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REVIEW OF MATHEMATICAL MODELING FOR EVALUATION OF SVE APPLICATIONS

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INTRODUCTION

Soil vapor extraction (SVE), a demonstrated technology, enhances the removal of volatile chemicals from the subsurface through application of a vacuum at an extraction well to induce air flow through the subsurface toward the well. As of 1991, SVE comprised 13% of selected remedies at Superfund sites, and approximately 7% of leaking underground storage tanks. The flow of air enhances volatilization of compounds from the residual NAPL phase in soil pores and from the dissolved phase in soil pore water. The technology is particularly applicable to relatively volatile organic compounds (Henry's law constant > 10^{-3} atm-m^3/mole) residing in the vadose zone. The technology may also be applicable for removal of volatile light non-aqueous phase liquids (LNAPLs) floating on the water table or entrained in the capillary fringe, if the chemicals of concern have high vapor pressures (e.g., benzene). During SVE, contaminant removal is expected to be enhanced by decreasing soil moisture. As percent moisture decreases, air permeability increases. Increased soil organic carbon content will increase sorption to the soil matrix, decreasing SVE efficiency. Heterogeneous flow conditions also affect the efficiency of contaminant removal, with higher flow zones (preferential flow zones) cleaning up faster than low flow zones (less permeable zones).

Air sparging, another SVE-related technology, generally involves use of injection wells to inject gas (typically air) into the saturated zone below areas of contamination. Ideally, dissolved, separate-phase and sorbed contaminants will partition into the injected air, effectively creating an in-situ air-stripping system. This can take place within a single-well system or the stripped contaminants can be transported in the gas phase to the vadose zone and collected by SVE wells. The advantage of such a system is that the treatment of groundwater and soil takes place in-situ, reducing the need for disposal of treated material. Although air sparging is a physical/chemical treatment process, the addition of air has the potential to promote biodegradation.

The SVE process involves installation of vacuum extraction wells or trenches at strategic locations and depths. Air extraction can also be combined with air injection. The spacing of wells or trenches depends on soil properties such as permeability and porosity. Where the objective is to remove both air and water, dual vacuum extraction wells may be used. The injection wells for air sparging can be vertical or inclined, ranging to horizontal. Effective design and prediction of system performance can be difficult, depending on site conditions.

Tools are now available, in the form of numerical models, that allow one to both screen for the potential feasibility of SVE, and design and estimate performance of the system. While modeling should not be considered an end in itself, it provides a means by which to quantify some of the important SVE operating processes. Modeling can provide estimated answers for numerous questions concerning the feasibility and usage of SVE. Screening models can be used in conjunction with site characterization data and best professional judgment to determine the potential feasibility of SVE at a contaminated site. Flow and transport models can then be used to enhance the system design

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process and estimate performance. The work performed as part of this effort included a review of models that can be applied to SVE applications. This review includes a summary of critical information required in a SVE application. It also includes a model selection process, model usage guidelines, and case studies.

METHODOLOGY

At an "Integrated In Situ Treatment System Design Workshop" that took place on August 10 and 11, 1993 in Edison, New Jersey, a need was identified to provide environmental managers with guidance on how models may be used to (1) determine the viability of using SVE, (2) if viable, help design the SVE system, and (3) estimate system performance. The methodology used to provide this guidance was a literature review and analysis of the various codes that may be applied to SVE. The literature review, and basic information on SVE system design, are provided. This includes introductory material, model selection tips, and example applications. In addition, information is provided on flow and transport theory.

Applicable codes were divided into the categories of screening, air flow, and compositional flow and transport. For each of these categories, currently available models were compiled and reviewed. Several example applications utilizing a number of the codes are presented, along with three case studies.

RESULTS

The results of this review is a guidance document that highlights the following topics and guide the user through the processes of selecting and applying models to SVE sites. Technical information is provided in order to: (1) Determine the types of problems that can be addressed by modeling; (2) Highlight the methods that are commonly used to solve such problems; (3) Assist potential users in determining the presence or absence of a need for modeling at their site and, if a need is shown to exist, selecting a model for their site; (4) Identify and illustrate the major processes governing air flow and contaminant transport in the subsurface; (5) Present a discussion of model data needs; (6) Review available commercial and public domain codes; and (7) Present a suite of example model applications and case studies.

CONCLUSIONS

Modeling can provide estimated answers for numerous questions concerning the feasibility and usage of SVE. Screening models can be used in conjunction with site characterization data and best professional judgment to determine if SVE at a contaminated site is feasible. Flow and transport models can be used to enhance the system design process and estimate performance. In some cases, no complex model is necessary, and decisions can be made based on simple analytical solutions and/or best professional judgment. Geographical information systems (GIS) can provide valuable assistance in organizing and presenting site data graphically in order to enhance the remedial alternative selection process.

Table 1 presents a summary of the screening, air flow, and compositional flow and transport codes that were evaluated. For screening, these models include the HyperVentilate and VENTING codes, as well as other analytical solutions. Air flow models available at this time include AIRFLOW, CSUGAS, and AIR3D. For compositional flow and transport, the VENT2D/VENT3D model is available and capable of simulating contaminant transport and removal via SVE.

The selection and application of any model will ultimately lie with the model user. This document attempts to guide the potential model user through a decision-making process that is intended to help decide how and when to select a model, to make users aware of the processes governing flow and transport in the vadose zone, and highlight the limitations of model results.

FOR MORE INFORMATION

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TABLE 1. SUMMARY OF THE SCREENING, AIR FLOW, AND COMPOSITIONAL FLOW AND TRANSPORT CODES THAT WERE EVALUATED.

Model	Type	Capabilities	Advantages	Limitations	Hardware/Software Requirements	Availability
Hyper-Ventilate, v2.0 (IBM PC) v1.01 (Apple Macintosh)	Screening	Calculates air permeability, well flow rates, mass removal rate, mass removal from several idealized diffusion-limited scenarios Calculates contaminant concentrations over time for multiple constituents	Provides rapid estimates for determination of the potential feasibility of SVE Provides rapid estimates of contaminant concentrations in extracted gas, allows comparison of removal rates of different constituents	Analytical air flow solution Should not be used to design SVE systems	IBM PC or Compatible: 80386/80387 coprocessor or 80486, 4 MB RAM, DOS 3.1 or higher, Microsoft Windows 3.x and runtime version of Object PLUS Apple Macintosh (Plus, SE, SE/30, II, IIX, or portable): 1 MB RAM, Apple HyperCard Software (v2.0 or greater)	Available from EPA as EPA/600/R-93/028 (EPA ORD Publications, 513-569-7562) Price: FREE while supplies last[1] Object PLUS available from Object PLUS Corp., 125 Cambridge Park Dr. Cambridge, MA 02140 Price: $100 (runtime version)[2]

[1]From NTIS: Report with disk (PB93-502664/AS) $140.00
Report only (PB93-134880/AS) $27.00

[2]From NTIS: IBM PC Disk (S/N 055-000-00427-7) $22.00
MacIntosh Disk (S/N 055-000-00403-0) $17.00

TABLE 1. SUMMARY OF THE SCREENING, AIR FLOW, AND COMPOSITIONAL FLOW AND TRANSPORT CODES THAT WERE EVALUATED (continued).

Model	Type	Capabilities	Advantages	Limitations	Hardware/Software Requirements	Availability
VENTING, v3.01	Screening	Calculates contaminant concentrations over time for multiple constituents	Provides rapid estimates of contaminant concentrations in extracted gas, allows comparison of removal rates of different constituents	User supplies flow rate to extraction well Simplistic one-dimensional representation of mass transport Should not be used to design SVE systems	IBM PC/AT or Compatible, DOS, 512 KB RAM, math coprocessor	Environmental Systems & Technologies, Inc. 2608 Sheffield Drive, Blacksburg, VA 24060-8270 703-552-0685 Price: $400.00
AIRFLOW^{EM} v2.07	Air flow	Calculates pressure distribution in a radial domain, calculates air flow pathlines and velocities	Easy-to-use 'CAD-type' graphical user interface which simplifies model input and setup Rapid setup aids in hypothesis testing for simple problems Many sample problems included with the code	Only allows for one extraction well No mass transport	IBM PC or compatible, 80386/80486, 4 MB RAM, DOS 2.0 or higher, mouse and math coprocessor for 80386-based machines recommended	Waterloo Hydrogeologic Software 19 McCauley Drive (RR#2) Bolton, Ontario, Canada L7E SR8 905-880-2886 Price: $650.00

TABLE 1. SUMMARY OF THE SCREENING, AIR FLOW, AND COMPOSITIONAL FLOW AND TRANSPORT CODES THAT WERE EVALUATED (continued).

Model	Type	Capabilities	Advantages	Limitations	Hardware/Software Requirements	Availability
CSUGAS	Air flow	Calculates vacuum distribution in the subsurface, in inches of water	Allows full, three-dimensional analysis of heterogeneous, multi-well air flow problems Text-based input/output is flexible and up to the user	Lack of easy-to-use input/output interface may intimidate beginners No steady-state solution option No mass transport	IBM PC AT/XT or compatible, 640 KB RAM, DOS 2.0 or higher	Dr. James W. Warner Department of Civil Engineering Colorado State University Fort Collins, CO 80523 303-491-5048 Price: $125
AIR3D	Air flow	Calculates pressure distribution in the subsurface	Easy-to-use 'CAD-type' graphical user interface which simplifies model setup and input Allows three-dimensional analysis of complex problems	Users need an awareness of the operation and limitations of the MODFLOW code No mass transport	IBM PC or compatible, DOS 3.3 or higher, 4 MB RAM, VGA card and color monitor, mouse is highly recommended	American Petroleum Inst. 1220 L Street Northwest Washington, DC 20005 Price: $500.00 The original version of AIR3D (without the GUI) is available free of charge from: USGS Book and Open File Reports BLDG 810, Box 25425 Denver, CO 80225 Price: FREE

TABLE 1. SUMMARY OF THE SCREENING, AIR FLOW, AND COMPOSITIONAL FLOW AND TRANSPORT CODES THAT WERE EVALUATED (continued).

Model	Type	Capabilities	Advantages	Limitations	Hardware/Software Requirements	Availability
VENT2D/ VENT3D	Air flow and multicom-ponent contam-inant transport	Calculates pressure distribution in the sub-surface, multi-component contaminant constituent concentrations over time in the subsurface	Only readily available compositional flow and transport code Source code is available Text-based input/output is flexible and up to the user	Grid size limited to 25 x 25 cells (can be increased with a different version available from the author)	IBM PC or compatible, 80X86 with math coprocessor, DOS 3.0 or higher, 525 KB RAM	David A. Benson 524 Claremont Street Reno, NV 98502 702-322-2104 Price: $495.00

REPRESENTATIVE SAMPLING AND ANALYSIS OF HETEROGENEOUS SOILS

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INTRODUCTION

Sampling and analysis presents specific problems with heterogeneous soils. These problems have been carefully evaluated in several projects for the Risk Reduction Engineering Laboratory (RREL), specifically Superfund Innovative Technology Evaluation (SITE) demonstrations. Of particular concern is the inability of standard analytical methods to account for heterogeneous samples. While a typical analytical method may normally accommodate only 2 grams (g) of sample (and therefore requires that "oversized material" be removed from a sample before analysis, potentially biasing analytical results), a representative sample aliquot from a heterogeneous site may require a sample size that is orders of magnitude greater than this. The inability to analyze representative samples may be the result of various factors, including the presence of oversized material (such as rocks or other debris); highly concentrated contaminants (such as lead chunks or tar balls), which may preclude taking large laboratory samples that would overwhelm instrument capabilities; or volatile contaminants which cannot be mixed to