44	1.6	0.4	0.2	0.005
45	48	1.6	0.4	0.25	0.005
49	50	1.6	0.4	0.35	0.005

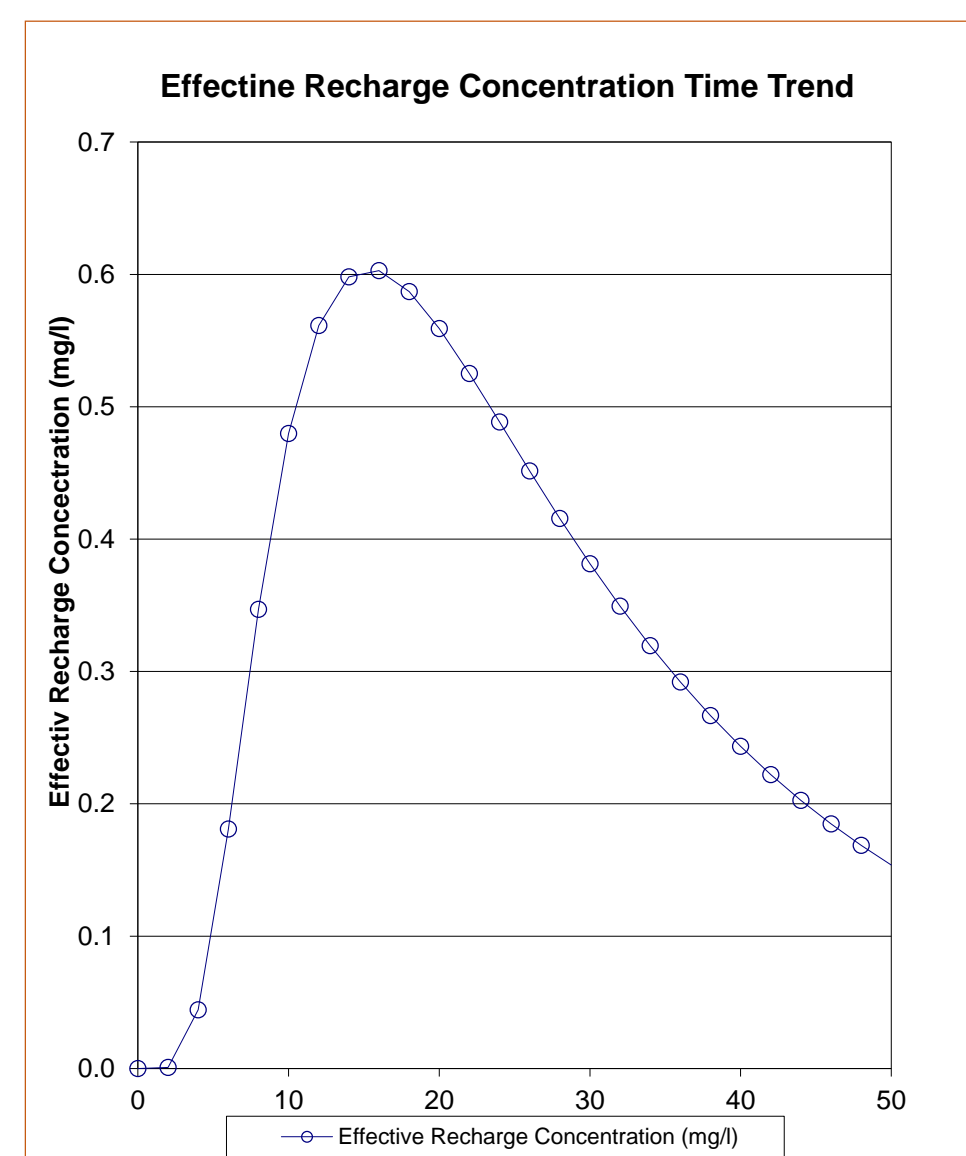
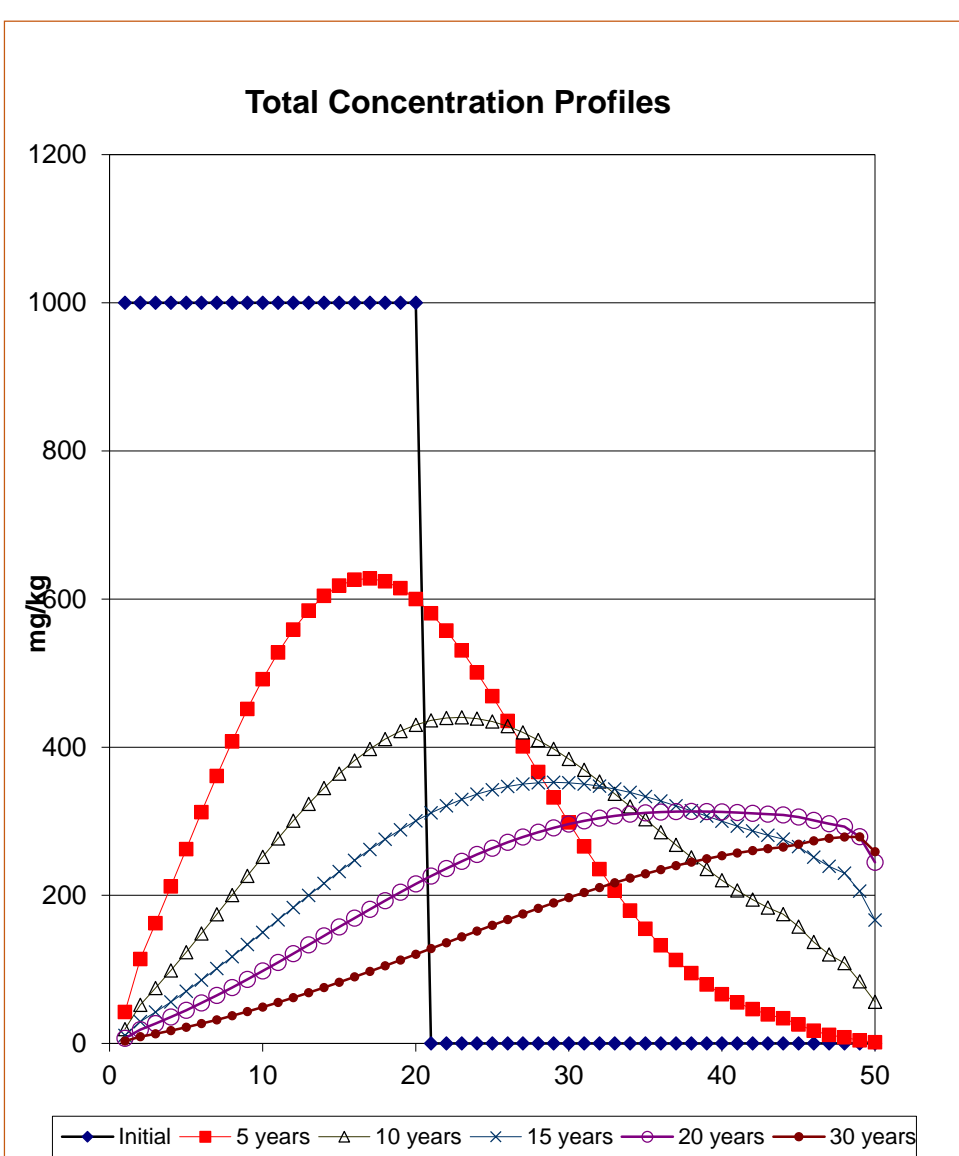
Right: Soil profile and concentration profiles for location without buried sawdust.

Left: Soil profile and concentration profiles for location with buried sawdust.

Vadose Zone Leaching Model Soil Properties					
from cell	to cell	Bulk Dry Density	Total Porosity	Moisture Content	Organic Carbon Content
1	30	1.6	0.4	0.2	0.005
31	40	1.6	0.4	0.25	0.005
41	45	1.6	0.4	0.3	0.005
46	48	1.6	0.4	0.34	0.005
49	50	1.6	0.4	0.39	0.005



At an industrial site in the United States, on-site disposal of sawdust had occurred, and further activities had covered it. A site investigation had shown highly elevated trichloroethene concentrations located at these depths. This VLX model shows how this can be have occurred from incremental surface releases, simulated here as contaminated influent.



Quantitative Estimation of Effect on Ground Water

Left: Concentration Profiles and Effective Recharge Concentration for Site affected by trichloroethene in upper 20 feet. The effective recharge concentration is the sum of the vapor diffusion plus dissolved solute infiltration to groundwater, divided by the water infiltration rate for the affected area. In this example, the release to soil shows detectable impact to groundwater starting at 4 years peaking at 16 years, and declining afterwards.

