VLX Introduction

ABSTRACT VLX is a spreadsheet 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 (pore water, soil organic carbon).

The concept: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 advection, phase change, and aqueous phase advection 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 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.

Conceptual Approach

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

It is present in the vadose zone in one of three fractions, dissolved in soil pore water, or vaporized into soil air.

It migrates within the vadose zone by:

- vapor phase diffusin,
- 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 change, 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.
- Alternatively, the water table can be made impermeable 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:

\[ M_{C_i}(t) = V C_{C_i}(t) \]

For each time step, the 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.
- Alternatively, the water table can be made impermeable to vapor phase diffusion.

Computation of Time Step

The length of the time steps 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 the next cell over two cells. According von Neumann, the stability criterion for diffusive flux is

\[ \frac{\Delta t}{\Delta z} \cdot \frac{\Delta^2 x}{\Delta x^2} < 1 \]

Similarly the stability criterion for advective flux is

\[ \frac{Q \cdot \Delta x}{\Delta z} \cdot \frac{\Delta^2 x}{\Delta x^2} < 1 \]

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

\[ \Delta t = \Delta t \cdot \min\left(1, \frac{\Delta z}{\Delta x}, \frac{\Delta x}{\Delta z} \right) \]
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 choose 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 chart 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.

Comparison between VLX and Analytic Solution of Example Problems

Comparison between VLX and VLEACH example problems

VLX Validation

Comparison between VLX and VLEACH example problems

VLX Operation

User input worksheet for VLX

<table>
<thead>
<tr>
<th>Vadose Zone Leaching Model</th>
<th>Vadose Zone Leaching Model</th>
<th>Vadose Zone Leaching Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>General Conditions</td>
<td>Soil Properties</td>
<td>Initial Concentrations in Soils</td>
</tr>
<tr>
<td>Title of Run</td>
<td>Demonstration Problem 3</td>
<td>From cell to cell</td>
</tr>
<tr>
<td>Site ID</td>
<td>Location with High Carbon Layer</td>
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<tr>
<td>Length of Time step</td>
<td>30 years</td>
<td>16</td>
</tr>
<tr>
<td>Length of Simulation Time</td>
<td>3 years</td>
<td>20</td>
</tr>
<tr>
<td>Length of Interval for Migration Output</td>
<td>3 years</td>
<td>25</td>
</tr>
<tr>
<td>Length of Interval for Profile Output</td>
<td>3 years</td>
<td>25</td>
</tr>
<tr>
<td>Constituent of Concern</td>
<td>TCE</td>
<td>45</td>
</tr>
<tr>
<td>Krc</td>
<td>100 mg/kg in soil per mg/l in water</td>
<td>15</td>
</tr>
<tr>
<td>Henry’s Law Constant</td>
<td>6.4 mg/l in vapor per mg/l in water</td>
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<tr>
<td>Solubility in air</td>
<td>0.000276 atm per mole</td>
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</tr>
<tr>
<td>Diffusivity in air</td>
<td>16.0 ft²/day</td>
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</tr>
<tr>
<td>Diffusivity in water</td>
<td>0.000276 atm per mole</td>
<td>15</td>
</tr>
<tr>
<td>Site Area</td>
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<tr>
<td>Cell Thickness</td>
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<tr>
<td>Number of Cells</td>
<td>50</td>
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<tr>
<td>Recharge Rate</td>
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</tr>
</tbody>
</table>

Concentration in Recharge Water (mg/l)

Concentration in Overlying Air (mg/l)

Concentration in Groundwater (mg/l)

Water Table Enhance Control Flag

0 Plus for fixed conc; 0 for free boundary, minus for impermeable

Hydraulic Conductivity of Underlying Soil

4.0 feet per day

Underlying Groundwater Gradient

0.00030 feet per foot

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

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### 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 dissolution of the initial TCE, because the capillary fringe retards vapor migration.

**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% o maximum within 8 years. 23 grams per day to enter 1000 square foot building.

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.

**Effect of Organic Rich Layer**

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

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

**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.