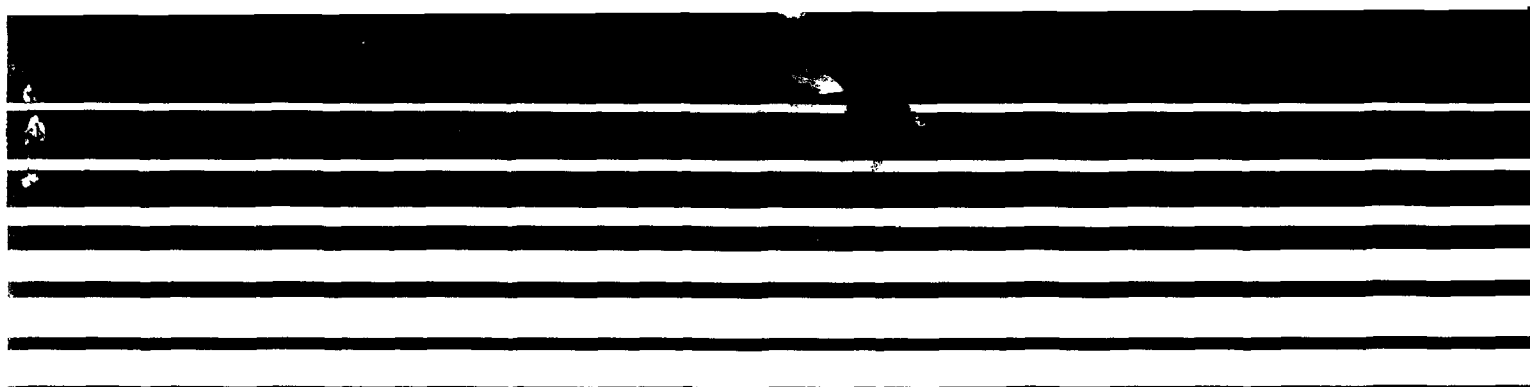


Air/Superfund



AIR/SUPERFUND NATIONAL TECHNICAL GUIDANCE STUDY SERIES

Estimation of Air Impacts for Soil Vapor Extraction (SVE) Systems (Revised)



**AIR/SUPERFUND NATIONAL TECHNICAL
GUIDANCE STUDY SERIES
ASF-22**

**ESTIMATION OF AIR IMPACTS
FOR SOIL VAPOR EXTRACTION
(SVE) SYSTEMS
(REVISED)**

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SECTION 1

INTRODUCTION

The U.S. Environmental Protection Agency's (EPA's) Office of Air Quality Planning and Standards (OAQPS) and the Regional Air Offices have been given the responsibility to evaluate air impacts from Superfund sites. An important part of this program is the analysis of air impacts from various alternatives for cleaning up Superfund sites. Since these analyses are frequently required for planning purposes prior to actual cleanup they depend on estimated emissions and ambient concentrations rather than on field measurements.

Soil Vapor Extraction (SVE) is also known as soil venting, vacuum extraction, aeration, or in-situ volatilization. It is a widely used technique for removing volatile organic compound (VOC) vapors from contaminated soil. This report provides several predictive emission models ranging from first-order gross estimates requiring little site-specific data, to refined models which calculate air flow through a porous medium as a result of the pressure gradient created by an extraction well and the vapor-phase concentration of the extracted air.

When evaluating the array of predictive models, a primary concern is the ability of each model to estimate time-dependent removal rates. This is especially important for SVE in that initial removal rates may be quite high (e.g., 500 to 600 kg/day). Typically, removal rates decrease with time as initial soil concentrations are depleted. Time-dependent removal rates may be critical for estimating other than long-term exposures, and thus short-term risks to the community and to site workers.

This document does not, however, include an analysis of the selection or use of air pollution control devices. The models reviewed are used to estimate contaminant

removal rates which are also synonymous with uncontrolled emission rates. Modeling results are therefore most useful to determine the need for air pollution controls.

The report also provides guidance on air dispersion model selection and use to help develop different modeling scenarios and estimate ambient air impacts. Model inputs, including source and receptor data can vary greatly. These data can have a direct bearing on ambient air concentrations, which are important both in risk assessments and compliance with air applicable or relevant and appropriate requirements (ARARs). Modeling several scenarios can allow for the adjustment of equipment size, design, control equipment, and location in a cost effective manner.

SECTION 2

PROCESS DESCRIPTION

Soil vapor extraction systems involve the removal of air containing volatile compounds from unsaturated soil. A general process schematic is shown in Figure 1. One or more extraction wells are placed in the vadose (unsaturated) zone at the site of the contamination. The extraction wells typically are constructed of slotted plastic pipe placed in permeable packing such as coarse sand. The wells are connected via a manifold that leads to an air blower or vacuum pump. The vacuum pump is used to withdraw air from the extraction wells and is typically capable of inducing a vacuum of about 30 in. Hg. The subsurface vacuum that is created and the resulting pressure gradient in the soil will dictate the rate at which vapors are withdrawn and the air flow patterns in the vadose zone.

As shown in Figure 1, air inlet wells can be used to introduce ambient air at the edge of the contaminated area. They serve to both increase the rate that contaminant-laden air is extracted and to control the direction of vapor migration. The air inlet wells can be passive or air can be forced into the ground using an air blower. Only a fraction of the extracted air comes from the air inlets, with the remainder of the air drawn from the surface through the soil. Therefore, it is important to have an impermeable cap in place at the top of each extraction well to prevent the direct inflow of ambient air down the well casing.

Several design options are available for increasing the air flow rate and removal efficiency of a SVE system. The inlet air can be heated to increase the partitioning of subsurface contaminants into the vapor-phase. The air blower used to inject air into the ground will heat the air to some extent due to compression; additional heat is added in some SVE systems by also injecting steam into the ground. In some cases, the air inlet

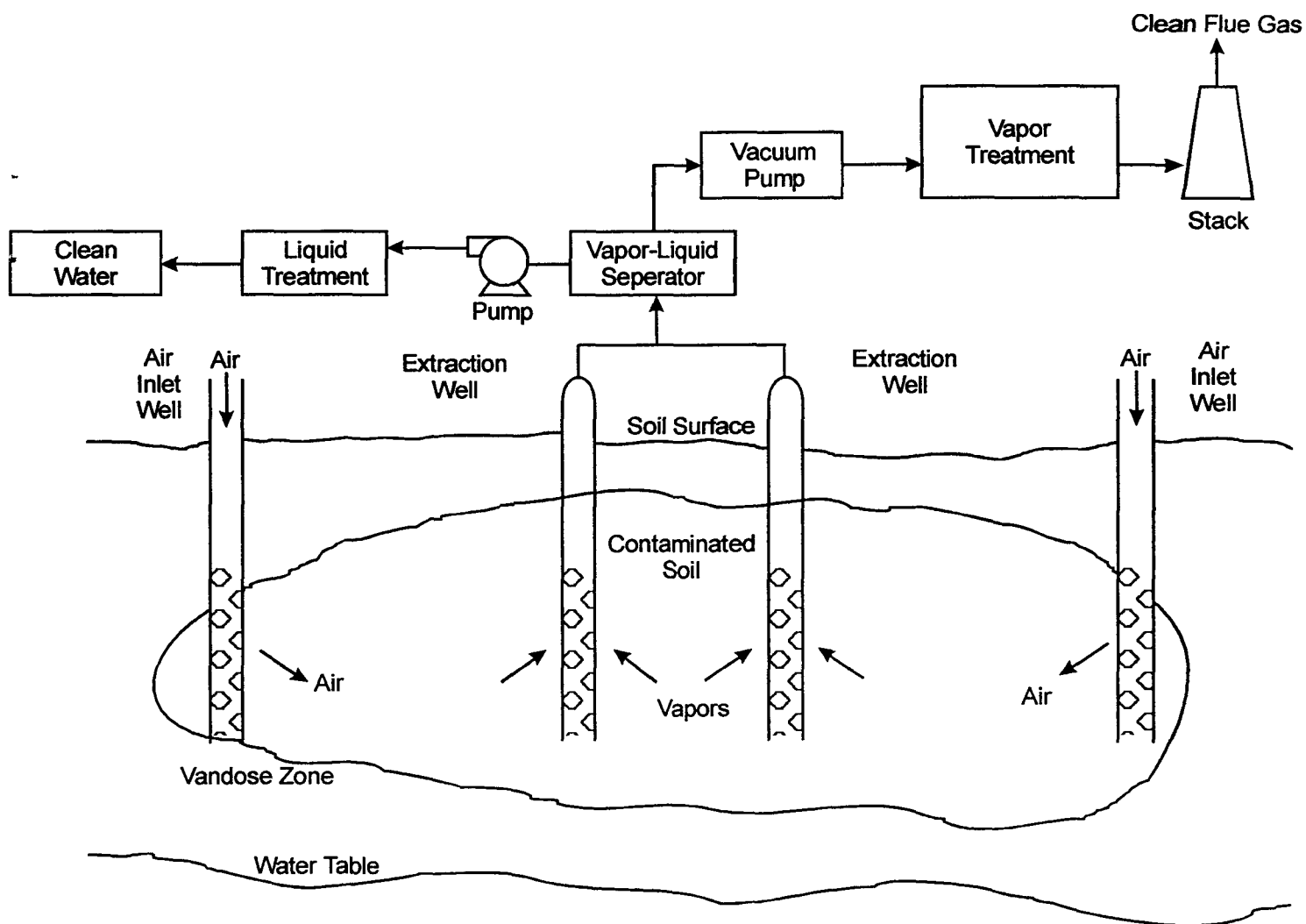


Figure 1. Generalized process flow diagram for soil vapor extraction.

wells extend down into the saturated zone. The inlet air bubbles up through the water table and this sparging action can enhance the removal of slightly soluble volatile organic compounds.

An air/water separator is typically employed if water is pulled from the extraction wells. The separator serves to protect the air blowers or pumps and to increase the efficiency of any vapor treatment system that is used. The condensate from the separator may require treatment prior to discharge. For the large-scale remediations done at Superfund Sites, the air stream will normally require treatment to reduce its VOC content prior to discharge into the atmosphere. Carbon adsorption, catalytic, or thermal oxidation are the most commonly used control technologies. Carbon adsorption systems may be present upstream or downstream of the vacuum pump. For SVE systems with small air flow rates (i.e., 30 to 100 scfm), internal combustion engines can also be used to control the air emissions.

SECTION 3

ESTIMATION OF AIR EMISSIONS

There are several alternative approaches for estimating the emissions from a SVE system. The best method is to directly measure the emissions from the system while it is in full-scale or pilot-scale operation. The next best method is to estimate the emissions using predictive equations with site-specific inputs. If site-specific inputs are not available, conservative estimates can be made by using default values for the input parameters.

This report describes several existing models for estimating the removal rate of volatile soil contaminants via SVE. Each model was evaluated based on theoretical approach, data requirements, ease of use, and the relative refinement of the removal rate estimates. Critical to the estimation of the emission rate, is a time-dependent estimate of the vapor-phase contaminant concentrations within the soil column. For this reason, the more refined models include equilibrium contaminant phase distribution estimates.

Each model was evaluated as to its usefulness for conducting risk evaluations and/or ARAR compliance evaluations at each step in the remedial process. Screening models were considered most useful during the detailed analysis of alternative remedial technologies and were therefore assessed as to the relative refinement of their predictions using limited site-specific and/or default data. Refined models are typically more useful during the remedial design/remedial action (RD/RA), when more data are available. In the case of computer models, availability and support were also considered as key criteria.

3.1 FIRST-ORDER ESTIMATES OF REMOVAL RATES

The most basic techniques for estimating SVE removal rates involve either an assumption of total contaminant mass removed over a given time period, or the product of estimated subsurface vapor flow and vapor concentration. The former assumes a constant removal rate and the latter a constant flow and vapor-phase concentration.

An estimate of the total emission potential for a site may be made using the following equation:

$$ER_i^{ave} = M_i/t = (V_s C_i (1 - \rho_b)/t) \quad (1)$$

where	ER_i^{ave}	= Average emission rate of component i, g/s
	M_i	= Total mass of i in soil, g
	t	= Duration of remediation, s
	V_s	= Volume of contaminated soil to be treated, m ³
	C_i	= Average concentration of i in soil, $\mu\text{g/g}$
	1	= Constant, $\text{g}/10^6 \mu\text{g} \times 10^6 \text{ cm}^3/\text{m}^3$
	ρ_b	= Average soil dry bulk density, g/cm^3 .

Equation 1 assumes complete recovery of the contaminant over the duration of the remediation and thus constitutes a gross estimate of the average emission rate. In addition, Equation 1 assumes that the concentration in soil is constant over time and relies on an estimate of the time required to remove all of the contaminant. In reality, the concentration will not remain constant and the time required for remediation cannot be determined without further site information. Therefore, Equation 1 may best be used as a check on the total mass lost over long time periods.

A better estimate of the removal rate can be obtained as the product of the subsurface vapor flow induced by the extraction well and the soil vapor-phase

concentration. Johnson et al. (1990a) estimate the maximum uncontrolled emission rate over relatively short time periods as:

$$ER_i^{\max} = C_{v,i} Q \quad (2)$$

where ER_i^{\max} = Maximum emission rate of component i, g/s
 $C_{v,i}$ = Vapor-phase concentration of i in the vent, g/cm³-vapor
 Q = Induced soil vapor flow rate, cm³-vapor/s.

Equation 2 estimates the maximum emission rate at the start of remediation and requires an estimate of the soil vapor concentration and flow rate. The soil vapor concentration may be estimated via soil gas measurements, however, this necessitates determining the lateral and vertical soil gas profile to estimate an average in situ soil gas concentration. Another option would be to extract headspace gas samples from bore hole samples. This requires careful core sample handling and sample preparation to avoid loss of analytes with low boiling points.

If soil gas measurements are not available or if data are not sufficient, a first-order estimate of vapor concentration in soil may be made using the ideal gas law. The maximum vapor concentration of any compound in extracted vapors is its equilibrium or saturated vapor concentration which is calculated as:

$$C_{v,i}^{eq} = \frac{x_i P_i^v(T_s) MW_i}{RT_s} \quad (3)$$

where $C_{v,i}^{eq}$ = Equilibrium saturation vapor concentration of component i, g/cm³-vapor
 x_i = Mole fraction of i in the residual mixture, unitless

$P_i^v(T_s)$	= Pure component vapor pressure of i corrected for system temperature, atm
MW_i	= Molecular weight of i, g/mol
R	= Gas constant (= 82.1 cm ³ -atm/mol-°K)
T_s	= System temperature, °K.

Equation 3 is applicable when the residual total hydrocarbons are present as nonaqueous phase liquids (NAPLs) or solids. At low soil concentrations, nonideal conditions exist and Equation 3 will overpredict the vapor concentration.

With a measured or calculated vapor concentration in soil, an estimate of the induced soil vapor flow is required to predict the maximum emission rate using Equation 2. Johnson et al. (1990a) give a range of vent vapor flow rates typically seen for SVE systems. The range of values is given as 10 to 200 ft³/min per well.

Emissions calculated using Equation 2 may give reasonable estimates at the start of venting, however, vapor concentrations decrease with time due to changes in the composition of the residual and due to mass-transfer resistances (Johnson et al., 1990). Because emissions calculated using Equation 2 are constant, an estimate of the time required to reduce residual soil levels to some target concentration cannot accurately be made.

3.2 ESTIMATION OF MULTICOMPONENT SYSTEM REMOVAL RATES

An estimate of the removal rate of an individual compound in a multicomponent system (i.e., one volatile compound in a mixture) may be obtained from the procedures of U.S. EPA (1994) and Johnson et al. (1990 and 1990a, b). In a single component system, the soil concentration at which the sorbed, dissolved and vapor-phases are saturated is commonly referred to as the soil saturation concentration (C_{sat}). The value of C_{sat} (mg/kg) can be estimated from U.S. EPA (1994) as:

$$C_{sat} = \frac{S}{\rho_b} (K_D \rho_b + \theta_w + H_T' \theta_a) \quad (4)$$

where S is the pure component solubility in water (mg/L); ρ_b is the soil dry bulk density (kg/L); K_D is the soil/water partition coefficient (L/kg); θ_w is the soil water-filled porosity (unitless); H_T' is the Henry's law constant corrected system for temperature (unitless); and θ_a is the soil air-filled porosity (unitless). Concentrations greater than C_{sat} indicate the presence of a residual-phase (e.g., NAPL). Although not as accurate as computer codes which solve for multicomponent thermodynamics, Equation 4 may be used as a preliminary estimate of the soil concentration above which a residual phase is present for individual components of a mixture.

Equilibrium vapor-phase soil concentrations during SVE can be calculated at discrete time-steps using either Raoult's law or Henry's law depending upon whether the soil concentration is greater than C_{sat} . If the soil concentration for any time-step is greater than or equal to C_{sat} , the vapor-phase concentration at equilibrium can be calculated using Equation 3. If the soil concentration at any time-step is less than C_{sat} , the vapor-phase concentration can be calculated from Johnson et al. (1990b) as:

$$C_v^{eq} = \frac{H_T' C_s \rho_b}{(H_T' \theta_a) + \theta_w + (K_D \rho_b)} \quad (5)$$

where H_T' is the dimensionless Henry's law constant corrected for system temperature; C_s is the soil concentration at each time-step; θ_a is the soil air-filled porosity; ρ_b is the soil dry bulk density; θ_w is the soil water-filled porosity, and K_D is the soil/water partition coefficient.

The pure component vapor pressure corrected for system temperature used in Equation 3 may be calculated using Antoine coefficients if available or may be estimated by:

$$P_i^v(T_s) = P_i^v(T_R) \exp \left[\left[\frac{T_B T_R}{T_B - T_R} \right] \left[\frac{1}{T_s} - \frac{1}{T_R} \right] \ln \frac{P_i^v(T_R)}{P_B} \right] \quad (6)$$

where $P_i^v(T_R)$ is the vapor pressure of i at the reference temperature (atm); T_B is the normal boiling point ($^{\circ}\text{K}$), T_R is the reference temperature ($^{\circ}\text{K}$), T_s is the system temperature ($^{\circ}\text{K}$), and P_B is the pressure at which the boiling point is measured (atm).

The Henry's law constant used in Equations 4 and 5 may be adjusted for system temperature by:

$$\ln \left(\frac{H_T}{H_R} \right) = - \frac{\Delta H_{v,T_s}}{R} \left(\frac{1}{T_s} - \frac{1}{T_R} \right) \quad (7)$$

where H_T is the Henry's law constant at the desired temperature ($\text{atm}\cdot\text{m}^3/\text{mol}$); H_R is the Henry's law constant at the reference temperature ($\text{atm}\cdot\text{m}^3/\text{mol}$); $\Delta H_{v,T_s}$ is the enthalpy of vaporization of the compound at the system temperature (cal/mol); R is the gas constant $1.987 \text{ cal/mol}\cdot^{\circ}\text{K}$; T_s is the system temperature ($^{\circ}\text{K}$); and T_R is the Henry's law constant reference temperature ($^{\circ}\text{K}$) (U.S. EPA, 1990). The enthalpy of vaporization at the system temperature may be estimated from Lyman et al. (1990):

$$\Delta H_{v,T_s} = \Delta H_{v,b} \left[\frac{(1-T_s/T_c)}{(1-T_b/T_c)} \right]^n \quad (8)$$

where $\Delta H_{v,b}$ is the enthalpy of vaporization at the normal boiling point (cal/mol); T_s is the system temperature ($^{\circ}\text{K}$); T_c is the critical temperature ($^{\circ}\text{K}$); T_b is the normal boiling point ($^{\circ}\text{K}$); and n is an exponential term given the value of 0.38. The dimensionless form of the Henry's law constant corrected for temperature (H_T') is simply H_T/RT_s where R is the gas constant $8.21\text{E-}05 \text{ m}^3\cdot\text{atm/mol}\cdot^{\circ}\text{K}$ and T_s is the system temperature ($^{\circ}\text{K}$).

With an estimate of the equilibrium vapor-phase concentration as a function of the degree of saturation, the removal rate at each time-step may be calculated using Equation 2. This also requires an estimate of the induced vapor flow rate from the SVE well (Q). Constant vapor flow rate may be estimated from Johnson et al. (1990) as:

$$Q = H \left[\frac{\pi k_v}{\mu} \right] P_w \frac{[1 - (P_{atm}/P_w)^2]}{\ln (R_w/R_i)} \quad (9)$$

where H is the length of the vacuum well that is screened through the vadose zone (cm), k_v is the permeability of the soil to vapor flow (cm^2), μ is the viscosity of air ($1.8\text{E-}04$ g/cm-s), P_w is the well absolute pressure (g/cm-s²), P_{atm} is the average atmospheric pressure (g/cm-s²), R_w is the vent well radius (cm), and R_i is the well radius of influence (cm) where the pressure is equal to atmospheric pressure.

For screening purposes, the screened interval (H) is assumed to be equal to the thickness of the contaminated zone. The removal rate (g/s) for each time-step is calculated using Equation 2. The initial total mass of the contaminant within the radius of influence of a single vacuum well at time-zero is estimated from the initial soil concentration and the well radius of influence by:

$$M_i = \pi R_i^2 H C_{o,i} \quad (10)$$

where M_i is the total initial mass of component i (g); R_i is the well radius of influence (cm); H is the screened interval (cm); and $C_{o,i}$ is the initial soil concentration of i (g/cm³) at time-zero.

For the first time-step, the initial soil concentration is compared to the value of C_{sat} calculated by Equation 4. Equation 3 or Equation 5 is then used to calculate the vapor-phase concentration, as appropriate. The vapor concentration is then multiplied by the

flow rate calculated by Equation 9 to obtain the removal rate (g/s). The removal rate is then multiplied by the time-step interval (s) to derive the total mass removed. This mass is subsequently subtracted from the initial mass calculated by Equation 10. The remaining mass is converted to a concentration by dividing the remaining mass by the volume determined from the values of R_i and H (i.e., $V = \pi R_i^2 H$). This concentration is then compared to the value of C_{sat} to determine the appropriate phase-partitioning for the next time-step. This procedure is duplicated for each succeeding time-step until a target soil concentration is reached.

During the transition from four to three phases (i.e., when the residual phase is depleted), the dissolved-phase concentration will not be at the solubility limit, as assumed in Equation 5, but will be at a reduced concentration such that the activity coefficients of the dissolved and residual phases are in local equilibrium as a function of the mole fraction. Therefore during the transition, Equation 5 will tend to overpredict the vapor-phase concentration and thus the emission rate. Once the soil concentration drops below the value of C_{sat} , the vapor-phase concentration predicted at each time-step is compared to that predicted at the previous time-step. If the vapor-phase concentration predicted by Equation 5 is higher than that predicted for the previous time-step, the vapor-phase concentration is multiplied by the mole fraction.

Appendix A contains a case example spreadsheet printout of the multicomponent estimation procedures for 10 contaminants. The spreadsheet is constructed in MICROSOFT EXCEL Version 5.0. Enclosed with this document is a diskette containing the EXCEL spreadsheet. In addition, this file has also been converted to a LOTUS 1-2-3 spreadsheet.

The spreadsheet may be used with the original 10 chemicals or new chemicals may be substituted. If analysis of more than 10 chemicals is needed, the spreadsheet must be altered to accommodate the additional compounds. If less than 10 chemicals are to be analyzed, the initial soil concentrations of the excess listed chemicals must be set to zero. To execute the analysis, the data entry sheet is filled-in first. The next step is to simply copy down row 14 starting at column AF (the column containing the time-steps for the first chemical) until the soil concentration remaining for each chemical is less

than the target soil concentration. Emission calculations for each chemical cannot be done separately because the computed mole fractions are based on the relative weight fractions of all chemicals.

Once the analysis is complete, the average emission rate of each chemical (\overline{ER}_i) over the operating time of the SVE system may be numerically estimated using the trapezoidal rule:

$$\overline{ER}_i = \frac{1}{\tau} \left[\frac{\Delta t}{2} (ER_0 + 2ER_1 + 2ER_2 + \dots + 2ER_{n-1} + ER_n) \right] \quad (11)$$

where τ is the averaging period (s), Δt is the constant time-step interval (s), $ER_{0,1,2 \dots n}$ are the emission rates at the initial and each succeeding time-step (g/s), and n is the number of time-steps. To ensure that a mass balance violation does not occur, the cumulative mass lost of each chemical ($\overline{ER}_i \times \tau$) must be compared with the initial mass in the soil at time-zero. If the cumulative mass lost is greater than the initial mass, the analysis is rerun with a shorter time-step interval.

The multicomponent estimation model, as well as the screening model computer codes described in the next section, require chemical properties for the contaminants to be analyzed. The following is a list of references which may be consulted to attain these chemical properties:

CHEMDAT8 Data Base of Compound Chemical and Physical Properties. U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards Technology Transfer Network (TTN), CHIEF Bulletin Board, Research Triangle Park, North Carolina.

CRC Handbook of Chemistry and Physics. CRC Press, Boca Raton, Florida. 1995.

Perry, R. H., and C. H. Chilton, eds. Chemical Engineering Handbook, 5th Ed. McGraw-Hill, New York, New York. 1973.

Soil Screening Guidance: User's Guide. U.S. Environmental Protection Agency, Office of Solid Waste and Emergency Response, Washington, D.C. OSWER Publication 9355.4-23. April 1996.

Soil Screening Guidance: Technical Background Document. U.S. Environmental Protection Agency, Office of Solid Waste and Emergency Response, Washington, D.C. EPA/540/R95/128.

Superfund Chemical Data Matrix and User's Guide. U.S. Environmental Protection Agency, Office of Emergency and Remedial Response, Washington, D.C. EPA/540/R-96-028 and EPA/540/R-96/029.

3.3 SCREENING MODEL COMPUTER CODES FOR MULTICOMPONENT SYSTEMS

The work of Johnson et al. (1990 and 1990a) are available as computer codes in two separate programs. The HyperVentilate code (Johnson, 1991) is available as public domain software free of charge from the U.S. EPA. The HyperVentilate application manual (U.S. EPA, 1993) is a software guidance manual for evaluating the feasibility of using SVE at specific sites. HyperVentilate operates in the APPLE MACINTOSH or the IBM PC-compatible MICROSOFT WINDOWS environment with OBJECT PLUS.

HyperVentilate is an educational and decision support tool consisting of several "stacks" of graphical reference "cards" within a hypertext framework. Based on user inputs and/or a range of default model parameters, HyperVentilate enables the user to decide whether SVE is practical, produce preliminary SVE system designs, and project system costs. Of particular interest to risk evaluations of remedial alternatives, HyperVentilate can estimate maximum removal rates. The analytical mass transfer equations used by the code are based on Raoult's law, and assume the presence of NAPL in the vadose zone. Therefore, it is not appropriate to apply HyperVentilate at sites where NAPL is absent because Henry's law rather than Raoult's law describes volatilization from the dissolved-phase. The program does not compute time-dependent removal rates. Program outputs include: 1) extraction well flow rate, 2) maximum estimated contaminant removal rates, 3) desired versus maximum removal rate, 4) soil permeability estimates, 5) relative removal efficiency based on diffusion-limited vapor transport, and 6) removal rates based on vapor flow outside of the contaminated zone.

VENTING is a program for estimating hydrocarbon recovery from SVE and is based on the VENTING fortran code of Johnson et al. (1990). VENTING is a commercial code available from Environmental Systems and Technologies, Inc. (ES&T, 1994). At the time of publication, the cost of the VENTING software was \$395. The code uses a MICROSOFT DOS based text menu interface for data input and provides ASCII output of the results in the form of phase partitioning and mass versus time at a series of user-specified time-steps. Graphical output is a series of plots for total mass and individual component mass versus time. VENTING calculates contaminant mass in the subsurface (averaged over the entire specified contaminated zone) over time during extraction from a single well or a multiwell system based on a user-defined SVE flow rate. The code will also calculate flow rate using Equation 9. Soil permeability may be specified by the user or calculated from air pumping tests.

VENTING partitions contaminant mass at each time-step following the procedures outlined in Johnson et al. (1990). The total initial mass of each contaminant in a mixture at each time-step is numerical calculated using a variable time weighted scheme. Using these procedures, the program is able to partition contaminants in four and three-phase systems. VENTING also incorporates the diffusion-limited solution of Johnson et al. (1990) by calculating a venting efficiency factor which accounts for vapor flow through uncontaminated soils. Finally, the code also includes a biodegradation scheme whereby the rate constant is calculated as a function of the amount of oxygen pulled through the contaminated zone and a default theoretical oxygen requirement for all contaminant species in dissolved-phase.

The multicomponent estimation procedures described in Section 3.2 were compared to the results of employing the VENTING model for an example mixture of benzene, toluene, and ethylbenzene. Figure 2 shows the results of this comparison. Overall, the comparison indicates similar results for the same vapor flow rate. Major differences may be attributed to the fact that the VENTING model repartitions the soil concentration at each time-step, and thus calculates mole fractions based only on the mass fractions in the residual phase. The multicomponent estimation procedures do not repartition at each time-step but compute mole fractions as a function of the total mass

SOIL CONCENTRATIONS REMAINING

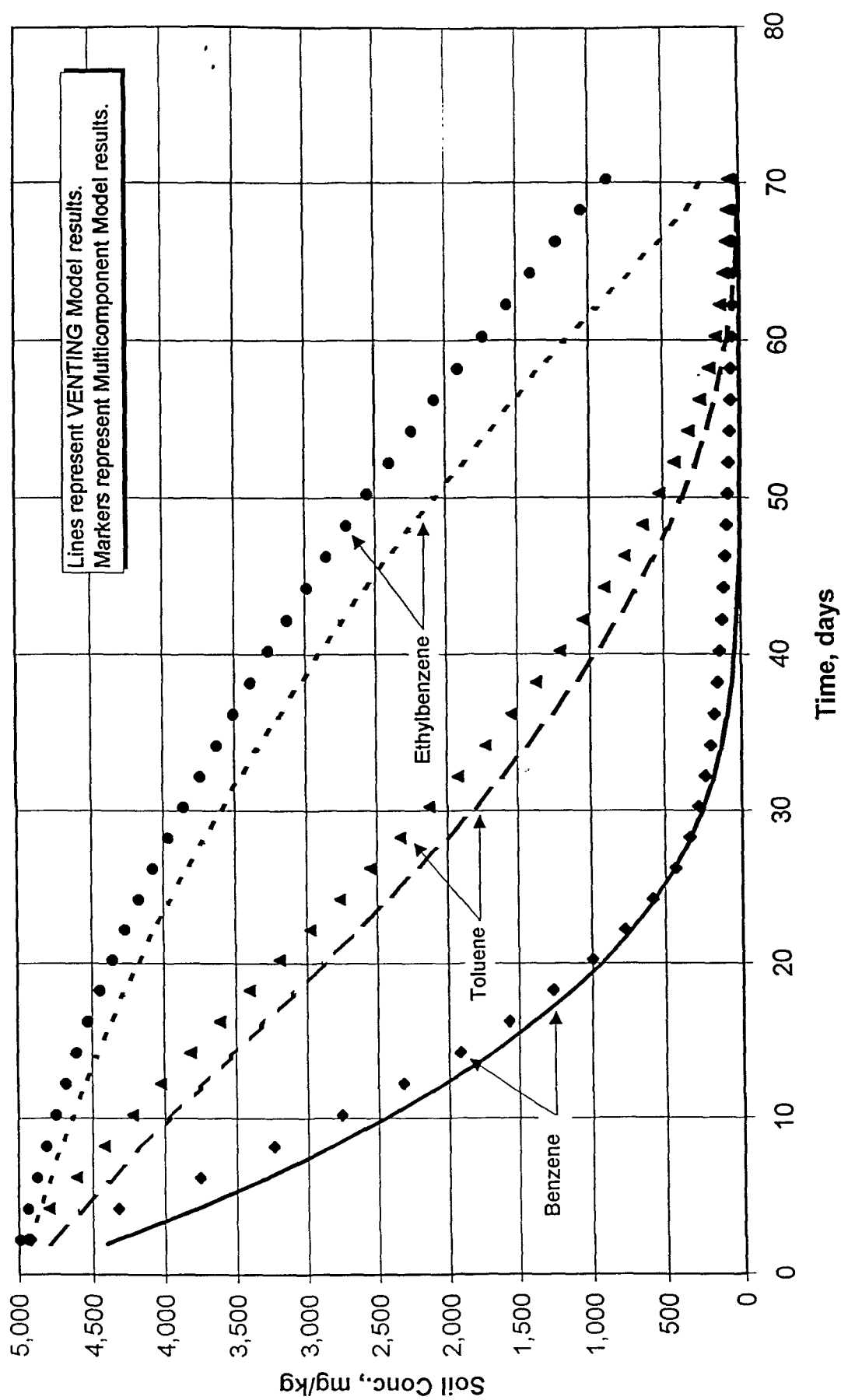


Figure 2. Comparison of time-dependent soil concentrations of benzene, toluene, and ethylbenzene.

fractions. In addition, the VENTING model accounts for the presence or absence of a residual phase as a function of phase saturation for the mixture of contaminants; the multicomponent estimation procedures estimate phase saturation for individual components rather than for the mixture. Finally, the VENTING model calculates Henry's law constants while the estimation procedures use published Henry's law constants and approximate four to three phase transition by assuming that activity coefficients are a function of the total mass mole fractions.

SECTION 4

REFINED ESTIMATES OF REMOVAL RATES

Refined models that are applicable to SVE systems can be categorized into 1) air flow models and 2) compositional flow and transport models. Air flow models generally are used to predict vapor flow rates and pressure distributions in the vadose zone due to the induced pressure differential of a single or multiple extraction wells. Compositional flow and transport models are also used to simulate SVE-induced air flow but included algorithms to estimate contaminant phase partitioning and multicomponent transport in the vadose zone. Because the main objective of modeling for risk evaluation is to determine SVE removal rates (i.e., uncontrolled emission rates), only compositional flow and transport models provide the vapor composition data needed to estimate air pathway exposure point concentrations.

Refined models are most useful for risk evaluation purposes during the RD/RA when more detailed site data are available. Compositional flow and transport models attempt to simulate pressure distributions, vapor distributions and vapor flow in complex two or three-dimensional domains and require detailed soil and contaminant distribution data. As a result, the predicted removal rate and time required to deplete site contaminants to target levels can be more rigorously estimated.

Recently, a review was performed of the mathematical models for evaluating SVE systems (U.S. EPA, 1995). The following discussion regarding refined compositional flow and transport models is taken from that review.

Compositional flow and transport models can be used to estimate both the subsurface air flow regime and the transport and removal of contaminants via SVE. These models can also be used to estimate post-remedial soil concentrations in order to determine if cleanup goals can be met. Flow and

transport modeling can be used to generate estimates for most aspects of SVE design, ranging from well placement to contaminant extraction rates. However, the level of complexity of the modeling and data requirements are also substantially greater than that associated with screening and air flow models.

A compositional flow and transport model should be used when it is necessary to attempt to estimate both the air flow regime and the transport of contaminants in the subsurface. The transport portion of the model allows more robust analysis of contaminant removal rates than simplified screening models, and provides estimates of contaminant levels in soil over the operating life of the SVE system. Compositional flow and transport models can be applied to estimate the concentration of a specified contaminant in the vadose zone for any given point in space and time. Thus, it may be advantageous to develop a transport model to examine mass removal trends given sufficient site characterization data.

Simulating vapor transport increases both the complexity and uncertainty associated with a modeling analysis. In addition to the parameters which affect air flow, transport simulation also requires characterization of the contaminant distribution and the contaminant media, and fluid properties which affect transport but not flow. Characterizing contaminant distribution, transport properties, and transport processes is typically subject to significantly greater uncertainty than characterizing flow properties and processes.

Results from a transport model consist of contaminant concentrations throughout the model region over time in soil and soil vapor. As such, transport models can be used to predict or evaluate contaminant removal rates and residual concentrations. These results can be used to assess the overall efficacy of an SVE system and identify problem areas where mass removal rates are inadequate. Areas where simulated contaminant concentrations remain at unacceptable levels for the duration of the planned SVE operation may require the installation of additional extraction or injection wells. Contaminant removal rates can be used to develop a general estimate of cleanup time. A determination of residual concentrations can be useful both in predicting possible

cleanup levels and determining which, if any, semivolatile compounds may remain in place after SVE has been completed. Such an analysis requires characterization of the existing contaminant distribution.

Two commercially available computer codes for refined modeling were reviewed for this report. The VENT2D model, Benson et al. (1993) simulates steady-state air flow and transient vapor-phase transport of multicomponent mixtures. Any number of vapor extraction or injection wells can be simulated, and grid-variable soil permeability, and initial contaminant distribution can be specified. An upper confining layer can be included to simulate the effects of surface boundary condition effects. The equilibrium partitioning distribution of contaminant in residual, sorbed, dissolved, and vapor-phases is calculated, as are the effects of contaminant retardation. The transport of soil moisture is simulated, and permeability is a time-and space-dependant function of soil moisture and NAPL saturation.

With the VENT2D model, Benson et al. (1993) take a convenient approach to the solution of the adjective-dispersive equation by neglecting mechanical dispersion in favor of diffusion. This allows a simpler finite difference numerical formulation to solve the transport equation, thus enabling transport modeling of multicomponent mixtures with retardation. Equilibrium phase partitioning is assumed and the presence of NAPL is indicated when all non-NAPL phases are saturated. Sorption to soil solids of individual constituents is calculated based on octanol/water partition coefficients and the soil fraction of organic carbon.

The model solves the steady-state equation of air flow based on the principle of conservation of mass. The concept of relative permeability in which effective permeability varies as a function of changing air-filled porosity is incorporated in VENT2D. Permeability increases with decreasing soil moisture and NAPL saturation due to drying induced by SVE. In order to save computational time, the permeability distribution is only recalculated when 10 percent or more of the active cells' permeability values have changed by 25 percent or more.

VENT2D operates in the DOS environment and does not provide any input or output interface or menu. The code author suggests that an effective approach to developing a simulation is to modify one of the example input files provided to suit the user's needs. A utility program is included that allows conversion of SURFER grid files to ASCII text so that site concentration contour maps can be used as initial concentration input to VENT2D. The code includes several composition files, including fresh and weathered gasoline, and common solvents.

The outer boundary of the model domain is set by default as follows: no-flow at the bottom of the domain (water table); and constant, atmospheric pressure and zero concentration elsewhere around the model perimeter. A surface confining layer is allowed, whereby the user can control vertical leakage by varying the vertical permeability of the confining layer. Extraction wells are represented by constant-flow cells. The pressure at an extraction well can be determined based on the pressure distribution output from the model. An additional feature of VENT2D allows placement of zero-concentration nodes at the model surface to simulate contaminant diffusion to the atmosphere.

VENT2D produces a wide range of output data, including distributions for pressure, permeability, air flow specific discharge (analogous to air flow velocity), soil moisture content, total VOC and individual component concentrations in soil and soil gas, and NAPL. A utility program included with the software will convert any of the parameter maps in the output file to a SURFER file format for contouring (U.S. EPA, 1995).

VENT2D allows two-dimensional (areal or cross-sectional) analysis of air flow and multicomponent transport with multiple extraction wells. A three-dimensional extension of this code called VENT3D has also become available recently. Some of the new features incorporated within VENT3D include the ability for individual layers to be given unique values of thickness, anisotropy, porosity, moisture content, organic carbon content, and distributions of permeability and contamination. At the time of publication of this report, VENT2D or VENT3D is available from the author at a price of \$495.

Recently, a new commercial model has become available with many of the same features as the VENT2D model but which offers a menu-driven operating environment.

AIRFLOW/SVE (Guiguer et al., 1995) simulates soil vapor flow in an axisymmetric cylindrical coordinate system whereby the vacuum extraction well is located at the center of a theoretical cylinder. The model boundaries are the ground water table, the ground surface, and the well radius of influence. The coordinate system results in a vertical axis representing elevation above the water table, and a horizontal axis representing the radial distance from the extraction well. The model simulates gas flow and vapor transport in the radial and vertical directions. All soil properties and water saturation are assumed to be homogeneous in the radial direction. Multiphase flow and transport are approximated using a finite difference solution to the governing partial differential equations.

AIRFLOW/SVE features a fully menu-driven operating system. From user-specified data, the model generates a finite difference grid of the SVE environment. The user is then transferred to a computer-aided design (CAD) environment where the grid can be altered and model parameters manipulated. After execution of the computational analysis, the results can be visualized and output to the screen, printer, plotter or to a graphics file. Output includes pressure contours, velocity vectors, flow path lines, isoconcentration contours, and NAPL distribution contours, as well as concentration, mass, and removal rate versus time. At the time of publication of this report, AIRFLOW/SVE is available from Waterloo Hydrogeologic Software at a price of \$1,195.

Air flow and compositional flow and transport models generally incorporate more assumptions and require more data input than simplified screening models. The user must be able to select and apply increasingly complex boundary and initial conditions effectively. As the complexity of the model increases, so does the complexity of the results and their potential uncertainty. Simulation results of a compositional flow and transport model for a multicomponent mixture depend on numerous properties of each component. In order to effectively interpret the results of the model, the modeler must understand the physics, chemistry, and mathematics of the model application (U.S. EPA, 1995).

To evaluate short-term risk during the remedial action and, if applicable, during the five-year review, perhaps the best use of refined modeling is to estimate the time for source depletion and the vacuum well vapor constituent distributions as a function of time.

This may best be accomplished by modeling the vacuum well removal rates at the start of SVE system operation to predict the decrease in component residual mass in the soil. At periodic intervals after the start of remediation, the SVE system can be shut down and the soil contaminants allowed to re-equilibrate. Upon restart of the system, measured contaminant concentrations and field measurements of pressure distributions are used to remodel the removal rates on a contaminant-specific basis. In this manner, the model may be calibrated to field conditions and afford more accurate predictions of vapor flow rate, total mass removed as a function of time, and the removal rates of individual contaminants. Calibration may be achieved by applying field pressure distribution data to the model variables affecting vapor flow rate, and by altering contaminant input variables (e.g., initial concentration) so that the calculated vapor-phase concentrations match measured values.

SECTION 5

LIMITATIONS AND ASSUMPTIONS OF MODELS REVIEWED

Three screening models were reviewed for this report: 1) HyperVentilate, 2) VENTING, and 3) a multicomponent estimation model. All three models are based on the work of Johnson et al. (1990 and 1990a). As such, the limitations and assumptions of the analytical vapor flow rate solution are identical. The three models vary, however, in the procedures used to estimate vapor-phase concentrations and distributions of contaminants.

5.1 GAS FLOW

The three screening models solve for steady-state radial flow in a one-dimensional confined porous medium using Equation 9. This solution is normally used to calculate a range of predicted vapor flow rates based on soil vapor permeability and well pressure. Equation 9 predicts the rate of vapor flow through an ideal isotropic soil column in that actual flow is assumed to be unimpeded due to diffusion mass transfer limitations between a contaminated soil layer and a gas flow field which passes parallel to but not through the contaminated layer (e.g., for a lens of floating product). In addition, the solution to vapor flow does not consider air flow variations due to impedances such as unconnected pore spaces, variations in pore size and volumetric water content, or variations in lateral and vertical permeability (leaky or confining layers).

The HyperVentilate and VENTING models attempt to account for nonideal flow with a user-specified or calculated venting efficiency factor. If part of the total gas flow does not pass through the contaminated soil, an efficiency factor (ϕ) will arise such that if the screened interval (H) is specified as the total unsaturated zone thickness, the factor will be equal to the ratio of contaminated zone thickness to total unsaturated zone thickness.

This accounts for the dilution effects of "clean" air flowing parallel to but not through the contamination.

To account for diffusion-limited mass transfer, HyperVentilate and VENTING employ the procedure of Johnson et al. (1990) to calculate a diffusion-limiting efficiency factor as:

$$\eta = \left[\frac{2 D_E \mu R_c^2 \ln (R/R_w)}{3 H^2 k_v (P_{atm} - P_w)} \right]^{1/2} \quad (12)$$

where D_E is the effective diffusion coefficient (cm^2/s) and R_c is the radius of the contaminated soil zone, $R_c \leq R_i$, (cm). The effective diffusion coefficient is given as $D_E = D_A (\Theta_a^{3.33}/n^2)$, where D_A is the diffusion coefficient in air (cm^2/s), Θ_a is the soil air-filled porosity (unitless) and n is the total soil porosity (unitless). The diffusion-limiting efficiency factor may be used to account for nonideal conditions within the soil column, such as a floating product layer at the top of the water table or a pocket of contamination within a clay lens of lower permeability. The factor relates venting efficiency as limited by diffusion from subsurface locations where the gas flow field passes parallel to, but not through the contaminated layer. In the event that multiple factors such as fractional swept volume and diffusion limitations occur simultaneously, the net efficiency is the product of each efficiency factor.

Calculation of the efficiency factors described above may also be applied to the multicomponent estimation model described herein such that

$$ER_i = (1 - \phi) \eta Q C_{i,v}^{eq} \quad (13)$$

where ER_i is the uncontrolled emission rate (removal rate) of component i (g/s); ϕ is the fraction of air flow through uncontaminated soil; η is the fractional efficiency due to diffusion-limited mass transfer (Equation 12); Q is the vapor flow rate calculated by

Equation 9 (cm^3/s); and $C_{i,v}^{\text{eq}}$ is the equilibrium vapor concentration (g/cm^3). Alternatively, the user may specify efficiency factors based on observation, experience, field measurements, or professional judgement.

5.2 VAPOR CONCENTRATION

The three screening models and the refined models reviewed for this report use multiphase partitioning of homogeneously contaminated soil to derive the vapor-phase concentration. The HyperVentilate code is applicable only when a residual phase is present and calculates the maximum vapor-phase concentration, and thus removal rate, by employing Raoult's law. Therefore, HyperVentilate cannot estimate removal rates as a function of time. The VENTING code, VENT2D and VENT3D, and AIRFLOW/SVE employ a molar mass-balance approach whereby the vapor-phase concentration is derived as a function of the degree of phase saturation. These programs are capable of equilibrating four and three-phase systems and can predict time-dependent removal rates. The multicomponent estimation model can also estimate four and three-phase equilibrium but is less accurate than the molar mass balance approach.

Most vapor transport models developed to date assume local equilibrium between phases to simplify calculation of chemical mass distribution, movement, and interphase transfer.

The local equilibrium assumption presumes: 1) the rate of chemical movement through any phase in the vadose zone is slow compared to the rate of mass transfer between phases, 2) chemical concentrations in all phases are therefore in thermodynamic equilibrium, 3) mass transfer is reversible, 4) phase equilibrium is independent of the presence of other phases, and 5) linear partitioning occurs which does not vary with chemical concentration (U.S. EPA, 1995).

The soil water partition coefficient, K_p , is a valid representation of the partitioning between dissolved and sorbed-phases only if partitioning is fast compared to vapor flow, reversible and linear. Although this is true for many organic compounds, it is not true for others. Karickhoff et al. (1979) investigated the sorption and desorption of organic

compounds and found that a very rapid component of sorption was followed by a slower component visualized as diffusive transport to the interior sorption sites that were inaccessible to the fluid (U.S. EPA, 1995). Sorption, therefore, appears to be a combination of adsorption to the surface of the sorbent as well as adsorption within the micropores of the soil particles. In combination with nonlinear desorption and confinement of contaminant in isolated layers (e.g., clays), this phenomenon may be responsible for much of the reported discrepancies between simulated removal rates and observed removal rates.

Typically, the rate of contaminant removal usually declines rapidly in the initial stage of remediation as the more volatile constituents are removed by advection. This initial stage is followed by a transitional stage between advective and diffusive mass transfer. Finally, a third stage marks the diffusion-limiting mass transfer which is characterized by the relatively slow process of contaminant diffusion from dead-end pores and stagnation zones, evaporation from the dissolved-phase, and desorption from the sorbed-phase. The mass balance approach to local phase equilibrium used by the computer models reviewed for this report and the approach used by the multicomponent estimation model do not account for nonlinear desorption nor for retarded desorption from the interiors of the sorbing clays and organic matter particles.

This combination of rate-limiting factors, including fractional vapor flow through the contaminated zone, diffusion-dominated mass transfer, and nonideal phase equilibria, may combine to produce a "tailing" effect whereby the actual time required to reduce the total contaminant mass in the soil may be significantly longer than predicted values.

SECTION 6

ESTIMATION OF AMBIENT AIR CONCENTRATIONS

Estimates of short-term or long-term ambient air concentrations may be obtained by using site-specific release parameters with the EPA SCREEN3 Model (Version 96043, EPA 1996), TSCREEN Model (Version 94133, EPA 1994), or the Industrial Source Complex (ISC3) Short-Term Model (Version 96113, EPA 1996).

The EPA OAQPS has developed an electronic bulletin board network to facilitate the exchange of information and technology associated with air pollution control. This network, entitled the OAQPS Technology Transfer Network (TTN), is comprised of individual bulletin boards that provide information on OAQPS organization, emission measurement methods, regulatory air quality models, emission estimation methods, Clean Air Act Amendments, training courses, and control technology methods. The dispersion model codes and user's guides referred to in this document, are all available on the TTN in the bulletin board entitled SCRAM, short for Support Center for Regulatory Air Models. Procedures for downloading these codes and documents are also detailed in the SCRAM bulletin board. The TTN may be accessed at the telephone number (919) 541-5742 for users with 1200 or 2400 bps modems, or at the telephone number (919) 541-1447 for users with a 9600 bps modem. The communications software should be configured with the following parameter settings: 8 data bits, 1 stop bit, and no (N) parity. The SCRAM is also available on the Internet via the world wide web through EPA's main website (<http://www.epa.gov/scram001>).

Depending upon time, resources, and modeling experience, one may use these dispersion models as an evaluation tool to quickly assess ambient air concentrations. Depending upon the contaminants involved, air concentrations can then be used to perform risk evaluations or ARAR compliance evaluations. The ISC3ST and TSCREEN

models can handle a variety of averaging times such as 1-h, 3-h, 8-h, 24-h, and annual. The SCREEN3 model only computes ambient concentrations for a 1-h averaging period. For compounds that have chronic toxicity values or long-term regulatory standards, ISC3ST and TSCREEN provide an annual ambient air concentration. If SCREEN3 is used, one must adjust the hourly concentration by applying a conversion factor of 0.08 to convert to an annual averaging period. The conversion factors for estimating an annual, 24-h, 8-h, and 3-h ambient air concentration are presented below in Table 1.

TABLE 1. CONVERSION FACTORS FOR 1-HOUR AMBIENT AIR CONCENTRATIONS

Convert to	Conversion factor
3-h	0.9
8-h	0.7
24-h	0.4
Annual	0.08

If the SVE site is located in an area with receptors located far enough away (critical distances vary according to contaminants involved, emission rates, and equipment parameters), the SCREEN3 or TSCREEN models may satisfy the necessary modeling requirements. If receptors are located nearby or if stringent regulatory standards are to be met, the ISC3ST model using actual meteorological data is recommended. Other advantages include more flexible averaging periods and more accurate handling of building downwash and complex terrain.

These air dispersion models can also be used to help assess design parameters for the SVE system as well as address the effects of control options, if needed. An SVE system is modeled as a point source in most cases, and the stack parameters used in the air dispersion models will be the same. Data required are as follows:

- Emission rate (g/s)
- Stack height (m)
- Stack inside diameter (m)
- Stack gas exit velocity (m/s)

- ° Stack gas exit temperature (° K).

Additional data required are use of either the urban or rural coefficients of dispersion, receptor coordinates or distances, and meteorological data (ambient temperature for the screening models and a meteorological data file for the ISC3ST model). If the SVE system will be operated for less than one year, the ISC3ST model includes an option (i.e., EMISFACT) that allows the user to zero emissions for any month (multiplies the emission rate by a factor), which will affect the annual ambient air concentrations accordingly. In addition, if the SVE system is shut down during the day or evening to allow the vapors to accumulate, the EMISFACT allows the user to zero emissions for any hour of a 24-h day, which allows for more accurate 24-h concentrations.

To help assess the effects of SVE size and/or evaluate the risks to receptors at the site, Tables 2 through 4 give typical SVE parameters according to control options. These scenarios were developed based on a review of the existing literature and discussions with researchers in the SVE area.

Four air emission control options are typically employed for SVE systems: 1) no controls, 2) activated carbon control systems, 3) catalytic oxidation control systems, and 4) thermal oxidation control systems. Thermal and catalytic oxidation emission control systems can reduce emissions by 90 to 95 percent. Activated carbon systems have control efficiencies that are compound specific. The reader is referred to U.S. EPA 1989 and 1992 for more information on control options for soil vapor extraction technologies.

TABLE 2. EXAMPLE SCENARIOS FOR SVE WITH NO CONTROLS BASED ON SIZE OF SYSTEM

Parameter	Units	Scenario			
		Very Small	Small	Medium	Large
Exhaust Gas Flow Rate	m ³ /min cfm	1.4 50	14 500	85 3,000	425 15,000
Exhaust Gas Velocity	m/sec	3.0	7.4	12.5	14.2 ^a
Exit Gas Temperature	°C	50	50	50	50
Stack Height	m	3.0	4.6	7.6	9.1
Stack Diameter	m	0.10	0.20	0.38	0.46

^a Assume three adjacent stacks each handling 5,000 cfm. The flow is split to lower the velocity of the exiting gas to typical design levels to minimize corrosion of the stack.

TABLE 3. EXAMPLE SCENARIOS FOR SVE WITH ACTIVATED CARBON CONTROLS BASED ON SIZE OF SYSTEM

Parameter	Units	Scenario			
		Very Small	Small	Medium	Large
Exhaust Gas Flow Rate	m ³ /min cfm	1.3 46	13 461	78 2,770	392 13,800
Exhaust Gas Velocity	m/sec	2.8	6.9	11.5	13.1 ^a
Exit Gas Temperature	°C	25	25	25	25
Stack Height	m	3.0	4.6	7.6	9.1
Stack Diameter	m	0.10	0.20	0.38	0.46

^a Assume three adjacent stacks each handling 4,600 cfm. The flow is split to lower the velocity of the exiting gas to typical design levels to minimize corrosion of the stack.

TABLE 4. EXAMPLE SCENARIOS FOR SVE WITH CATALYTIC OR THERMAL OXIDATION CONTROLS BASED ON SIZE OF SYSTEM

Parameter	Units	Scenario			
		Very Small	Small	Medium	Large
Exhaust Gas Flow Rate	m ³ /min cfm	2.6 92	26 918	156 5,510	780 27,500
Exhaust Gas Velocity	m/sec	5.5	13.8	22.9	26.1 ^a
Exit Gas Temperature	°C	320	320	320	320
Stack Height	m	3.0	4.6	7.6	9.1
Stack Diameter	m	0.10	0.20	0.38	0.46

^a Assume three adjacent stacks each handling 9,200 cfm. The flow is split to lower the velocity of the exiting gas to typical design levels to minimize corrosion of the stack.

SECTION 7

RECOMMENDATIONS

The following procedures are recommended for estimating uncontrolled emissions from SVE systems for the purposes of conducting an air pathway evaluation. The recommendations are categorized as to when the evaluation is performed within the remedial process. When applied, these procedures will provide theoretical predictions of removal rates of individual contaminants based on increasingly rigorous estimates of vapor flow in the vadose zone and contaminant phase partitioning.

7.1 ESTIMATING EMISSIONS DURING THE FEASIBILITY STUDY

During the feasibility study (FS), a range of remedial alternatives is identified, if necessary, and each alternative is evaluated with respect to effectiveness, implementability, and cost. This process typically involves development of alternatives and screening of technologies. Those alternatives that are clearly unfavorable relative to other alternatives in terms of effectiveness or implementability, or that are grossly excessive in cost are dropped from consideration after the screening. During the detailed analysis of alternatives, more site-specific data are typically available to refine the screening procedures to evaluate the potential risks to the community and to workers. Screening-level models are therefore more applicable during the FS in making preliminary assessments of SVE feasibility at contaminated sites. Screening models can be applied with very limited site data, and thus can be used early in the remedial process.

The HyperVentilate model is perhaps best used during the initial identification and screening of remedial alternatives. This model is designed primarily to assess the feasibility of SVE and to grossly estimate costs. HyperVentilate is capable of estimating subsurface vapor flow under ideal conditions and capable of estimating the maximum

uncontrolled emissions of individual contaminants. HyperVentilate does not compute time-dependent emissions, and is only applicable at sites where NAPL is present. HyperVentilate does not predict the time required to deplete initial soil concentrations to a target concentration. If NAPL is present at the site, and if the soil target concentration is above the soil saturation concentration, HyperVentilate can be used to estimate maximum emissions for a user-specified remediation time interval.

The VENTING model is a better choice for estimating 1) time-dependent emissions, 2) time required for initial soil contaminant depletion, and 3) residual contaminant soil concentrations as a function of time. VENTING may be employed at sites where NAPL is not present or when target soil cleanup concentrations are below the soil saturation concentration. VENTING uses the same subsurface vapor flow algorithms as the HyperVentilate code but is capable of four and three-phase contaminant partitioning.

Finally, the multicomponent estimation model described in this document and detailed in Appendix A may be used if the VENTING commercial code is not available. This model uses the same radial flow algorithms as the VENTING code but simplifies phase partitioning.

The HyperVentilate model directs the user through a step-by-step approach for estimating SVE feasibility and maximum contaminant removal rates. Therefore, the user is referred to the model user's manual (U.S. EPA, 1993) for specific guidance. The following guidance is applicable for estimating time-dependent uncontrolled emissions from SVE systems using either the VENTING model or the multicomponent estimation model.

Application of the VENTING model or the multicomponent estimation model involves estimating a range of predicted emissions based on a typical range of values for the most sensitive model parameters. The most sensitive variables in calculating the subsurface flow rate are soil permeability to vapor flow, vacuum well pressure, and soil temperature.

Table 5 gives the flow rate model variables, the practicable range of variable values, and the default variable values from U.S. EPA (1993 and 1995).

TABLE 5. VAPOR FLOW RATE MODEL VARIABLES

Variable	Practical range	Default value(s)
Permeability (k_v)	0.01 to 100 Darcys	
- Medium sand		10 - 100 Darcys
- Fine sand		1 - 10 Darcys
- Silty sand		0.1 - 1 Darcys
- Clayey silts		0.01 - 0.1 Darcys
Well pressure (P_w)	5 - 200 in. H_2O	20 - 120 in. H_2O
Radius of influence (R_l)	3 - 12 m	12 m
Well radius (R_w)	5.08 - 60.96 cm	10.16 cm
Soil temperature (T_s)	0 - 30°C	11°C
Screened interval thickness	0.3 - 6 m	Set H equal to thickness of contamination

Vapor flow rates should be calculated using the range of default values unless site-specific data are available.

Contaminant phase distributions are calculated by both models based on the initial soil concentration (total volume) and soil properties. Table 6 gives the soil properties required for phase partitioning and the default values for subsurface soils from U.S. EPA (1994) if site-specific data are not available.

Once a range of vapor flow rates have been calculated, the subsurface equilibrium vapor concentration of each contaminant is estimated for a series of time-steps. If site-specific information is available, an estimate of the fraction of subsurface vapor flow through uncontaminated soil (ϕ) can be made. In addition, a fractional system efficiency (η) can be calculated using Equation 12 to account for diffusion-limited mass transfer, if applicable.

TABLE 6. SOIL PROPERTY VARIABLES FOR PHASE PARTITIONING

Variable	Default value
Soil dry bulk density (ρ_b)	1.5 g/cm ³
Soil particle density (ρ_s)	2.65 g/cm ³
Total soil porosity (n)	0.434 cm ³ /cm ³
Soil moisture content (w)	0.20 g/g
Soil water-filled porosity (Θ_w)	0.300 cm ³ /cm ³
Soil air-filled porosity (Θ_a)	0.134 cm ³ /cm ³
Soil organic carbon (f_{oc})	0.002 g/g

7.2 ESTIMATING EMISSION DURING THE RD/RA

Because more data are generally available during the remedial design, a compositional flow and transport model may be more useful for estimating uncontrolled emission rates. VENT2D, VENT3D, or AIRFLOW/SVE allow for solution of radial flow in stratified soils for multiwell systems and attempt to compensate subsurface vapor flow due to nonconfined boundaries and variations in site permeability.

Perhaps the best use of these types of models is to perform calibrated estimates of removal rates and vapor concentrations throughout the life of the remediation. This may best be accomplished by periodically recalibrating the model with measured pressure, soil contaminant concentration, and vapor concentration distribution data. After recalibration, the models may be rerun to examine unexpected variations in system performance, to re-evaluate the time required to complete remediation, or the extent to which SVE can attain the target soil concentrations.

7.3 DISPERSION MODELING TO ESTIMATE AMBIENT AIR IMPACTS

As in estimating emissions during the feasibility study, screening-level models are used to make preliminary assessments of ambient air impacts from the site. Depending upon site location with respect to receptors, contaminants involved, and/or equipment

design and controls, a screening model may be all that is needed to conservatively predict short- or long-term, ambient air concentrations. The SCREEN3 or TSCREEN models offer quick results for a first look at ambient air impacts and in some cases may be all that is needed to assess the risks associated with a SVE unit. If refined modeling is desired or needed to predict more accurate ambient air concentrations, the ISC3ST model is recommended to provide short-term or annual average impacts. The major advantage of the ISC3ST model is the use of actual meteorological data as well as options to zero out emissions (e.g., EMISFACT) for any hour, month, or season the SVE system is not operated.

With time-dependent uncontrolled emissions and an estimate of the time to deplete the initial soil concentrations to target levels, atmospheric dispersion modeling can be used to estimate exposure point concentrations from which potential risks can be assessed. With these data, a decision can be made as to the need for air pollution control equipment. If controls are required, an estimate can then be made of controlled emission rates and the relative risks of remediation via soil vapor extraction.

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;

APPENDIX A

MULTICOMPONENT ESTIMATION MODEL (CASE EXAMPLE)

COL	B	C	D	E	F	G	H	I	J	K	L	M	N
ROW	DATA ENTRY SHEET												
3													
4	ENTER Chemical Properties												
5													
6				Organic carbon partition coefficient, K_{oc}	Vapor pressure at 25°C, p^*	Henry's law constant at 25°C, H	Enthalpy of vaporization at the normal boiling point, ΔH_{vap}	Normal boiling point, T_b	Critical temperature, T_c	Diffusion coefficient in air, D_a	Initial soil conc., C_o	Target soil conc., C_T	Initial soil conc., C_o
7													
8		Molecular weight, MW	Solubility in water, S										
9													No
10													Entry
11	Chemical	(g/mol)	(mg/L)	(cm ³ /g)	(mmHg)	(atm-m ³ /mol)	(cal/mol)	(°K)	(°K)	(cm ² /s)	(mg/kg)	(mg/kg)	Required
12													
13	Benzene	78.12	1750	61	95.2	5.55E-03	7342	353.24	562.16	8.70E-02	5000	120	5.00E-03
14	Toluene	92.14	526	139	30	6.84E-03	7930	383.78	591.79	8.70E-02	5000	120	5.00E-03
15	Ethylbenzene	106.16	169	180	10	7.88E-03	8501	409.34	617.20	7.50E-02	5000	120	5.00E-03
16	m-Xylene	106.16	161	196	8	7.34E-03	8523	412.27	617.05	7.00E-02	5000	120	5.00E-03
17	Trichloroethylene	131.40	1100	94	75	1.03E-02	7505	360.36	544.20	7.90E-02	5000	120	5.00E-03
18	Tetrachloroethylene	165.85	200	268	19	1.84E-02	8288	394.40	620.20	7.20E-02	5000	120	5.00E-03
19	Chloroform	119.39	7920	56	208	3.87E-03	6988	334.32	536.40	1.04E-01	5000	120	5.00E-03
20	Carbon Tetrachloride	153.84	793	152	113	3.04E-02	7127	349.90	556.60	7.80E-02	5000	120	5.00E-03
21	1,2-Dichloroethane	98.96	8520	38	80	9.79E-04	7643	356.60	561.00	1.04E-01	5000	120	5.00E-03
22	1,1,1-Trichloroethane	133.42	1330	137	123	1.72E-02	7137	347.27	545.00	7.80E-02	5000	120	5.00E-03
23													
24	ENTER Soil Properties												
25	a	a		a	a								
26													
27	Soil dry bulk density, ρ_b	Average soil temp., T_s	Soil vapor permeability, k_v	Average soil moisture content, w	Soil organic carbon, f_{oc}	Average thickness of contamination, D_c							
28													
29													
30													
31	(g/cm ³)	(°C)	(darcy)	(g/g)	(fraction)	(m)							
32													
33	1.5	11	10	0.2	0.002	3							
34													
35	ENTER Default or Calculated SVE System Conditions												
36	a	b		a	a	a	a	c	d	d, e			
37	Vent well radius, R_w	Screened interval thickness, H	Well absolute pressure, P_w	Absolute atmospheric pressure, P_{atm}	Well radius of influence, R_i	Air viscosity, μ	Vapor flow through uncontaminated soil, ϕ	Consider diffusion-limited mass transfer? (Enter YES, NO, or User Defined)	Minimum initial time-step (i.e., time-zero), t_0	Maximum time-step interval, Δt			
38													
39													
40													
41													
42	(cm)	(cm)	(ft H ₂ O)	(ft H ₂ O)	(cm)	(g/cm-s)	(fraction)	Fractional Efficiency	(days)	(days)			
43													
44	10.16	300	24	34.8084	1200	1.80E-04	0	NO	0.25	2			
45													
46	a = default value												
47	b = [H = D _c x 100]=default. If H > D _c , enter fraction of vapor flow through uncontaminated soil (ϕ).												
48	c = entering YES assumes diffusion-limited mass transfer across the areal extent of contamination (i.e., $R_i = R_l$); entering NO results in a fractional efficiency of 1.0; user-defined efficiency should be entered as a fraction.												
49	d = shorter time-step intervals may be necessary when numerical integrations yield greater cumulative mass lost than initial mass at time-zero.												
50	e = longer time-step intervals may be necessary for any or all of the following: 1) high initial soil concs., 2) less volatile compounds, 3) low permeability soils, 4) low extraction well vacuum, and 5) fractional flow or diffusion-limited mass transfer.												
51													
52													

COL ROW	O	P	Q	R	S	T	U	V
CHEMICAL PROPERTY CALCULATIONS								
3								
4								
5								
6								
7		Enthalpy of vaporization at T_s	Henry's law constant at T_s	Henry's law constant at T_s	Vapor pressure at 25°C,	Vapor pressure at T_s	Soil/water partition coefficient,	Soil saturation conc.,
8								
9								
10		$\Delta H_{v,T_s}$	H_i	H_i'	P^v	P^v	K_D	C_{sat}
11		(cal/mol)	(atm·m ³ /mol)	(unitless)	(atm)	(atm)	(cm ³ /g)	(mg/kg)
12								
13	Benzene	8186	2.81E-03	0.1204	0.1253	0.0651	0.122	582
14	Toluene	9203	3.09E-03	0.1324	0.0395	0.0194	0.278	258
15	Ethylbenzene	10171	3.38E-03	0.1449	0.0132	0.0060	0.360	97
16	m-Xylene	10253	3.13E-03	0.1341	0.0105	0.0047	0.392	97
17	Trichloroethylene	8564	5.05E-03	0.2165	0.0987	0.0510	0.188	448
18	Tetrachloroethylene	9641	8.25E-03	0.3536	0.0250	0.0119	0.536	154
19	Chloroform	7604	1.95E-03	0.0836	0.2737	0.1520	0.112	2530
20	Carbon Tetrachloride	7917	1.57E-02	0.6745	0.1487	0.0789	0.304	447
21	1,2-Dichloroethane	8579	4.79E-04	0.0208	0.1053	0.0536	0.076	2367
22	1,1,1-Trichloroethane	7931	8.89E-03	0.3812	0.1618	0.0860	0.274	676
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COL	W	X	Y	Z	AA	AB	AC	AD	AE
ROW	SOIL PROPERTY AND WELL CALCULATIONS								
3									
4									
5									
6									
7	Volume of	Total	Water-filled	Air-filled	Soil	Well	Absolute	Vapor	Diffusion- limited efficiency factor, η
8	contaminated	soil	soil	soil	vapor	absolute	atmospheric	flow	
9	soil per well,	porosity,	porosity,	porosity,	permeability,	pressure,	pressure,	rate,	
10	V_s	n	θ_w	θ_a	k_v	P_w	P_{atm}	Q	
11	(cm ³)	(cm ³ /cm ³)	(cm ³ /cm ³)	(cm ³ /cm ³)	(cm ²)	(g/cm-s ²)	(g/cm-s ²)	(cm ³ /s)	(unitless)
12									
13	1.3572E+09	0.434	0.300	0.134	1.00E-07	6.9859E+05	1.0132E+06	84593	1.000
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COL ROW	AF	AG	AH	AI	AJ	AK	AL	AM
3	Benzene	EMISSION CALCULATIONS						
4								
5		Total						
6		mass of						
7		contaminant	Soil	Soil	Mole	Estimated	Uncontrolled	Uncontrolled
8		per well,	conc.,	conc.,	fraction,	vapor	emission	emission
9	Time	M	C _s	C _s	x _i	conc.,	rate	rate
10	(days)	(g)	(mg/kg)	(g/g)	(fraction)	C _v ^W	per well,	per well,
11						(g/cm ³)	ER _w	ER _w
12	0.25	1.0179E+07	5.000	5.00E-03	0.144	3.15E-05	2.66E+00	5.78E+04
13	2.25	1.0121E+07	4.972	4.97E-03	0.144	3.15E-05	2.66E+00	4.60E+05
14	4.25	9.6610E+06	4.746	4.75E-03	0.143	3.12E-05	2.64E+00	4.56E+05
15								
16	COPY DOWN ROW 14 STARTING WITH							
17	COLUMN "AF" THROUGH COLUMN "DG"							
18	UNTIL THE CALCULATED SOIL							
19	CONCENTRATION REMAINING							
20	FOR EACH COMPOUND IS LESS THAN							
21	THE RESPECTIVE TARGET SOIL							
22	CONCENTRATION SPECIFIED IN COLUMN "M".							
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COL	AN	AO	AP	AQ	AR	AS	AT	AU
ROW	EMISSION CALCULATIONS							
3	Toluene							
4								
5		Total					Uncontrolled	Uncontrolled
6		mass of					emission	emission
7		contaminant	Soil	Soil	Mole	Estimated	rate	rate
8		per well,	conc.,	conc.,	fraction,	vapor	per well,	per well,
9	Time	M	C _s	C _s	x _i	C _v ^{eq}	ER _w	ER _w
10	(days)	(g)	(mg/kg)	(g/g)	(fraction)	(g/cm ³)	(g/s)	(g/unit T)
11								
12	0.25	1.0179E+07	5,000	5.00E-03	0.122	9.37E-06	7.92E-01	1.71E+04
13	2.25	1.0162E+07	4,992	4.99E-03	0.123	9.40E-06	7.95E-01	1.37E+05
14	4.25	1.0024E+07	4,924	4.92E-03	0.126	9.62E-06	8.14E-01	1.41E+05
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COL	AV	AW	AX	AY	AZ	BA	BB	BC
ROW	EMISSION CALCULATIONS							
3	Ethylbenzene							
4								
5		Total				Estimated	Uncontrolled	Uncontrolled
6		mass of				vapor	emission	emission
7		contaminant	Soil	Soil	Mole	conc.	rate	rate
8		per well,	conc.,	conc.,	fraction,		per well,	per well,
9	Time	M	C _s	C _s	x _i	C _s ^M	ER _w	ER _w
10	(days)	(g)	(mg/kg)	(g/g)	(fraction)	(g/cm ³)	(g/s)	(g/unit T)
11								
12	0.25	1.0179E+07	5,000	5.00E-03	0.106	2.91E-06	2.46E-01	5.31E+03
13	2.25	1.0173E+07	4,997	5.00E-03	0.107	2.92E-06	2.47E-01	4.27E+04
14	4.25	1.0131E+07	4,976	4.98E-03	0.110	3.01E-06	2.55E-01	4.41E+04
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COL	BD	BE	BF	BG	BH	BI	BJ	BK
ROW	EMISSION CALCULATIONS							
3	m-Xylene							
4								
5		Total					Uncontrolled	Uncontrolled
6		mass of					emission	emission
7		contaminant	Soil	Soil	Mole	Estimated	rate	rate
8		per well,	conc.,	conc.,	fraction,	conc.,	per well,	per well,
9		M	C _o	C _o	x _i	C _o ^{eq}	ER _w	ER _w
10	Time	(g)	(mg/kg)	(g/g)	(fraction)	(g/cm ³)	(g/s)	(g/unit T)
11	(days)							
12	0.25	1.0179E+07	5,000	5.00E-03	0.106	2.27E-06	1.92E-01	4.14E+03
13	2.25	1.0175E+07	4,998	5.00E-03	0.107	2.28E-06	1.93E-01	3.33E+04
14	4.25	1.0141E+07	4,982	4.98E-03	0.110	2.35E-06	1.99E-01	3.44E+04
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COL	BL	BM	BN	BO	BP	BQ	BR	BS
ROW	EMISSION CALCULATIONS							
3	Trichloroethylene							
4								
5		Total						
6		mass of						
7		contaminant	Soil	Soil	Mole	Estimated	Uncontrolled	Uncontrolled
8		per well,	conc.,	conc.,	fraction,	vapor	emission	emission
9		M	C _o	C _o	x _i	conc.,	rate	rate
10	Time	(g)	(mg/kg)	(g/g)	(fraction)	C _v ¹⁴	per well,	per well,
11	(days)					(g/cm ³)	ER _w	ER _w
12	0.25	1.0179E+07	5.000	5.00E-03	0.086	3.06E-05	2.59E+00	5.59E+04
13	2.25	1.0123E+07	4.973	4.97E-03	0.086	2.47E-05	2.09E+00	3.61E+05
14	4.25	9.7621E+06	4.795	4.80E-03	0.086	2.47E-05	2.09E+00	3.61E+05
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COL	BT	BU	BV	BW	BX	BY	BZ	CA
ROW	EMISSION CALCULATIONS							
3	Tetrachloroethylene							
4								
5								
6		Total				Estimated	Uncontrolled	Uncontrolled
7		mass of				vapor	emission	emission
8		contaminant	Soil	Soil	Mole	conc.,	rate	rate
9		per well,	conc.,	conc.,	fraction,	per well,	per well,	per well,
10	Time	M	C _o	C _o	χ	C _v ^a	ER _w	ER _w
11	(days)	(g)	(mg/kg)	(g/g)	(fraction)	(g/cm ³)	(g/s)	(g/unit T)
12								
13	0.25	1.0179E+07	5.000	5.00E-03	0.068	8.98E-06	7.60E-01	1.64E+04
14	2.25	1.0162E+07	4.992	4.99E-03	0.068	5.77E-06	4.88E-01	8.44E+04
15	4.25	1.0078E+07	4.951	4.95E-03	0.070	5.94E-06	5.02E-01	8.68E+04
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COL	CB	CC	CD	CE	CF	CG	CH	CI
ROW	EMISSION CALCULATIONS							
3	Chloroform							
4								
5		Total					Uncontrolled	Uncontrolled
6		mass of				Estimated	emission	emission
7		contaminant	Soil	Soil	Mole	vapor	rate	rate
8		per well,	conc.,	conc.,	fraction,	conc.,	per well,	per well,
9	Time	M	C _o	C _o	x _i	C _v ⁴⁴	ER _w	ER _w
10	(days)	(g)	(mg/kg)	(g/g)	(fraction)	(g/cm ³)	(g/s)	(g/unit T)
11								
12	0.25	1.0179E+07	5.000	5.00E-03	0.095	8.27E-05	7.00E+00	1.51E+05
13	2.25	1.0028E+07	4.926	4.93E-03	0.094	7.29E-05	6.16E+00	1.07E+06
14	4.25	8.9625E+06	4.403	4.40E-03	0.087	6.75E-05	5.71E+00	9.87E+05
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COL	CJ	CK	CL	CM	CN	CO	CP	CQ
ROW	EMISSION CALCULATIONS							
3	Carbon Tetrachloride							
4								
5		Total						
6		mass of						
7		contaminant	Soil	Soil	Mole	Estimated	Uncontrolled	Uncontrolled
8		per well,	conc.,	conc.,	fraction,	vapor	emission	emission
9	Time	M	C _o	C _o	x _i	C _v ^W	rate	rate
10	(days)	(g)	(mg/kg)	(g/g)	(fraction)	(g/cm ³)	ER _w	ER _w
11							(g/s)	(g/unit T)
12	0.25	1.0179E+07	5.000	5.00E-03	0.073	5.54E-05	4.68E+00	1.01E+05
13	2.25	1.0078E+07	4.950	4.95E-03	0.073	3.80E-05	3.22E+00	5.56E+05
14	4.25	9.5220E+06	4.677	4.68E-03	0.072	3.73E-05	3.15E+00	5.45E+05
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COL ROW	CR	CS	CT	CU	CV	CW	CX	CY
EMISSION CALCULATIONS								
3	1,2-Dichloroethane							
4								
5		Total						
6		mass of						
7		contaminant	Soil	Soil	Mole	Estimated	Uncontrolled	Uncontrolled
8		per well,	conc.,	conc.,	fraction,	vapor	emission	emission
9	Time	M	C _o	C _o	x	conc.,	rate	rate
10	(days)	(g)	(mg/kg)	(g/g)	(fraction)	C _v ^M	per well,	per well,
11						(g/cm ³)	ER _w	ER _w
12	0.25	1.0179E+07	5,000	5.00E-03	0.114	2.42E-05	2.04E+00	4.42E+04
13	2.25	1.0135E+07	4,978	4.98E-03	0.114	2.60E-05	2.20E+00	3.79E+05
14	4.25	9.7552E+06	4,792	4.79E-03	0.114	2.59E-05	2.19E+00	3.79E+05
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COL	CZ	DA	DB	DC	DD	DE	DF	DG
ROW	EMISSION CALCULATIONS							
3	1,1,1-Trichloroethane							
4								
5		Total					Uncontrolled	Uncontrolled
6		mass of					emission	emission
7		contaminant	Soil	Soil	Mole	Estimated	rate	rate
8		per well,	conc.,	conc.,	fraction,	vapor	per well,	per well,
9	Time	M	C _o	C _o	x _i	C _v ^{eq}	ER _w	ER _w
10	(days)	(g)	(mg/kg)	(g/g)	(fraction)	(g/cm ³)	(g/s)	(g/unit T)
11								
12	0.25	1.0179E+07	5.000	5.00E-03	0.085	5.23E-05	4.42E+00	9.55E+04
13	2.25	1.0083E+07	4.953	4.95E-03	0.084	4.14E-05	3.50E+00	6.06E+05
14	4.25	9.4776E+06	4.656	4.66E-03	0.082	4.04E-05	3.42E+00	5.90E+05
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TECHNICAL REPORT DATA*(Please read Instructions on reverse before completing)*

1. REPORT NO. EPA-451/R-96-007	2.	3. RECIPIENT'S ACCESSION NO.
4. TITLE AND SUBTITLE Air/Superfund National Technical Guidance Study Series, Estimation of Air Impacts for Soil Vapor Extraction (SVE) Systems (Revised)		5. REPORT DATE August 1996
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16. ABSTRACT The purpose of this document is to provide both screening level and refined models for estimating the uncontrolled emissions from soil vapor extraction systems and resulting ambient air concentrations. The document references several public domain and commercially available emission models. In addition, the document is accompanied by a PC computer diskette containing a screening emission model for multiple contaminants. This model is written in the form of a spreadsheet.		
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