



Project Summary

Forced Air Ventilation for Remediation of Unsaturated Soils Contaminated by VOC

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Many cases of soil vacuum extraction (SVE) applications in the field have been reported, but very few systematic studies about physical and chemical processes in soil air are found. Parameters which were expected to control the removal process of VOCs from contaminated soil during the SVE operation were studied by means of numerical simulations and laboratory experiments in this project.

Experimental results of SVE with soil columns in the laboratory indicated that the removal efficiency of VOCs from soil columns was a complicated function of air flow and the hydrogeometry inside. The partition process between air and the immobile liquid was not an equilibrium one, and the interfacial mass transfer varied with the residual amount of VOCs in the soil. Additional experiments under various conditions should be conducted to obtain further insight into the SVE process.

Two computer models were developed to study soil air and VOC movement during the SVE process. The first one was an analytical approximate model which could be used for the simulation of air movement in the SVE operation with multiple wells in homogeneous soil media. The second one was a numerical model in three-dimensional geometry which used a finite difference solution scheme. A simple pneumatic pump test was conducted, and parts of test data were used for the validation of the simple analytical model.

This Project Summary was developed by EPA's Robert S. Kerr Environmental Research Laboratory, Ada, OK, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

Fuel leakage and spills are the most frequent sources of soil and ground-water contamination at service stations and underground storage tank areas. A large portion of released hydrocarbon infiltrates the subsurface and remains bound under capillary pressure as a residual immiscible phase liquid. The residual hydrocarbon serves as a continuous source for ground-water contamination. Therefore, the reclamation of the contaminated aquifer should include removal of the long-term contamination source. The cleanup of soil contaminated by Volatile Organic Contaminants (VOCs) is generally an expensive operation due to the high cost associated with excavation, transportation, and disposal. Classic methods such as soil removal, forced percolation, encapsulation, or trenching are frequently impossible or prohibitively expensive, especially in the midst of an industrial or residential area.

An alternative method to remediate soils is the use of the soil vacuum extraction (SVE) system. This process has proven to be inexpensive and effective for the cleanup of soil and ground water contaminated by solvents and volatile components of petroleum products. The cost of installation and



operation of an SVE system is usually lower than the cost of other methods. Another major advantage is that this method is an *in-situ* process. The contaminated soil remains in place and is not excavated and disposed of in other locations. The SVE system is also used for the control of methane gas migration from landfills. Methane and carbon dioxide, which are generated by microbial decomposition of organic materials, can migrate a long distance from the landfill and build up to explosive levels. The SVE wells, sometimes with interdiction walls, are installed to prevent the migration of methane gas. In spite of many field applications, very few scientific or systematic studies have been reported. Therefore, the design of the SVE system has been mainly dependent on experience and rough estimations. Sometimes, prototype or pilot-scale systems are used to obtain design parameters such as well depths, well spacings, and extraction rates.

The objective of this project was to investigate the movement of VOCs in soil air during the SVE process. Several physical and chemical processes are involved in the movement of VOCs in soil air, including convective and diffusive transport, interfacial mass transfer between immiscible phases, and biological/chemical transformations. Physical and chemical properties of soil and VOCs are expected to control these processes. The ultimate goal of this project was to obtain knowledge on relationships among the various properties and processes of VOC transport in soil air. These relationships were integrated in computer models. This report includes laboratory experiments and field tests of SVE in relatively simple systems. The model development procedures are also included in this report.

Process of Soil Vacuum Extraction

The basic principle of SVE is very simple. Air flow is induced in the subsurface by a pressure gradient applied through vertical wells or horizontal trenches. The flowing air sweeps out VOCs by vaporizing highly volatile components from soil pores, and the contaminated soil air is collected by extraction wells. Effluent air from extraction wells is often treated by off-air treatment systems, i.e., an activated carbon tank or catalytic converters. A typical SVE system consists of air pumps or blowers connected to a series of wells located in contaminated soil. The lower pressure inside the extraction well generated by pumps causes soil air to move to the well. Sometimes air injection wells are added for the further control of air flow. VOC

movement in convective and diffusive modes is considered as the main process of chemical transport during the SVE operation. When there is an induced pressure gradient, the bulk phase of soil air moves and carries a large amount of VOCs in the convective transport mode. Especially in the close vicinity of wells and trenches, a large pressure gradient is developed and the convective transport dominates the movement of VOCs. At remote areas from wells, the pressure gradient becomes very small. VOC transport in these remote locations from the wells is expected to be slow because of the diffusive transport. In addition to the convective and diffusive movements, VOC transport in soil air during SVE is expected to be influenced by several other processes including the partition process among gas, liquid and solid soil matrices, and biological/chemical transformations. Biological/chemical transformation processes of VOCs were not investigated in this project.

Soil Air Flow

The VOC concentration in soil air is usually low, and the changes in thermodynamic and transport properties of soil air due to the concentration change are not significant. Therefore, air flow is considered to be independent of the VOC concentration in soil air and treated explicitly from VOC transport. In cases where changes of physical and chemical properties due to the high concentration of VOCs in soil air are significant, iterative or updating computational procedures should be used to solve the coupled problems.

Three basic equations are considered in the description of air flow: the mass balance equation of soil air, the flow equation due to pressure gradients, and the equation of state. The mass balance of soil air is expressed by the equation of continuity.

$$\phi_a \frac{\partial \rho_a}{\partial t} = -\nabla \rho_a \mathbf{V} \quad (1)$$

where the ϕ_a is the air-filled porosity in soil, ρ_a is the density of soil air, and \mathbf{V} is the velocity vector of air flow. The air flow velocity due to the pressure gradient can be expressed by Darcy's law when the slip flow is negligible. In the case of air flow in sand and gravel, the slippage of air on the soil wall is negligible and Darcy's law for the flow in porous media can be applied.

$$\mathbf{V} = \frac{k_a}{\mu_a} \nabla p \quad (2)$$

where k_a is the soil-air permeability tensor and μ_a is the viscosity of air.

The density of air is a function of pressure and temperature. The relationship among these parameters is expressed by the equation of state. One of these equations of state is the ideal gas law, which is simple and applicable for soil air at low pressure. The ideal gas law can be used because the operating pressure of the conventional SVE is close to ambient or lower. The ideal gas law for soil air is

$$\rho_a = \frac{\rho \text{ MW}}{R T} \quad (3)$$

where MW is the molecular weight of soil air, R is the ideal gas law constant, and T is the absolute temperature. By combining the above equation, a general soil air flow equation can be obtained.

$$\phi_a \frac{\partial \left(\frac{M W}{R} \frac{\rho_a}{T} \right)}{\partial t} = \nabla \left(\frac{\rho_a k_a}{\mu_a} \nabla p \right) \quad (4)$$

This equation is nonlinear because the air density, ρ_a , in the right hand side of the equation is a function of pressure.

VOC Fate and Transport

VOCs can be present in the subsurface soil in five basic ways: (1) as a residual immiscible liquid phase in the soil pore spaces, (2) as a floating product above the water table in the case of light hydrocarbon or as a pooled or continuously migrating liquid of a dense nonaqueous phase to the bottom of the ground water, (3) as a vapor in soil air, (4) as dissolved components in soil pore water and ground water, and (5) as adsorbed hydrocarbons on soil particles or organic compounds on the particle surfaces. When soil air remains undisturbed after spillage and infiltration to the subsurface, it becomes saturated by the VOC vapor evaporated from the liquid phase. This highly saturated air will be removed initially after SVE starts. As the vapor is purged from soil pores, the concentration of VOCs in soil air begins to decrease as the process shifts away from equilibrium. At this stage, the interfacial mass transfer between the liquid and flowing air is expected to control the removal of the VOC from soil. Soil air in the SVE system moves much faster than the liquid phase inside soil pores. Therefore, residual immiscible liquid, soil pore water, and solid particles are considered as an immobile phase.

The convective transport by bulk air flow and diffusive transport due to the concentration gradient are the major transport processes. The mass flux of the VOC component A is

$$N_A = c_A V - \phi_a D \nabla c_A \quad (5)$$

where c is the concentration of the component A in soil air, V is the velocity vector of air flow, ϕ is the air-filled porosity in soil, and D is the diffusivity.

The mass balance of the component A in soil air becomes

$$\begin{aligned} \phi_a \frac{\partial c_A}{\partial t} &= -\nabla N_A + S_a \\ &= -\nabla c_A V + \nabla \phi_a D \nabla c_A + S_a \end{aligned} \quad (6)$$

where S_a is the source/sink term of soil air.

The mass balance of the component A in the immobile phase becomes

$$\phi_l \frac{\partial C_A}{\partial t} = -S_l \quad (7)$$

where ϕ_l is the pore volume occupied by the immobile phase, C_A is the concentration in the immobile phase, and S_l is the source/sink term for the immobile phase. The source/sink terms both in the mass balance of component in soil air and the immiscible phase include the interfacial mass transfer and biological/chemical transformations.

Several parameters are used in the description of the VOC movement and therefore are needed to obtain solutions of the air flow and VOC transport equations. Properties of soil and VOCs should be measured for the accurate design of the SVE operation on the specific site. Most thermodynamic and transport properties of VOC components in air can be obtained from reported data. These properties may change depending on the operating condition of the SVE. The property changes caused by operating conditions sometimes give considerable variations in the efficiency of the SVE. Thermodynamic and transport properties of VOCs in various conditions can be estimated from theoretical and empirical relationships. These parameters are the soil air permeability, molecular weight of soil air, viscosity of gas mixture, diffusivity in gas mixture, vapor pressures and aqueous solubilities of VOCs.

Interfacial Mass Transfer

One of the empirical correlations for the interfacial mass transfer between immiscible phases is the first order kinetics expression. The rate of mass exchange between immiscible phases is expressed

by the mass transfer potential and the mass transfer coefficient. The difference of the concentration at equilibrium and the actual concentration in the main body is defined as the mass transfer potential. The mass transfer rate is expressed as

$$n_A = K_G (\hat{c}_A - c_A) \quad (8)$$

where \hat{c}_A is the concentration of A at equilibrium, c_A is the actual concentration in the main body of fluid, and K_G is the mass transfer coefficient. The mass transfer coefficient, K_G , is expected to be a function of Reynolds' number, Schmidt's number, and the air saturation, θ_a , which is the ratio of the air-filled porosity to the total porosity of soil.

$$K_G = K_G(\text{Re}, \text{Sc}, \theta_a) \quad (9)$$

Effect of Parameters

Analytical solutions in one-dimensional systems have been obtained for the soil air flow and contaminant transport equations under simplifying assumptions. Those solutions were applicable for analysis of simple soil column operations. Effects of parameters on the VOC movement have been studied through simulations and comparisons with soil column experiments.

Analysis of SVE Processes

The pressure distribution calculated from the analytical solution of the air flow equation showed variations with location inside a one-dimensional soil column, but was not a function of the air permeability at steady state. The pressure and corresponding velocity distributions obtained from the linearized and nonlinear equations showed discrepancies between calculated values. The maximum difference in pressure distributions inside the column was about 20% when the ratio of the inlet pressure, p_{in} , and the outlet pressure, p_{out} , was 0.6. But the corresponding air flow velocity showed a significant difference between calculated values from the linearized and nonlinear equations. When the pressure ratio was 0.9, the maximum difference was about 10%, and it was about 70% at the location of the lowest pressure when the pressure ratio was 0.6. Errors in the air flow velocity generate errors in the estimation of the convective movement term in the transport equation. Therefore, one should be very careful when the linearized equation is used.

Air and liquid saturations in soil pores were expected to have significant effects on both the air flow and VOC transport. The relative permeability of soil air was a function of the air saturation. If the liquid

saturation, including the water and immiscible nonaqueous phases, was high, then the relative permeability became so small that a large pressure drop was expected. The effect of the air saturation on the transport of the VOC impacted the diffusivity, as did the interfacial mass transfer from the immobile phase to the air flow. The liquid saturation was also considered to determine the effective interfacial area for the mass transfer. As the liquid saturation increased above the residual saturation, the mass transfer coefficient was expected to increase due to the increased interfacial area between contacting phases. After passing the maximum point, the interfacial area decreased, and so did the mass transfer coefficient. The change of contacting area was considered to be a complicated function of the hydrogeometry inside soil pores and was expected to vary continuously as the removal process of the VOC and soil water continues. Additional efforts should be made in this area of research. Systematic studies in the laboratory and field should be conducted to gain better knowledge of the process.

Temperature Effect on the Removal Efficiency

To investigate the temperature effect on the performance of the SVE process, the soil column experiment was simulated at three different temperatures. In comparing property changes at different temperatures, the largest differences were found in vapor pressures. At a 15°C increase of temperature in the ambient condition, the vapor pressure of TCE doubled. The major contributing factor to the performance of the SVE process at increased temperature was the vapor pressure increase. The removal rate doubled when the operating temperature increased 15°C. In future studies, it may be worthwhile to consider increased temperature operation.

VOC Removal Rate Measurements

One of the controlling processes in SVE is the partitioning among gas, liquid, and solid soil phases. When the convection dominates the transport of VOCs and its rate is fast, local equilibrium assumption is not accurate; and a kinetics model seems to be more appropriate to describe partition processes. Experimental investigations of two parameters, the air flow rate and the liquid distribution including the nonaqueous phase liquid and water, on the removal rate of VOCs from soil columns are presented.

Soil Column Experiments

Nine soil columns made of 2-inch, Schedule 80, PVC pipe were used. Each column had a soil-packed section 28 to 30 cm long and two additional empty sections with a cap on each end. Brass fittings were attached on the top and bottom sections of the columns. Both 1/4 inch I.D. plastic and copper tubings were used; plastic tubings were used where VOC did not contact. The Oil Creek sand was packed in the columns. The sand was white and very uniformly sized with very small amounts of organic content on the surface. These columns were set up in a constant temperature room. Pure toluene was used as a VOC and was applied on top of the soil-packed section of each column drop by drop through a hypodermic syringe to minimize the disturbance of soil packing. The same method was used for water application to control water content. After application of each liquid, a 24-hour equilibrium period was set to achieve uniform distribution of liquid. The air flow rate was monitored with a rotameter and adjusted as necessary with two needle valves. The vacuum pressure and the pressure drop through the column were measured with manometers. An in-house vacuum line was attached to the column for the vacuum source. The vacuum pressure and corresponding air flow rate fluctuated about 10 % from the set point. Air was saturated with moisture by passing it through water baths before it entered the columns to minimize the water content change in the soil. Samples of effluent air from each column were taken directly by a gas-tight chromatograph syringe and injected into an HP 5840A gas chromatograph equipped with an FID. A 6 ft, 1/4 inch O.D. custom packed stainless steel column (Supelco, EPA Method 602) was used for analysis of toluene concentration in air. Nitrogen served as the carrier gas at a flow rate of 36 ml/min. The injector and FID temperatures were set at 110°C and 150°C, respectively. The column oven temperature was fixed at 90°C. A specialty gas mixture (Blend 3, Scott Specialty Gas) was used as a standard for calibration.

Results and Discussion

Two major parameters investigated in this experiment were the air flow rate and liquid phase contents of the immiscible nonaqueous VOC and water in soil. The effluent concentration decreased as the time passed even in the case where only pure toluene was applied. This decrease of effluent concentration suggests that the interfacial mass transfer is a function of residual liquid contents inside soil pores.

Also these decreasing rates of effluent concentrations varied with respect to the air flow rate. At a lower flow rate, the effluent concentration change was slower than at the higher air flow rate. These trends were maintained through different water content and distributions inside soil columns. To verify the VOC and water distribution effects on the removal, the effluent concentration changes at different initial liquid VOC and water were investigated. Throughout these experiments, the amount of toluene applied on each column was far above the water solubility, and, therefore, toluene existed as an immiscible nonaqueous liquid. The vapor pressure was expected to be that of pure toluene. Nevertheless, the effluent rate was seriously affected by the water content in the soil. Increasing water contents reduced the removal rate. This may be due to the entrapment of residual VOCs inside soil pores by water and thereby reducing contacting area between the air and VOC phase. However, this could not be verified.

Even though the air flow rate and the liquid distribution of VOCs and water were distinctive parameters verified through these experiments, it was not possible to obtain quantitative correlations among them. The main reason was that throughout these experiments, mass balances of VOCs and water could not be checked. Another unexpected result was the non-uniform distribution of VOCs and water inside soil columns. It was found that liquids, including toluene and water, moved upward as air flowed up from the bottom of the column and accumulated in the upper part of the soil packed section of the column. Redistribution of liquids and experimental results suggest the necessity for a new design of soil column and experimental procedures which include the control and measurement of liquid content changes.

Removal Rate Model

A similarity of physics involved in the moisture removal from a wet solid by dry air and the VOC removal from soil pores by uncontaminated air suggests the same conceptual model. The moisture removal model consists of the constant rate period and the falling period. The constant rate period is at the first stage of the drying process in which the moisture removal rate remains constant and is mainly controlled by external factors like air flow, temperature, and the moisture content in the air. The falling rate period represents the second stage of the removal process in which the removal rate decreases as the moisture content reduces after a critical point.

In this stage, the moisture removal rate is controlled by internal factors such as the liquid diffusion, the capillary flow of liquid, or the flow by shrinkage of solid pores. The capillary movement of liquid water due to the change of the suction potential by evaporation of moisture inside pores is expected to control the drying rate of sand soil or granular materials by air flowing through pores. The moisture removal rate is approximated by first order kinetics. The removal rate of VOCs from soil pores can be expressed with the same concepts of physical process. During the first stage after air flow begins, the removal rate from soil pores remains constant until the VOC content is reduced to a critical value.

$$\phi_l \frac{\partial C_A}{\partial t} = S_1 \text{ when } \phi_l C_A \leq \phi_l C_{A,c} \quad (10)$$

(critical amount)

At the second stage, after the critical point of the VOC content has been reached, the removal rate decreases as the VOC contents decreases. It is expressed by a first order kinetics model of the removal of VOC from the soil pores.

$$\phi_l \frac{\partial C_A}{\partial t} = K_1 (C_A - C_{A,\theta}) \quad (11)$$

where $K_1 = \frac{-S_1}{(C_{A,c} - C_{A,\theta})}$, and $C_{A,\theta}$ = low-

est obtainable amount of liquid VOC under the given operating conditions. The solution of the above equation for the falling rate period can be obtained.

$$t = \frac{(C_{A,c} - C_{A,\theta})}{-S_1} \ln \frac{(C_A - C_{A,\theta})}{(C_{A,c} - C_{A,\theta})} \quad (12)$$

The semilogarithmic plot of $\frac{(C_A - C_{A,\theta})}{(C_{A,c} - C_{A,\theta})}$

vs. t should give a straight line and the slope of the curve is related to the constant rate. The constant rate S_1 , and the coefficient, K_1 , are expected to be complex functions of the liquid saturation, θ , and various operating conditions.

$$K_1 = K_1 (Re, Sc, \theta) \quad (13)$$

Soil Air Flow Model with Superpositions of Analytical Solutions

The development of a three-dimensional analytical approximate model to simulate the air flow during the SVE operation and a simple pneumatic pump test conducted on an aviation gasoline-contaminated site are

presented. The model used a superposition of the analytical solutions obtained from potential theory in a three-dimensional space. This model is only applicable to homogeneous media. Pneumatic pump tests were conducted to obtain soil air flow characterization around an air injection and vacuum extraction well in relation to a field demonstration project for bioremediation. The result revealed the importance of the pneumatic pump test prior to the design of a full scale operation. A part of the test results was used for the validation of the model.

Analytical Solutions

At steady state, the equation describing the pressure distribution of soil air is

$$\nabla K_a p \nabla p = 0 \quad (14)$$

Three appropriate boundary conditions are a constant pressure boundary, like soil surface exposed to the atmosphere, a zero flux boundary for the impermeable layer, and the continuous flux condition at the interface between different permeability layers.

The superposition of exact solutions is possible only for the linear equations. By applying the Kirchoff transformation on the above equation as follows,

$$\frac{dm}{dp} = K_a P \text{ or } m = \frac{K_a}{2}(p^2 - p_f^2) \quad (15)$$

the equation becomes a Laplace type equation

$$\nabla^2 m = 0 \quad (16)$$

where m is defined as the discharge potential at location x .

One of the exact solutions which satisfies the Laplace equation is the point source

$$m = \frac{Q}{4\pi} \frac{1}{r} \quad (17)$$

where Q is the source strength and r is the distance from the source point. A finite length well in the subsurface can be modeled as a line source with finite length. The discharge potential at x due to the line source can be obtained by integration. When the source strength Q is assumed to be constant through the well length, the potential becomes

$$m = \frac{Q}{4\pi} \ln \frac{u+v-2h}{u+v+2h} \quad (18)$$

where u , v , h are lengths of vectors to the point x from various points on the well. Another useful solution for the Laplace

equation is the point dipole which is defined as a point potential of combined point source and point sink of same strength at an infinitesimally short distance. The potential at x due to a point dipole is

$$m = \frac{q \cdot c \cdot r}{4\pi r^3} \quad (19)$$

where q is the dipole strength, c , the unit orientation vector of dipole, r , the vector from dipole point to location x , and r , the length of vector r . Potentials due to the line dipole and dipole panel could be obtained by integration. Boundary conditions mentioned above can be satisfied by superposition of line and panel dipoles on boundaries. Unknown variables are the strength terms on sources and dipoles. These unknowns can be obtained from simultaneous equations satisfying boundary conditions and potential values at selected control points.

Pneumatic Pump Test

A series of pneumatic pump tests were conducted on an aviation gasoline-contaminated site. The soil type at the site was categorized as a fine sand which had a grain size distribution of 0.35 mm average and 90% in the range of 0.1 to 1 mm. The intrinsic permeability of this sand was reported as $5.2 \times 10^{-10} \text{ ft}^2$. The thickness of this sand layer was about 47 ft, and a thick clay was located underneath. The water table was 17 ± 2 ft from the surface, and the ground-water flow direction was north-east. An injection well and an extraction well were installed 20 ft apart. Both wells were made of 5 inch schedule 40 PVC pipe and had a 1 ft screened section 15 ft from the soil surface. Each well was connected to a separate blower pump. To control the pressure and air flow into/out of the well, a bypass line, which had an opening to the atmosphere with a ball valve, was attached to each connecting pipe. Several different pressures and air flow rates could be applied to each well by controlling valve openings. The pressure inside the well was measured by a pressure gauge installed on the top of each well. The volumetric flow of air inside the well was measured with pitot tubes installed on 4 inch schedule 40 PVC pipe that connected the well and the blower pump. The maximum capacity of blower pumps was 176 scfm at the positive pressure of 52.3 inch water inside the injection well. The pressure distribution in the subsurface around the well was measured with Magnahelic pressure gauges. Gauges were connected through quick release connectors on probe clusters located 5, 10, 12.5, 15, and 30 ft away from the injection

well along a straight line between injection and extraction wells. Each cluster had three probes. Each probe had a screened opening at the bottom of 1/4 inch O.D. copper tubing and a quick release connector at the top. The probes were 3, 10, and 15 ft in length.

Test Results

A series of tests of air injection, extraction, or combined operation were conducted. The same procedure was applied to each set of tests. The blower pump connected to the well was powered on and the pressure and air flow were controlled by the control valve. Due to the high permeability and low moisture content in the soil, the transient pressure change around the well reached the steady state very rapidly. Only the pressure distribution at the steady state could be obtained.

The pressure change was large within 15 ft from the well; beyond this distance, the pressure gradient became very small. Because the air flow is proportional to the pressure gradient, the air flow rate is expected to decrease sharply as the distance from the well increases. The vertical pressure gradient and air flow also decrease at distant locations from the wells. Conventionally, field engineers set up a pilot scale test of a single extraction well and measure the pressure distribution and estimate the zone of influence from the measured pressure distribution. The most important factor in determining the zone of influence and the well interval should be the pressure gradient and the air flow velocity. The tests showed that the wells should be spaced less than 30 ft apart to induce sufficient air flow in this site.

The pressure distribution at a depth of 15 ft for the combined operation of injection and extraction wells with various combinations of positive and negative pressures inside the wells was investigated. The maximum injection pressure was 52 inch water and the volumetric air flow was 176 scfm. The pressure at the extraction well was -48 inch water and the volumetric flow was 140 scfm. Large pressure gradients in vertical and horizontal directions in the vicinity of wells (within 5 ft) were seen, and a large volume of air exchange around the wells was expected. At the midpoint, a very small gradient and air flow in both directions existed. But the pressure gradient was very small compared to the pressure difference between the two wells (100 inch water). The efficiency of horizontal air flow and the rate of sweeping VOC in that direction should be low. Therefore, it might not be an efficient way to induce horizontal air flow with distantly located wells and large pressure differences.

Very important information on design of an SVE system can be obtained from pneumatic pump tests. Design parameters in the SVE system should include the zone of influence in which the pumps can produce the sufficient air flow. Estimation from the measurable vacuum pressure can cause overestimation of the radius of the zone of influence. The major factor in determining the zone of influence should be the pressure gradient and corresponding air flow. The pumping efficiency could be measured from the tests. A single high vacuum pumping well does not have a larger zone of influence than the low vacuum pumping well because a large pressure gradient exists only in the vicinity of the well. The SVE system with multiple low vacuum wells may be more efficient than one with a single high vacuum well. Combined operation of extraction and injection wells could induce horizontal air flow, but still a large vertical flow is expected in the vicinity of wells. Therefore, the system should be carefully engineered to obtain reasonable efficiency. A tightly covered soil surface may help to induce more horizontal flow. Additional field tests are suggested to measure the pressure distribution of the operation with a tightly covered soil surface and also with various lengths and locations of well screens.

Three-Dimensional Finite Difference Model

A mathematical model was developed for the simulation of the soil vacuum extraction process in field scale. This model consisted of a soil air flow equation, the contaminant transport equation and the mass balance equation of residual hydrocarbon inside soil matrices. The air flow equation was transformed to a Laplace type equation to obtain the soil air pressure distribution and the flow velocities. The calculated air flow velocities were used in the transport equation to describe the convective movement of VOC. In addition to the convective movement, the transport equation included the diffusive movement and the interfacial mass transfer between the air and the residual hydrocarbon contacting the flowing air. The mass balance equation for the residual hydrocarbon was also used. The numerical method to solve these differential equations with boundary conditions was the finite difference method in a three-dimensional space domain and the unsteady state time process.

Finite Difference Solutions

The soil air flow arrives at steady state quite rapidly after the SVE system is initiated by pumping the air into/out of the subsurface. The contaminant movement

usually is a non-steady state problem until all the contaminant mass is removed from the system. Therefore, it is reasonable to assume that the air flow is at steady state during the operating period. In this project, a finite difference method with central spatial difference scheme was adopted to solve this air flow equation. Replacing the differential equations with the difference operators results in the difference equations for the air flow equation. By applying the above finite difference operator on all the interior nodal points, excluding the boundary points, w , where specific conditions are assigned, the total number of linear algebraic equations becomes $(M-1) \times (N-1) \times (L-1) - w$. The number of equations increases rapidly as the nodal points increase. For example, $100 \times 100 \times 100$ system generates 100,000 simultaneous algebraic equations which need a tremendous amount of computational time. In this project, the point Jacobi iterative method was selected to solve the equations because it uses considerably less CPU memory than the direct solution method, allowing the large physical problems to be simulated. Additional refinement adopting various preconditioner and accelerator schemes is needed to make the program faster and more stable.

Several finite difference schemes have been developed to solve these convective diffusion equations of the VOC transport. In this project period, two simple schemes have been tested, the explicit method and the alternating direction implicit (ADI) schemes; only the explicit scheme was implemented in the program. The advantage of the explicit scheme over the implicit scheme is that each node is computed explicitly and the computations need less memory and processor time. The disadvantage is that the selection of time step increment is severely dictated by the stability conditions. Usually, the ADI scheme is unconditionally stable and has second-order convergence error. One would have to invert a set of three tridiagonal matrices for each time step with the ADI scheme.

Computer Implementation

Very often, the modeling of fluid flow and contaminant transport in the subsurface is dictated by availability of computer resources. Because of limited computational resources at Kerr Laboratory, the point Jacobi method for the air flow equation and the explicit scheme for the VOC transport equation were selected. Both methods require less memory and computational time; but because of limited time step allowed, they may not be suitable for the long period of simulation. Currently, the algorithms and controlling program discussed above are implemented in FOR-

TRAN 77 on an Apollo DN4500 using Unix system V as the primary operating system. The sampling array used by this model is $101 \times 101 \times 51$ which calculates to 520,251 physical nodes. Given this amount of nodes, the program requires approximately 10 megabytes (MB) of memory which is not suitable for personal computers. Through implication, a larger model would require even greater memory to function. Provided with the main program is a postprocessor program which is for graphical display of data generated by the main program. It is specifically designed with an XWindows interface and will require an XWindows server be available to run the postprocessor.

Conclusions and Recommendations

From analyses of experiments and model simulations, very valuable information could be obtained. The observation of simulated results based on soil column experimental conditions showed several physical and chemical properties influencing the efficiency of the SVE operation. Among VOC chemical properties, the vapor pressure was the most sensitive factor that controlled the efficiency of total operations. Air flow rate and liquid distribution were very important parameters which controlled the removal rate of VOCs from soil columns. A conceptual model was proposed to describe the evaporative process of VOCs from the residual liquid in soil pores. The pneumatic pump test gave very important information for design of SVE systems, including the zone of influence, soil characterization, and pumping efficiencies. Two computer models for soil air flow and VOC transport in the SVE system were developed. The analytical solution model developed was very simple and easy to use. Simulations of pneumatic pump tests with this model revealed that the model generated reasonable results and could be used as an initial design tool. A fully three-dimensional finite difference model was developed. Various solution methods have been tried, and explicit schemes were selected to reduce the computational time and memory requirements. A graphical postprocessor was attached to enhance the visualization of output results.

The proposed future works are as follows: A large number of studies on mass transfer have been reported in engineering literature, but very few pertain to soil systems. Soil particles and pore sizes are not uniform, and the Reynolds' number is usually less than 0.1 in soil systems. The extrapolation of empirical correlations to unmeasured operating conditions is not desirable, and further studies are required

to obtain more precise correlations suitable for soil systems. More experiments are suggested with modified columns and procedures for quantitative analyses. The proposed model for VOC removals from soil pores needs to be verified through additional experiments. More research on the enhancement of SVE by increased temperature is also needed to achieve better efficiency of the SVE operations. Pneumatic pump tests are recommended under various operating conditions before full scale implementations of SVE systems. Tracer gas tests will help further. A main reason for the lack of field scale model developments is the expense of the model validation with field scale data. It is very costly to perform tests for the model validation, but this is a very necessary step. A simple pneumatic pump test, like the one reported in this project, will give very important information for model validation and optimal design of the SVE system. Additional refinement and validation of the analytical solution model are necessary for further field applications. The finite difference model is still in the developmental stage and needs a rigorous validation through numerical experimentations and comparison with field data. In addition to the validation, alternative schemes should be tested to accelerate the computation.

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