The impact of fuel spills on the unsaturated zone are one of the main environmental issues when licensing new fuel stations or industrial facilities where Underground Storage Tanks (UST) are used. The development and use of fate and transport models of organic pollutants (BTEX) on the vadose zone can therefore be used to understand the behavior of these pollutants under different scenarios.

This paper describes the results obtained when using a simple one-dimensional finite difference vadose zone leaching model that describes the movement of organic contaminants within and between three different phases: (1) as a solute dissolved in water, (2) as a gas in the vapor phase, and (3) as an adsorbed compound in the soil phase. The model uses a numerical approximation of the Millington Equation, a theoretical based model for gasous diffusion in porous media. This equation has been widely used in the field of soil physics and hydrology to calculate the gaseous or vapor diffusion in porous media.

Initially, the equilibrium distribution of contaminant mass between liquid, gas and sorbed phases is calculated. Transport processes are then simulated. Liquid advective transport is calculated based on values defined by the user for infiltration and soil water content. The contaminant in the vapor phase migrates into or out of adjacent cells based on the calculated concentration gradients that exist between adjacent cells. After the mass is exchanged between the cells, the total mass in each cell is recalculated and re-equilibrated between the different phases. At the end of the simulation, (1) an overall area-weighted groundwater impact for the entire modeled area and (2) the concentration profile of BTEX on the vadose zone are calculated. The distribution of total mass of pollutants between the three phases is shown. A sensitivity analysis of the model parameters is used to set soil contamination scenarios caused by a set of BTEX spills from synthetic underground storage tanks is presented. Results demonstrate the applicability of simple numerical models for the environmental analysis of new industrial sites where soil contamination may be caused by organic pollutants.

Study area and available data

Fig. 1. Location of the study area
Fig. 2. Water extraction wells
Fig. 3. Geological schematic cross-section

Theory

VLEACH calculates the equilibrium distribution of contaminant mass between the liquid, gas and sorbed phases. Transport processes are then simulated.

- Liquid advective transport is calculated based on values defined by the user for infiltration and soil water content
- The contaminant in the vapor phase migrates into or out of adjacent cells based on the calculated concentration gradients that exist between adjacent cells. After the mass is exchanged between the cells, the total mass in each cell is recalculated and re-equilibrated between the different phases.
- These steps are conducted for each time step, and each polygon is simulated independently.
- At the end of the model simulation, the results from each polygon are compiled to determine an overall area-weighted groundwater impact for the entire modeled area.

Assumptions and limitations of the model

For computational purposes each polygon is divided vertically into a series of cells. When developing a model simulation the following assumptions are made:

- Linear isotherms describe the partitioning of the pollutant between the liquid, vapor and soil phases. Local or instantaneous equilibrium between these phases is assumed within each cell.
- The vadose zone is in a steady state condition with respect to water movement.
- The moisture content profile within the vadose zone is constant.
- Moisture gradients cannot be simulated.
- The impact of various moisture contents can be estimated by comparing results from several simulations that cover the common or possible ranges in soil moisture conditions.

Definition of scenarios - Soil and contaminant properties

<table>
<thead>
<tr>
<th>Type of soil</th>
<th>Sandy Silt</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ksat</td>
<td>0.30–2.04 (m/d)</td>
</tr>
<tr>
<td>Dry density</td>
<td>2 (g/cm³)</td>
</tr>
<tr>
<td>Effective porosity</td>
<td>0.485</td>
</tr>
<tr>
<td>Water content</td>
<td>0.278</td>
</tr>
<tr>
<td>Organic carbon content</td>
<td>0.0068</td>
</tr>
</tbody>
</table>

Table 1. Soil properties

<table>
<thead>
<tr>
<th>Type of pollutant</th>
<th>Benzene</th>
<th>Toluene</th>
<th>Ethylbenzene</th>
<th>Xylenes</th>
</tr>
</thead>
<tbody>
<tr>
<td>MW (g/mol)</td>
<td>78</td>
<td>94</td>
<td>106</td>
<td>109</td>
</tr>
<tr>
<td>Henry’s constant</td>
<td>0.221</td>
<td>0.389</td>
<td>0.921</td>
<td>0.244</td>
</tr>
<tr>
<td>Solubility (mg/l)</td>
<td>1790</td>
<td>126</td>
<td>109</td>
<td>109</td>
</tr>
<tr>
<td>App. diff. coeff (cm²/s)</td>
<td>0.904</td>
<td>0.786</td>
<td>0.657</td>
<td>1.618</td>
</tr>
</tbody>
</table>

Table 2. Contaminant properties

Scenario 1 – One-time release
- Recharge rate = 10 feet/year
- Recharge concentration = 0 ml/l
- Initial contaminant conc = 1 g/kg

Scenario 2 – One-time release
- Recharge rate = 100 feet/year
- Recharge concentration = 0 ml/l
- Initial contaminant conc = 1 g/kg

Scenario 3 – UST permanent leaking
- Recharge rate = 10 feet/year
- Recharge concentration = 100 ml/l
- Initial contaminant conc = 1 g/kg

Model results

Summary

- Scenario 3 (permanent leaking) induces greater contaminant concentration in soil for every species
- Scenarios 1 and 2 show that greater recharge rates (K) imply faster transference of contaminant through the vadose zone
- MTBE is the contaminant with greater mobility potential
- Biodegradation processes have not been taken into account in the analysis


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