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MATHEMATICAL MODELING OF BTEX CONCENTRATIONS ON THE UNSATURATED ZONE USING A SIMPLE FINITE DIFFERENCES MODEL: EVALUATION OF THE MASS DISTRIBUTION BETWEEN PHASES

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Abstract

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 different 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 absorbed compound in the soil phase. The model uses a numerical approximation of the Millington Equation, a theoretical based model for gaseous 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 to a set of 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

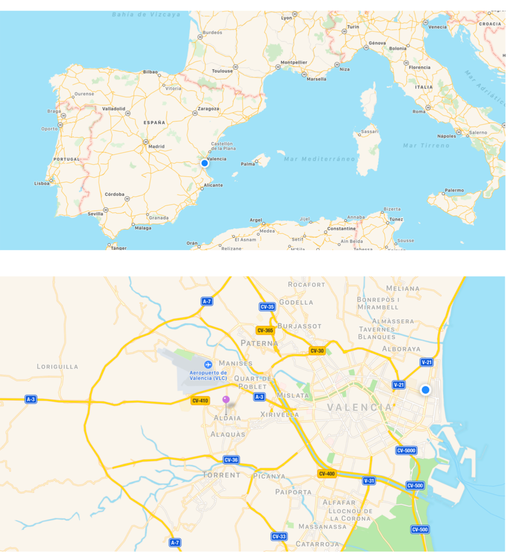


Fig. 1.- Location of the study area

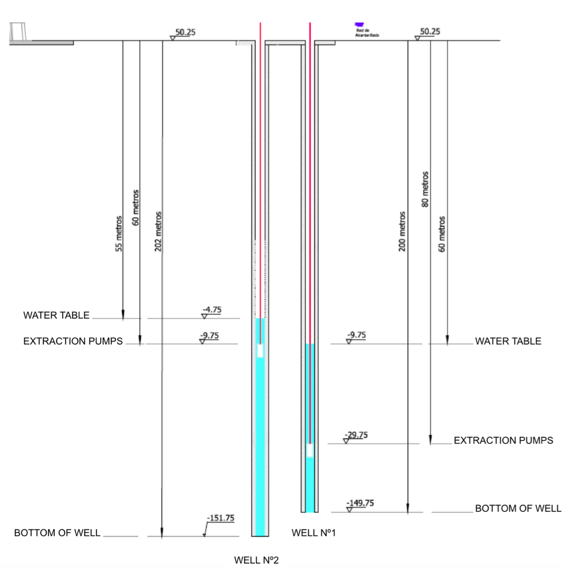


Fig. 2.- Water extraction wells

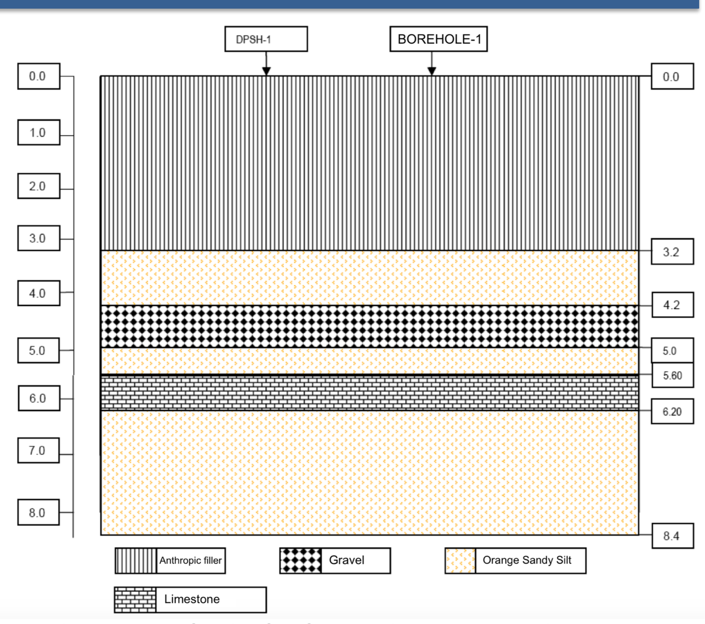


Fig. 3.- Geological schematic cross-section

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.

$$C_l(z,0) = M(z,0)\,\rho_b/\theta$$
Total initial contaminant mass

$$\frac{\partial C_1}{\partial t} = \frac{-q}{\theta}\frac{\partial C_1}{\partial t}$$
Advection equation

$$\frac{\partial C_g}{\partial t} = D\frac{\partial^2 C_g}{\partial z^2}$$
Diffusion equation

$$M_t\,(z,t) = \left[\theta C_1 + (\emptyset - \theta)C_g + \rho_b C_s\right]$$
Total mass in soil

$$C_g\,(z,t) = \frac{K_H\,M_T\,(z,t)}{[\theta + (\emptyset - \theta)K_H + K_d\rho_b]}$$

$$C_l\,(z,t) = \frac{M_T\,(z,t)}{[\theta + (\emptyset - \theta)K_H + K_d\rho_b]}$$

$$C_s = \frac{K_d\,M_T\,(z,t)}{[\theta + (\emptyset - \theta)K_H + K_d\rho_b]}$$
Individual concentrations in each phase

$C_1(Z, O)$	initial concentration in the liquid (g/ml)	q	Darcy's velocity	D	Gas diffusion coefficient (m^2/day)
M(z, 0)	initial mass per unit soil mass (g/g)	D	Gas diffusion coefficient	C_g	Concentration in the gas phase
θ	volumetric water content	Ø	Soil porosity	C_l	Concentration in the liquid phase
ρ_b	soil density (g/ml)	K_d	Distribution coefficient (ml/g)	C_s	Concentration in the solid phase

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

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

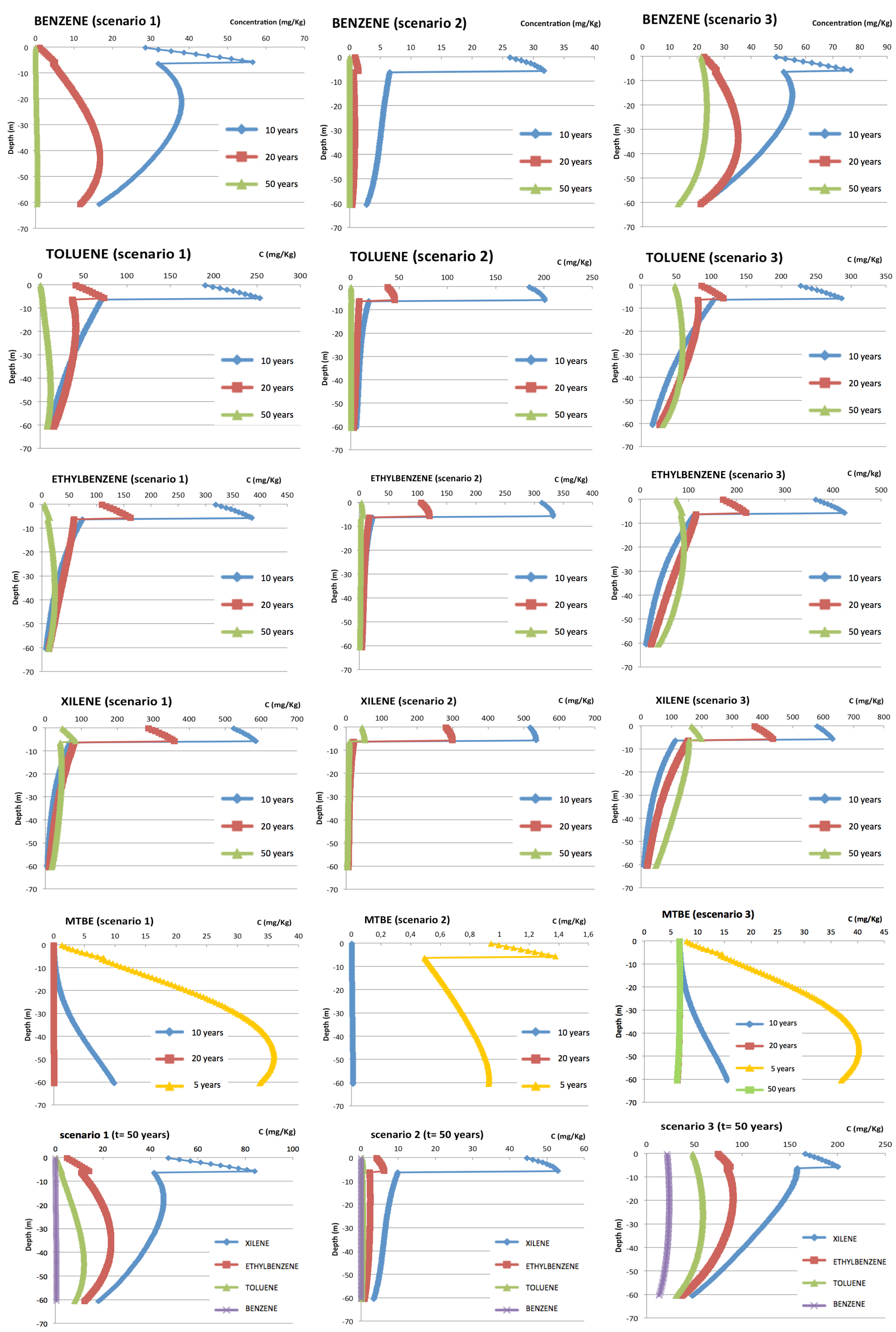
Type of soil: Sandy Silt		
K_{sat}	0,35-2,04	(feet/day)
Dry density	2	(g/cm^3)
Effective porosity	0.485	
Water content	0.078	
Organic carbon content	0.0058	

Table 1.- Soil properties

	Benzene	Toluene	Ethylbenzene	Xylene	MTBE
K_{oc} (ml/g)	58	139	220	350	12
Henry's constant	0.221	0.269	0.321	0.244	0.0224
Solubility (mg/l)	1790	526	169	106	51000
Air diff coeff (m^2/day)	0.804	0.736	0.657	0.622	0.889

Table 2.- Contaminant properties

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

References: Ravi, V. and Johnson, J.A. VLEACH, A One-Dimensional Finite Difference Vadose Zone Leaching Model. Version 2.0. USEPA

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