

Estimation of Volatile Organic Compound (VOC) Transport through Subsoil to Groundwater Using VLEACH Model

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ABSTRACT: This paper presents the transport of volatile organic compounds (VOC) through contaminated subsoil to groundwater using one dimensional vadose zone transport model, VLEACH. The model is applied using field specific data for a typical Toluene at Fuel pumping station and Transformer dumping yard. Laboratory column leaching studies were conducted to assess the mass flow rate of Toluene flux through subsoil and compared with VLEACH model output. The research also focused on the sensitivity of the model output with the varying input parameters, one at a time, across its maximum range of values identified from the study area. The observed Toluene fluxes are not consistent with the experimentally input concentrations and may not be valid due to its lower density of 0.865 g/ml. Hence, liquid phase transport of Toluene for experimental column leaching studies is not suitable. The sensitivity analysis results reveals that, model output is a function of fractional organic carbon content as well as water content.

KEYWORDS: VOC, Toluene, VLEACH, Vadose zone model.

I. INTRODUCTION

Over the past centuries, organic compounds have been used widely in industries, and large amounts of organic wastes are expelled carelessly into the subsurface from leaking storage tank, accidental spill of petroleum hydrocarbons, agricultural pesticides usage, etc. Most of these volatile organic compounds (VOCs) are toxic even when the concentrations are in several part-per-billion (ppb) (Kehua et al., 2013). One dimensional vadose zone transport model VLEACH is one of the models used to simulate the behaviour VOC is subsoil. VOCs are organic compounds that have high enough vapor pressures under normal conditions to significantly vaporize and enter the atmosphere. They are called organic because they contain carbon. VOCs are used as fuels and are components of many common house hold items like polishes, cosmetics and cleansers. Many numbers of models have been developed to know the fate and transport of VOCs through vadose zone. But, endure from uncertainties associated with input conditions. Uncertainties are due to subsoil structure and future activity in the site. This paper describes the use of one dimensional vadose zone transport model VLEACH to estimate the transport of VOC to groundwater at Fuel pumping station and Transformer dumping yard, Mysore. VLEACH is a simple model which was useful to these sites.

The transport mechanisms that govern the fate and transport of any contaminant released depends on a wide range of variable factors which are complex in nature. The transport mechanisms vary from place to place and time to time. Hence, prediction of VOC transport in subsoil need extensive and detailed field and lab studies with precise knowledge on basics of subsoil modeling concepts. The available literature and number of studies in this respect are very limited (Shahul Hameed et al., 2014).

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II. MATERIALS AND METHODS

This research applies VLEACH, a one dimensional vadose zone transport model, to predict transport of VOCs through contaminated subsoil. First, laboratory column leaching studies were carried out to know the mass flow rate of Toluene flux in subsoil. Six columns of 34 mm diameter and 250 mm length were taken and packed with sand up to 200 mm which had been baked to remove the organic carbon content. Distilled water was added to the column in order to bring it to the saturated condition. Toluene with six different concentrations for different columns was allowed to flow through soil, and was monitored periodically every hour. The laboratory column leaching studies result was compared with VLEACH model output. Secondly, VLEACH was used to predict the transport of VOC through subsoil in two study areas for field specific values. Finally, the research evaluates the sensitivity of the model output to variation in input parameters of the study areas. The parameters are replaced one at a time so as to know the effect of these parameters in the model output. The parameters are field specific values.

A. ANALYSIS

VLEACH is a one dimensional finite difference unsaturated zone transport model. The model incorporated multiple processes, including liquid phase advection, vapor phase diffusion and adsorption. These processes are conceptualized as occurring in a number of distinct user-defined polygons that are vertically divided by user defined cells. The polygons differ in soil properties, recharge rate and depth of water. At the end of the model simulation, the results of each polygon are compiled to determine an overall area weighted groundwater impact for the entire modeled area. The model produces a concentration profile of VOC as a function of depth below the contaminated zone for a selected site conditions.

B. APPLICATION OF VLEACH MODEL TO STUDY AREAS

VLEACH model is applied for site-specific conditions using field data for Fuel pumping station and KPTCL Transformer dumping yard, Mysore, Karnataka for VOC, Toluene. Field investigations of the study area have been conducted. In Fuel pumping station, the depth of groundwater is 130 ft, and varies over time. For KPTCL Transformer dumping yard, the groundwater depth is 120 ft. The soil type in both the study areas is sandy soil, which is ideal to promote downward transport of any VOCs present in the subsurface. The various parameters which are field and laboratory data were considered. Soil physical property data, consisting of soil bulk density, soil porosity, soil moisture content and soil organic Carbon content (f_{oc}); characteristics of pollutants, consisting of organic carbon partition coefficient (K_{oc}) and Henry's law constant (K_H) and recharge rate, obtained by laboratory infiltration test. The study area is divided into two polygons. The soil samples from the study area have been analyzed for one or more of the soil parameters obtained separately from polygons of the study area. The two parameters organic carbon partition coefficient (K_{oc}) and Henry's law constant (K_H) were taken from scientific literature. The sorption parameter is modeled by combining distributions of field data for f_{oc} and literature data for K_{oc} . For Toluene, K_{oc} has been considered as 139 ml/l and for K_H reported value in literature is 0.269.

III. RESULTS AND DISCUSSIONS

A. COMPARING VLEACH MODEL OUTPUT AGAINST LABORATORY COLUMN LEACHING DATA

VLEACH has been tested against experimental or field data. In one prominent case, Rosebloom et al. (1993) compared VLEACH simulations with measured field concentrations of Freon 11 and Freon 12 at a site characterized by silty and clayey soils, finding close agreement with field data. VLEACH was simulated by controlled experiments conducted by Cho and Jaffe (1990). The experiments of Cho and Jaffe characterized gas phase transport of a VOC volatilizing and diffusing counter current to a steady infiltration of water. The experimental columns were packed with sand that had been baked to remove the organic carbon content. Water was introduced from the top of the column and allowed to percolate downward. An aqueous solution of TCE was placed at the bottom of the vertical column such that TCE could diffuse upwardly. The TCE flux was monitored at the top of the column. The VLEACH simulated the

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observed fluxes reasonably well in five of seven cases. In six cases, VLEACH over predicted the TCE flux, supporting the expectation that VLEACH will provide conservative results.

This section evaluates VLEACH by simulating controlled experiments, liquid phase transport of Toluene. The experimental columns were packed with sand that had been baked to remove the organic carbon content. Water was introduced from the top of the column and allowed to percolate downward to bring soil to saturated condition. An aqueous solution of Toluene was introduced from the top of the column and Toluene flux was monitored at regular interval of time. Table 1 compares VLEACH derived Toluene fluxes with laboratory observed fluxes, the laboratory results fail to reproduce the results reported by VLEACH, the reported Toluene fluxes are not consistent with the experimentally input concentrations and may not be valid. This is because the volatile compounds like Toluene are less dense with density of 0.865 g/ml. so, liquid phase transport of Toluene for experimental column leaching studies is not suitable.

Table 1 Comparison of laboratory column studies result with VLEACH output

No. of columns	Column length (ft)	Infiltration rate (ft/year)	Toluene input concentration (mg/l)	Toluene flux	
				Lab observation	VLEACH (g/hr)
1	0.7	173.45	230	7.87	0.0098
2	0.7	173.45	280	6.23	0.0121
3	0.7	3448	320	56.00	0.0110
4	0.7	173.45	138	13.62	0.0057
5	0.7	173.45	160	1.90	0.0062
6	0.7	173.45	190	5.62	0.0081

B. VLEACH CALCULATIONS FOR FUEL PUMPING STATION

The soil samples collected from the site was analysed for the type of VOC present, Toluene was the compound traced with 159 mg/kg. Field data's were incorporated to VLEACH model. The area of contaminated soils was divided into two polygons which were simulated as one dimensional column with VLEACH. It provides the sum of mass loading per year for the two polygons as output. Mass loading predicted by VLEACH is shown in Figure 1 and it refers to the mass per unit time (g/year) estimated to reach the groundwater table from the entire area of contaminated soils. More than 4218 g/year of Toluene is estimated to be entering the groundwater from the vadose zone due to existing soil contamination. The mass loading is estimated to decrease with time.

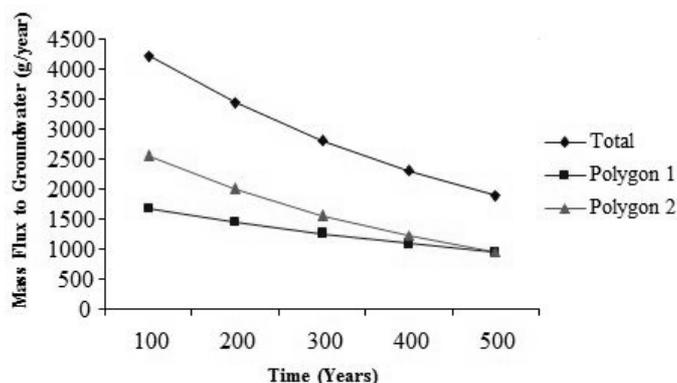


Figure 1 Plot of Mass Flux to Groundwater versus Time

C. VLEACH CALCULATIONS FOR KPTCL TRANSFORMER DUMPING YARD

The soil samples collected from the site was analyzed for the type of VOC present, Toluene was the compound traced with 1993 mg/kg. Field data's were incorporated to VLEACH model. The area of contaminated soils was divided into two polygons which were simulated as one dimensional column with VLEACH. VLEACH provided the sum of mass loading per year for the two polygons as output. Mass loading predicted by VLEACH is shown in Figure 2 and it refers to the mass per unit time (g/year) estimated to reach the groundwater table from the entire area of contaminated soils. More than 12631 g/year of Toluene are estimated to begin entering the groundwater from the vadose zone due to existing soil contamination. The mass loading is estimated to decrease with time.

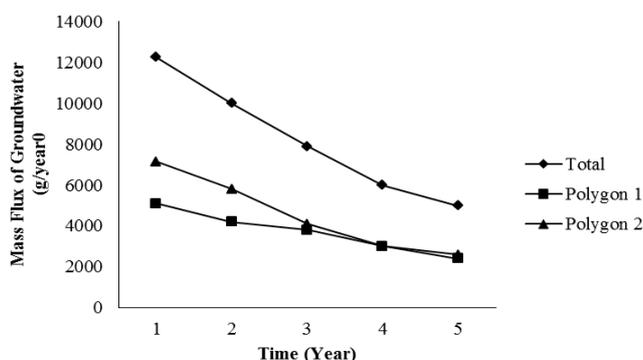


Figure 2 Plot of Mass Flux to Groundwater versus Time

D. SENSITIVITY ANALYSIS

Sensitivity analysis is the study of how the variation (uncertainty) in the output of a model can be apportioned, qualitatively or quantitatively, to different sources of variation in the input of the model. VLEACH output evaluates; maximum liquid phase contaminant concentrations in the vadose zone at the postulated depth to groundwater; and the number of years past initiation when those maximum concentrations will occur.

Results of the sensitivity analysis, in general Toluene transport in the vadose zone is slower with an increase in the soil organic content fraction (f_{oc}). This would promote sorption onto soil particles, and therefore retards transport. Increasing infiltration rate q produces faster VOC transport, because water movement downward through the soil carries VOCs in the liquid phase by the advective driving force, but in this study whatever may be the infiltration rate it doesn't affect Toluene transport. Increasing soil bulk density produces slower Toluene transport by effectively increasing retardation by sorption. Increasing soil porosity leads to faster Toluene transport by similarly increasing retardation and increasing water content in soil leads to slower Toluene transport because soil water occupies soil pores, inhibiting gaseous phase diffusion. These results may be compared to the VLEACH sensitivity analysis performed by Donald Duke et al. (1998).

IV. CONCLUSIONS

This research evaluates the transport of volatile organic compound namely Toluene through subsoil has been studied. Based on the results obtained from laboratory and field data's the following conclusions are made.

- VLEACH model is widely used in areas with deep vadose zones, low rainfall areas, and deep surficial deposits of coarse grain sandy, alluvial sediments; validation and testing of vadose zone transport models are difficult due to uncertainties associated with soil contaminant release time and quantity, soil sampling, sample transport and model assumptions.
- The validation of VLEACH is still limited because laboratory soil column studies in liquid phase are not suitable for the compound like Toluene because of its lower density.

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- The variability in the estimate of soil water content and fraction organic carbon content was found to be most significant among the key modeling parameters.
- Groundwater contamination due to long term migration of VOC exist indirectly from thick vadose zones.
- The results obtained from laboratory and field test suggest that model outcomes based on best estimate values of parameters are not adequate to characterize future VOC transport in the vadose zone.

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