

An Effective Soil Vapour Extraction / Bioventing Model

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ABSTRACT

Leaking underground storage tanks are one of the largest sources of soil contamination, and are considered an international problem. Soil remediation through soil vapour extraction (SVE) and bioventing (BV) are popular in situ technologies for the treatment of the hydrocarbon contaminated soil. The design of both systems involves a complex interplay of physical, chemical and biological processes, which together can address the problem of tailing. Tailing is one of the most important phenomena governing the clean-up achievement. When tailing is observed during SVE operation, the conversion to a BV system is a feasible and efficient method in reducing remediation time. However, the optimum time to start BV is not known, accordingly the need of an overall accurate mathematical representation is required.

To address the modelling efficiency, a comprehensive three-dimensional model is being developed. It is specifically designed to simulate SVE and BV. In this model, equations describing multiphase flow, single component advective diffusive transport, and biodegradation are coupled in a framework that allows for numerical simulation of advective gas phase fluxes, typical of remediation applications. First order biodegradation kinetics will be used to describe the growth of microorganisms. In addition, independent mass transfer models of hydrocarbons in the soil, mass transfer of oxygen, and biochemical reaction in an aqueous solution will be incorporated in to the model to represent an accurate SVE/BV system. The resulting non-linear equations are solved using HEMLAB, a commercial package that uses the iterative finite element method. Data for model calibration comes from the laboratory work of the Soils Research Group at the School of Engineering. Having an appropriate 3 D model will improve prediction capabilities and permit the prediction of the time to switch from SVE to BV. It will also reduce the cost of the remediation process. This paper will present the progress made on the model.

Key words: soil vapour extraction, bioventing, soil remediation, modelling

INTRODUCTION:

Leaking underground storage tanks are one of the largest sources of soil contamination, and are considered an international problem. Soil remediation through soil vapour

extraction (SVE) and bioventing (BV) are popular *in situ* technologies for the treatment of the hydrocarbon contaminated soil. Soil vapour extraction (SVE), also known as soil venting or vacuum extraction, is an *in situ* remedial technology that reduces concentrations of volatile constituents in petroleum products dispersed throughout the soil in the unsaturated (vadose) zone.

In SVE, a vacuum is applied through wells near the source of soil contamination. The vacuum evaporates the volatile constituents of the contaminant and the vapours are drawn toward the extraction wells. The extracted air is then treated as necessary before being released to the atmosphere. Some of the factors that determine the effectiveness of SVE include soil structure and stratification, soil moisture and soil permeability.

Soil structure and stratification affect SVE because they can impact how and where soil vapors will flow through the soil matrix under extraction conditions. Permeability of the soil further impacts the rate of air and vapor movement through the soil, where higher the soil permeability, faster the movement and greater the amount of vapors that can be extracted. However, high water content can reduce soil permeability, and consequently, the effectiveness of SVE.

A great deal of SVE studies are being conducted from an experimental and modeling standpoint. All models vary great in the level of complexity and in the processes included (Abriola et al., 1996). However, these SVE models suffer from the lack of testing against appropriate data, which affects their ability to predict performance at other conditions. At the 3 D level, a major drawback is the lack of validation with real site data that represent soil type, subsurface layering, contaminate type and moisture content (Wilson, 1995). Further impacting the models is the lack of mass transfer coefficients to represent rate-limitations in SVE that has been demonstrated in the literature. Obtaining the required mass transfer coefficients currently requires calibration against laboratory experiments (Gidra, 2003).

Without the proper mass transfer coefficient, it is difficult to study the cause of tailing or make predictions on how effective SVE would be to remediate a given site. Generally though, it is understood that SVE is effective in removing the light fractions found in petroleum products (USEPA, 1995). The difficulty arises with the weathered or heavier fractions, which are considered the main causes of tailing. Fortunately, petroleum products are biodegradable to a certain degree, and consequently the heavier petroleum fractions products may be suitable for removal by bioventing.

Bioventing is an *in situ* remediation technology that aerate soils to stimulate indigenous microorganisms to biodegrade organic constituents adsorbed to soil in the unsaturated zone and to promote bioremediation (Leeson and Hincee, 1997). In bioventing, the

activity of the indigenous bacteria is enhanced by inducing air (or oxygen) flow into the unsaturated zone (using extraction or injection wells), and if necessary, by adding nutrients.

Bioventing differs from SVE in one fundamental way, in that the objective is to induce only sufficient airflow to enhance natural biodegradation of the contaminants and not cause the contaminants to volatilize. According to the literature, the most important factors that control the effectiveness of bioventing are the permeability of the petroleum-contaminated soils and biodegradability of the petroleum constituents. Permeability affects the rate at which oxygen can be supplied to the hydrocarbon-degrading microorganisms found in the subsurface, while degradability affects the rate and degree to which the constituents will be metabolized by the microorganisms.

The proposed research is being completed in two phases. Phase I was designed to formulate a 3 D SVE model based on the governing equations used by Armstrong et al. (1997). This model was then calibrated with 3-D lab data generated in the School of Engineering (Duggal and Zytner, 2004). Phase II of this research is the development of bioventing model. It will incorporate biodegradation kinetics according to lab data. Having an effective SVE-bioventing model will give researchers and consultants the ability to evaluate different remediation scenarios and will reduce the cost of the remediation process. This paper will concentrate on the progress of Phase I of the research and provide an overview of Phase II.

METHODOLOGY

Developing a 3 D model to describe both SVE and bioventing requires equations that describe the conditions in the subsurface environment and yet simplify the study region. A numerical solution technique is then needed to solve the system of equations. For this research, FEMLAB was selected to solve the system of equations. FEMLAB is based on the finite element method, and incorporates MATHLAB, giving maximum flexibility to the researcher. FEMLAB is a package provided by COMSOL Inc., Burlington, MA.

The following sections outline the system of equations used to represent the important spatial and temporal variations in the site conditions.

Soil Vapour Extraction

Soil vapour extraction in unsaturated porous media involves several physical and chemical processes. These processes include volatilization, diffusion, residual saturation, and multiphase transport of hydrocarbons. The design of an efficient SVE system is a complex process due to the number of parameters and variables in the physico-chemical

processes. The SVE process is described by two main partial differential equations. Equation 1 represents vapour flow through the porous medium, while Equation 2 represents the advective and diffusive transport of the vapours.

$$\begin{aligned} & \left[\frac{\partial}{\partial x} (K_s \cdot \frac{\partial P}{\partial x}) + \frac{\partial}{\partial y} (K_s \cdot \frac{\partial P}{\partial y}) + \frac{\partial}{\partial z} (K_z \cdot \frac{\partial P}{\partial z}) \right] + \frac{\mathbf{m}}{K_{xy}} \cdot Q_v \\ & = \left(\frac{\mathbf{m}}{K_{xyz}} \right) \cdot \left(\frac{Sc}{\mathbf{r} \cdot \mathbf{g}} \right) \cdot \frac{\partial P}{\partial t} \end{aligned} \quad (1)$$

where

- Sc = storage coefficient (cm⁻¹)
- K_S = relative permeability (dimensionless)
- K_{xyz} = intrinsic permeability (cm²)
- P = pressure (g/cm·s²)
- ρ = gas density (g/cm³)
- g = acceleration constant due to gravity (cm/s²)
- Q_v = source term (cm³/cm³-s)
- μ = viscosity of air (g/cm·s)

$$\begin{aligned} & \frac{\partial}{\partial x} (\mathbf{q}_g \cdot D_{xx} \cdot \frac{\partial C}{\partial x}) + \frac{\partial}{\partial y} (\mathbf{q}_g \cdot D_{yy} \cdot \frac{\partial C}{\partial y}) + \frac{\partial}{\partial z} (\mathbf{q}_g \cdot D_{zz} \cdot \frac{\partial C}{\partial z}) - \mathbf{q}_g \cdot V_x \frac{\partial C}{\partial x} \\ & - \mathbf{q}_g \cdot V_y \frac{\partial C}{\partial y} - \mathbf{q}_g \cdot V_z \frac{\partial C}{\partial z} + Q_c = R \cdot \frac{\partial}{\partial t} (\mathbf{q}_g \times C) \end{aligned} \quad (2)$$

where,

- V_i = gas velocities in x, y and z direction (cm/s)
- D_i = coefficient of dispersion x, y and z direction (cm²/s)
- q_g = volumetric content of gas (cm³/cm³)
- R = retardation coefficient (dimensionless)
- Q_c = source term due to volatilization (g/sec-cm³)

An important step in coupling Equations 1 and 2 is the mass balance. Assuming that the NAPL phase is immobile, the mass balance equation for fluid phases can be written as:

$$\frac{\partial(\mathbf{q}_l \cdot \mathbf{r}_l)}{\partial t} = Q_c \quad (3)$$

where,

$$\begin{aligned}\theta_l &= \text{volumetric liquid content (cm}^3\text{/cm}^3\text{)} \\ \rho_l &= \text{liquid density (g/cm}^3\text{)} \\ t &= \text{time (s)}\end{aligned}$$

Biodegradation Kinetics

In order to incorporate bioventing into the model, biodegradation kinetics need to account for a variety of parameters including temperature, soil moisture, carbon source and soil pH. These all affect the amount of compound transformed per unit time. Obtaining the appropriate mathematical expression that describes the transformation is the challenge given the variety of metabolism in the laboratory or field.

For Phase II, lab data from related work in the School of Engineering will be reviewed to develop the kinetic equation. Based on the initial results, a first order expression will be tried as indicated by:

$$-\frac{dS}{dt} = k_1 \cdot S \quad (4)$$

where:

$$\begin{aligned}t &= \text{time (sec)} \\ S &= \text{substrate concentration at time } t \text{ (mg/L)} \\ k_1 &= \text{first order rate constant (sec}^{-1}\text{)}\end{aligned}$$

When using the first order decay model, it is considered that the substrate concentration is much less than the half-saturation constant, there are no excess microorganisms and the rate is proportional to the concentration of a single substrate (Cookson, 1995; and Hers et al., 2000). As Phase II evolves, other factors and conditions will be evaluated and the degradation kinetics modified.

RESULTS AND DISCUSSION

The importance of having an accurate model to describe SVE and bioventing is shown by Figure 1. Figure 1 shows that when tailing occurs, the continued running of remediation removes successively smaller amounts of contaminant. This is seen through the off gas concentrations which are initially high followed by a gradual decrease due to the development of mass transfer limitations, which may persist for extended times. In some cases when the SVE system is shut off, the off gas concentrations slowly rebound due to

equilibrium conditions being restored. The tailing phenomenon caused by SVE makes it a challenge to close the site as the soil concentrations remain above the required clean-up level.

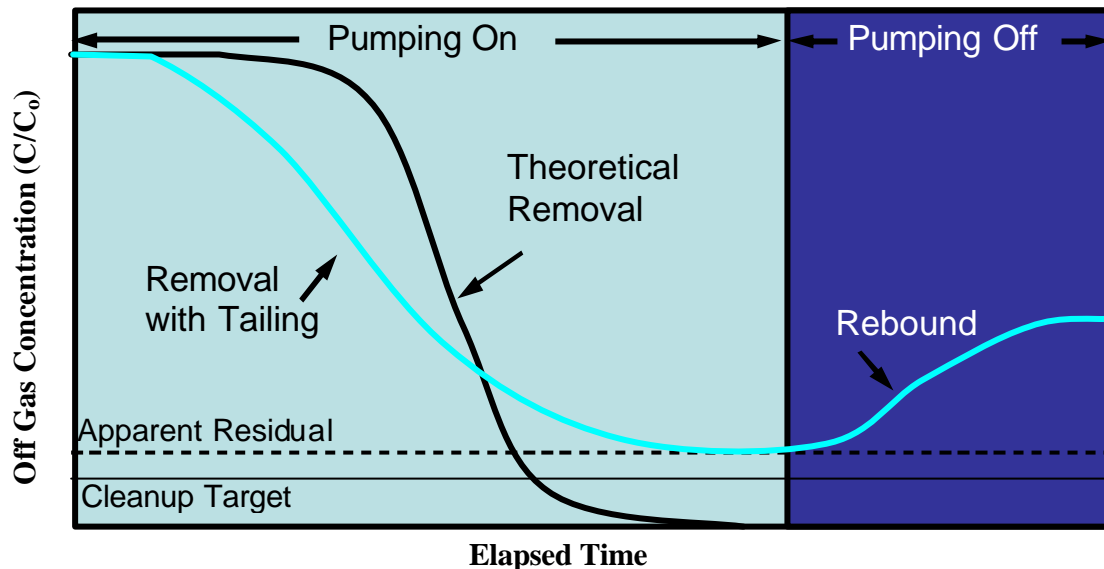


Figure 1: Tailing phenomena in soil remediation

Tailing is also evident in the lab work conducted by Harper et al. (2003), as seen in Figure 2. The work shown here is based on 1-D lab work and modelling with Elora Silt Loam soil. It can easily be seen that as the water content increases, so does the evidence of tailing. In the high water case, continued SVE would be very inefficient in remediating the site. Ideally bioventing could be used, but insufficient knowledge is available to know when to switch from SVE to bioventing.

Research completed to-date has shown that tailing in SVE and bioventing is the result of many factors, either in isolation or in combination. These factors include:

- Lower airflow rate in low permeability, finer-grained soils media
- High soil water content that blocks contaminant from the advecting airflow and restricts oxygen from getting to the degrading microorganisms
- Sorption of contaminant to organic matter which causes retardation of chemical movement from one phase to another
- Age of spills which causes lower overall vapour pressure and increased sorption of contaminant with the soil
- Development of preferential airflow patterns in heterogeneous soils which may create lower airflow rates.
- Diffusion controlled mass transfer
- Insufficient nutrients to stimulate the microorganisms
- High levels of contaminant which inhibit the growth of the microorganisms

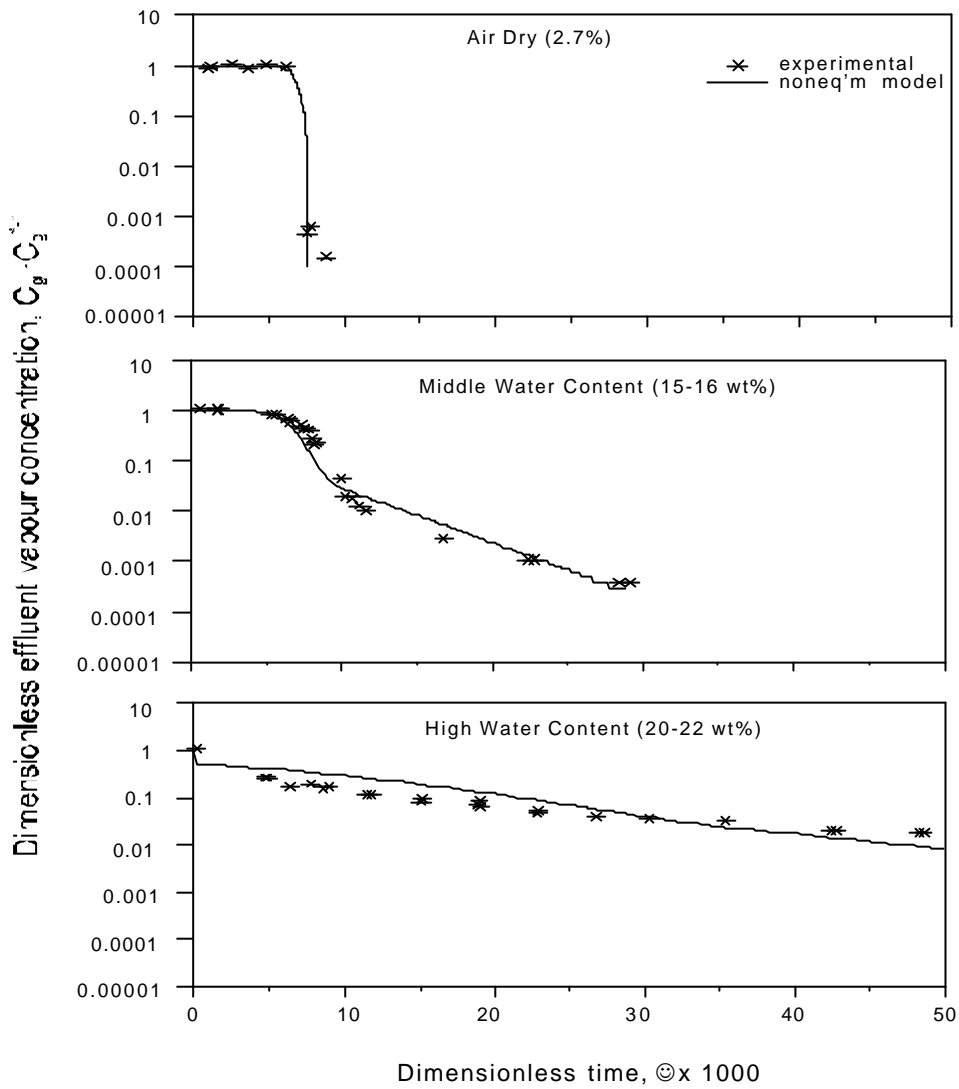


Figure 2: Behaviour of toluene at different water contents

Source: Harper et al, 2003

SVE Model

The initial step in model development was the creation of a 2 D model using FEMLAB. The model was based on the work of Armstrong et al. (1997), which included the overall mass transfer expression given in Equation 5. Table 1 gives the input data.

$$a = b \cdot (K_L a) \cdot q_o^{0.67} \quad (5)$$

where

- K_{La} = overall mass transfer coefficient of the particular constituent in free atmosphere (sec-1)
 β = shape factor as function of pore geometry and residual liquid distribution in the media
 θ_o = volumetric content of residual liquid (dimensionless).

Table 1. Values used in simulations

	Parameter	Armstrong et al. (1997)	Duggal and Zytner(2004)
ρ_b	Bulk Density	1.67 g/cm ³	1.55 g/cm ³
V	Soil volume	18000 cm ³	60000 cm ³
K_x, K_y	Intrinsic permeability	2.5x10 ⁻⁸ cm ²	3.1x10 ⁻⁸
R	The Gas law constant	83.145 cm ² .g/s ² .mole. ^o K	83.145 cm ² .g/s ² .mole. ^o K
T	The absolute Temperature	72.0 ^o F	72.0 ^o F
g	Gravity acceleration	980.665 cm/s ²	980.665 cm/s ²
a_L	Longitudinal dispersivity length	2.0 cm	2.0 cm
a_T	Transverse dispersivity length	2.0 cm	2.0 cm
P_{in}	Pressure at nodes	1.0x10 ⁶ g/cm.s ²	1.01325x10 ⁶ g/cm.s ²
P	Pressure at well	1.0x10 ⁵ -1.0x10 ⁷ g/cm.s ²	1.00531x10 ⁶ g/cm.s ²
μ	Air viscosity	1.86x10 ⁻⁴ g/cm.s	1.86x10 ⁻⁴ gm/cm.s
ρ_{air}	Air density	1.20x10 ⁻⁵ g/cm ³	1.20x10 ⁻⁵ g/cm ³
θ	Total porosity	0.37	.416
θ_r	Irreducible moisture content	0.01 cm ³ /cm ³	0.01 cm ³ /cm ³
P_c	Critical pressure	40.0 atm	40.0 atm
M	Molecule weight of Toluene	92.13 g/mole	92.13 g/mole
D_o	Diffusion coefficient in air	0.84 cm ² /c	0.84 cm ² /sec
ρ	Toluene density	0.8669 g/cm ³	0.8669 g/cm ³
C_o	Initial concentration in soil	60 g/g-soil	0.027 g/g- soil

The solved model was able to match the results of Armstrong et al. (1997). In doing so, it was determined that the overall mass transfer coefficient was estimated to be constant value of 5.5x10⁻⁴ (1/s).

The next part of Phase I was to convert the model to 3 D. After making the necessary code changes, the laboratory work of Duggal and Zytner (2004) was used to calibrate the model. The data was based on a large scale SVE reactor that had a height of 46.5 cm,

diameter of 41 cm and with a well diameter of 4.2 cm. Ottawa Sand and Elora Silt soils were used. The experiment was conducted at different flow rates and pressure drops at the suction well. The initial contaminant concentration in the soil was 0.027 g-toluene/g-soil, with the initial steady state vapour concentrations of toluene at 20 C° at 110.06 g-toluene/L-air.

For the initial runs, the same mass transfer coefficient used in the Armstrong et al (1997) runs were used. Table 1 gives the values of the remaining parameters.

Using the 3 D model developed and the data collected by Duggal and Zytner (2004), it was possible to predict the general behaviour of the SVE system as shown in Figures 3 and 4. Even though the simulation used a constant mass transfer coefficient the fits were reasonable, with the model being able to match the tailing behaviour of the experiments. It is believed that when the mass transfer coefficients measured by Gidda (2003) are incorporated, the predictions will improve and capture the complete data trend. The promising part is that a 3 D model has been developed that can be used to model 3 D data generated in the laboratory. It is also expected that the model will work favourably when data from field sites is used.

When working on a numerical model, it is always important to check sensitivity of the model. Sensitivity studies have shown that the model is highly sensitive to changing values of intrinsic permeability. This is important as the soils most likely to show tailing are those with low permeability. Additionally, the change in the volumetric gas content and the liquid content (NAPL phase) versus the time was explored. Figure 5 shows that the liquid content reaches a constant value at time of 50 hours, which is similar to when the off gas concentration is constant. This shows that SVE research should concentrate on accessing the NAPL contamination that is dispersed through the soil. While obvious, it will be difficult due to the complexity of unsaturated soil and all the physical-chemical parameters that affect how the NAPL is dispersed and retained in the soil.

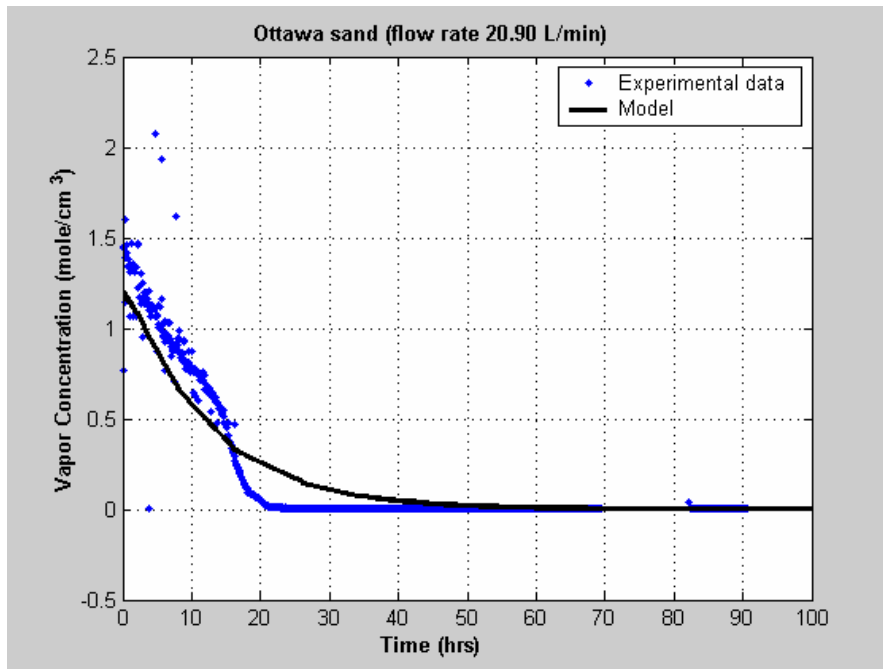


Figure 3: Vapor Concentration vs. Time (hrs) for excremental data and model prediction

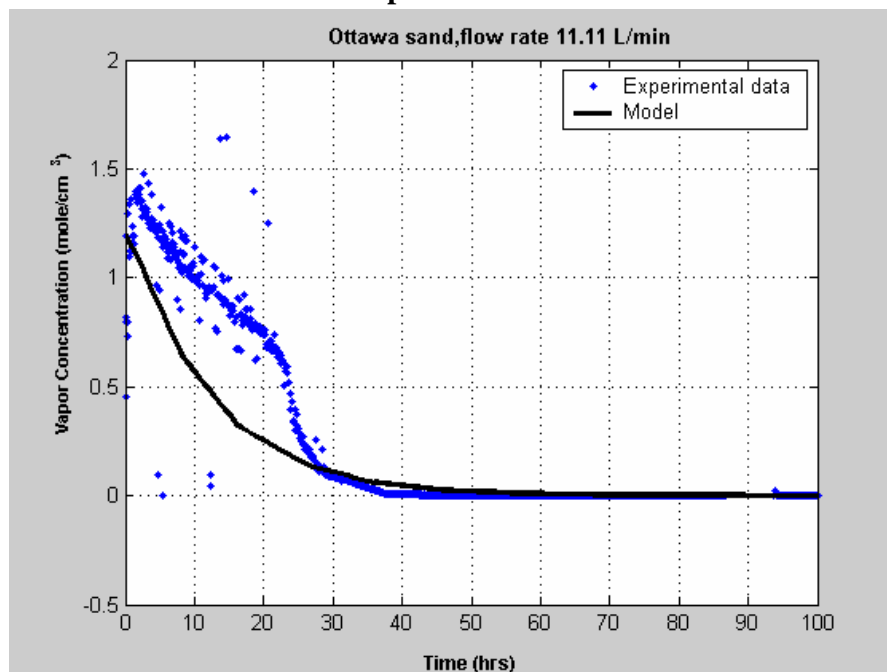


Figure 4: Vapor Concentration vs. Time (hrs) for excremental data and model prediction

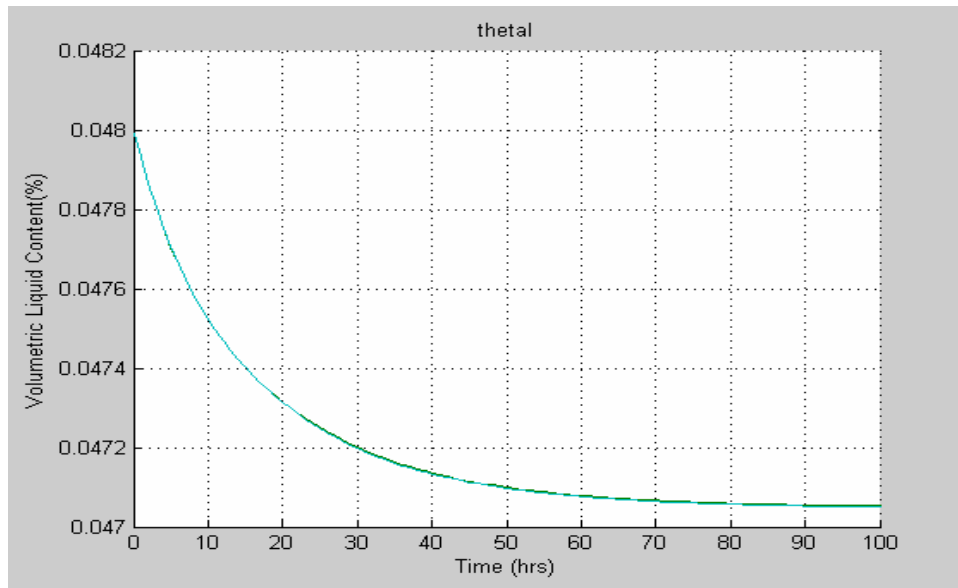


Figure 5: Changing of Volumetric gas content during the experiment.

Once Phase I of the research is complete, work will begin on the 3 D model that incorporates bioventing. The initial step of determining the biodegradation rate coefficients has been completed. Work is also progressing on a large scale bioreactor that will provide calibration data for bioventing portion of the model. Having the user friendly model will assist researchers and consultants with improving their understanding of SVE and bioventing remediation. It will assist consultants in predicting when to convert from SVE to bioventing and ultimately how long the entire remediation process will take. The end result being an improved soil environment, with a lower remediation cost.

CONCLUSIONS:

Research has been conducted in two phases. Phase I concerned the development of a 3 D SVE model which has been calibrated with 3 D lab data. On going work is the incorporation of the appropriate mass transfer coefficients that help explain all parts of the remediation cycle. Phase II involves the incorporation of a biodegradation component. Having an overall SVE/BV model will give remediation consultants an important tool to predict the time to switch from SVE to bioventing and the time required to achieve clean-up. Finally, at the end of this project, the better understanding of SVE/BV performance will result in lower remediation costs.

ACKNOWLEDGEMENTS

The authors wish to acknowledge the support of the NSERC of Canada in the form of a Strategic Research Grant and a Discovery Grant.

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