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Estimation of Air Impacts for the Excavation of Contaminated Soil

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Estimation of Air Impacts for the Excavation of Contaminated Soil

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INTRODUCTION

The U.S. Environmental Protection Agency's Office of Air Quality Planning and Standards 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.

This report provides procedures for roughly estimating the ambient air concentrations associated with the excavation of contaminated soil. These procedures are analogous to procedures for air strippers and soil vapor extraction systems that have previously been published[1,2]. Excavation is an integral part of any Superfund site remediation that involves removal or ex-situ treatment such as incineration, thermal desorption, bioremediation, or solidification/stabilization. Procedures are given to evaluate the effect of concentration and physical properties of the contaminants in the soil on the emission rates and on the ambient air concentrations at selected distances from the the excavation site.

Health-based ambient air action levels are also provided for comparison to the estimated ambient concentrations. Many of the health levels have not been verified by EPA or are based on extrapolations of oral exposures or occupational exposures. Their indiscriminate use could either under or over estimate the potential health effects. The statements and conclusions presented in this report are those of the authors and do not reflect U.S. EPA policy.

PROCESS DESCRIPTION

Excavation and removal of soils contaminated with Volatile Organic Compounds (VOCs) is a common practice at Superfund sites. Excavation and removal may be the selected remediation approach or it may be a necessary step in a remediation approach involving treatment. If removal is the preferred approach, the excavated soil is typically transported off-site for subsequent disposal at a landfill. If the soil contains large amounts of fuel or highly toxic contaminants, the soil may need to be treated off-site prior to final disposal. Excavation activities are also typically part of on-site treatment processes such as incineration, thermal desorption, batch biotreatment, landtreatment, and certain chemical and physical treatment methods. The soil is excavated and transported to the process unit and the treated soil is typically put back into place on the site.

VOC emissions from handling operations result from the exchange of contaminant-laden soil-pore gas with the atmosphere when soil is disturbed and from diffusion of contaminants through the soil. There are multiple potential emission points for each of the various soils handling operations. For excavation, the main emission points of concern are emissions from:

- exposed waste in the excavation pit;
- material as it is dumped from the excavation bucket; and
- waste/soil in short-term storage piles.

An idealized excavation scenario is shown in Figure 1 and assumes that each scoop of excavated soil has dimensions of 1m x 2m x 1m and that the soil is removed as a series of blocks that retain their shape and are stacked in a temporary storage pile.

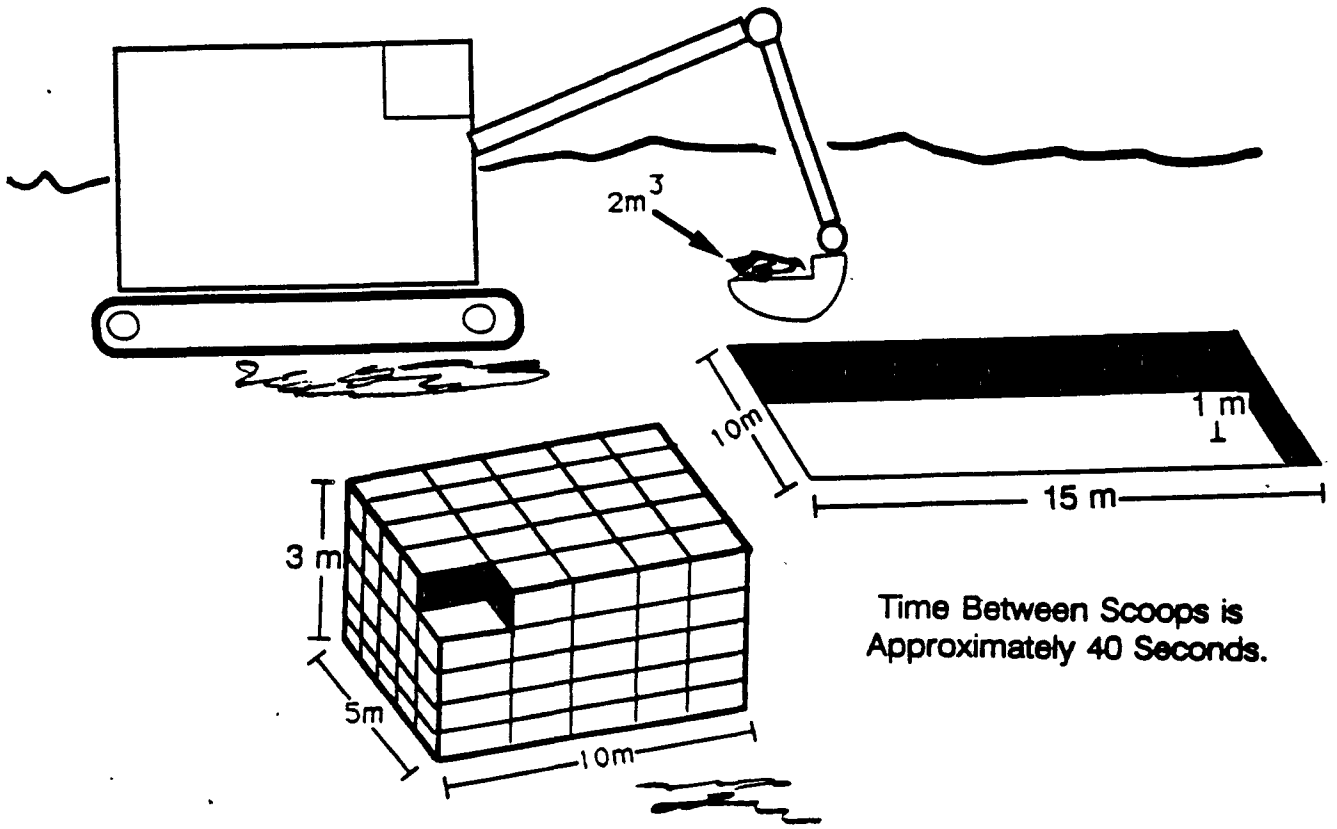

Figure 1. Idealized Excavation Scenario

The magnitude of VOC emissions depends on a number of factors, including the type of compounds present in the waste, the concentration and distribution of the compounds, and the porosity and moisture content of the soil. The key operational parameters are the duration and vigorousness of the handling, and the size of equipment used. The longer or more energetic the moving and handling, the greater likelihood that organic compounds will be volatilized. The equipment size influences volatilization by affecting the mean distance a volatilized molecule has to travel to reach the air/solid interface at the surface of the soil. In general, the larger the volumes of material being handled per unit operation, the lower the percentage of VOCs that are stripped from the soil.

The success of excavation for a given application depends on numerous factors with the three key criteria being: 1) the nature of the contamination; 2) the operating practices followed; and 3) the proximity of sensitive receptors. Each of these criteria is described below.

The magnitude of emissions from soils handling operations will vary with the operating conditions. Add-on control technologies are available for minimizing VOC emissions, but they are relatively ineffective and costly to implement. VOC emission control can also be achieved by controlling the operating conditions within preset parameters. The rate of excavation and dumping, the drop height, the amount of exposed surface area, the length of time that the soil is exposed, the shape of the storage piles, and the dryness of the surface soil layers will all influence the levels of VOC emissions. Large reductions in emissions can be achieved by identifying, and operating within, acceptable ranges of operating conditions.

Since some release of volatile contaminants is inevitable during excavation and removal unless extreme measures are taken (e.g. enclose the remediation within a dome), the proximity of downwind receptors (i.e. people) will influence whether or not excavation is an acceptable option. Excavation of contaminated areas that abut

residential areas, schoolyards, etc. may require more extensive controls, relocation of the affected population, or remediation only during certain periods (e.g. summertime for school sites).

ESTIMATION OF AIR EMISSIONS

Only limited guidance is currently available for estimating the air emissions from soils handling operations. The emissions of concern from soils handling operations such as excavation, dumping, grading, transport, and storage are typically volatile organic compounds (VOCs), though emissions of particulate matter and associated metals and semi-volatile compounds may be of concern at some sites.

There are several alternative approaches for estimating the emissions from excavation. The best method is to directly measure the emissions during full-scale or pilot-scale soils handling activities. The next best method is to estimate the emissions using predictive equations with site-specific inputs. If site-specific inputs are not available, a very conservative estimate can be made by using default values for the input parameters. Equations are given below for estimating an average long-term emission rate and a short-term emission rate.

Average Long-Term Emission Rate

A simple check of the total emissions potential for the site should be made by dividing the total mass of a given contaminant to be removed by the expected duration of the clean-up:

$$ER = (S_V)(C)(\beta)(1) / t_R \qquad \text{(Eq. 1)}$$

where:
- ER = Average emission rate (g/sec);
- S_V = Volume of contaminated soil to be excavated (m^3);
- C = Average contaminant concentration (ug/g);

β = Bulk density of soil (g/cm^3);
1 = Constant ($g/10^6ug * 10^6cm^3/m^3$); and
t_R = Duration of remediation (sec).

The volume of contaminated soil and the total mass of each contaminant of concern present are typically determined during the remedial investigation (RI) of the site, while the fraction of contaminated soil that must be removed or treated is typically determined during the feasibility study (FS) of the site. Final clean-up criteria should also be considered when calculating the volume of soil to be excavated. The duration of the clean-up will usually be limited by the rate at which contaminants can be transported off-site or treated on-site. For Equation 1, a typical default value for bulk density of uncompacted soil is 1.5 g/cm^3. The following paragraphs discuss the key variables influencing air emissions from the excavation of contaminated soil and present an empirical equation for estimating a short-term emission rate.

Short-Term Emission Rate

A number of assumptions were made to develop a typical scenario for soil excavation. It is assumed that an infinite, homogeneous body of waste or contaminated soil exists under a cap of clean soil. The cap is removed and then contaminated soil/waste is excavated for 50 min/hour. Each scoop of soil contains 2 m^3 of soil and 75 scoops moved per hour (= 150 m^3 of soil moved per hour). Each scoop has dimensions of 1m x 2m x 1m and adds 2 m^2 of surface area to the pile of excavated material. The pit, after one hour has dimensions of 10m x 15m x 1m. Furthermore, each scoop of dumped soil is assumed to maintain its 1x2x1 dimensions (the pile of dumped soil is equivalent to a series of stacked blocks). After one hour, a pile 5m x 10m x 3m is established. The total exposed surface area is 140 m^2 for the pile and another 150 m^2 for the pit. The pile is assumed to thereafter be covered with some type of impermeable cover that acts as a barrier to further emissions. Both soil and air temperatures are assumed to be near 25°C.

Since it is rarely feasible or efficient to dig soil and immediately transfer the soil directly to transport vehicles or treatment systems, the equations presented below must be applied to each event in which the soil is handled. In most cases, soil will be excavated and placed in a temporary holding area and then moved one to two more times on-site. Elevated levels of VOC emissions are possible each time the soil is handled. When estimating emissions from sequential soil handling steps, it may be important to adjust the starting concentrations for each step to account for contaminants emitted during prior steps.

The detailed equation (model) for estimating emissions from excavation is given below followed by a simple screening equation to estimate excavation emissions. Appendix A presents the derivation of the simple screening equation, contains a discussion of the various input variables, and has an example calculation. The more detailed equation should be used in place of the screening equation whenever there are significant deviations from the assumptions used for air-filled porosity, air temperature, or the time that the soil is exposed to the atmosphere before being covered with additional soil. Field data should be used whenever possible and default values used only when no valid data are available.

Average Emission Rate (Detailed Model)

The average emission rate (ER, with units of g/sec) from excavation is equal to the sum of emission rates from the soil pore space (ER_{PS}, g/sec) and from diffusion (ER_{DIFF}, g/sec):

$$ER = ER_{PS} + ER_{DIFF} \qquad \text{(Eq. 2)}$$

$$ER_{PS} = \frac{P\ MW\ 10^6\ E_a\ Q\ ExC}{R\ T} \qquad \text{(Eq. 3)}$$

$$ER_{DIFF} = \frac{(C)(10{,}000)(SA)}{\left(\frac{E_a}{K_{eq}\, k_g}\right) + \left(\frac{\pi t}{D_e\, K_{eq}}\right)^{1/2}} \qquad \text{(Eq. 4)}$$

The term ExC in Equation 3 is the fraction of the VOC in the pore space that is emitted to the atmosphere during excavation. All variables in Equations 2, 3, and 4 are defined in Table 1. Also shown in Table 1 are the units of each variable and a typical default value to use if valid field data are not available. Values of molecular weight, vapor pressure at 25°C, and diffusivity in air at 25°C are given in Appendix B. Equation 3 is based on the assumption that the soil pore gas is saturated with the compound of interest. If this is not the case, then Equation 3 may overpredict the emission rate. The output from Equation 3 should be multiplied by the duration of excavation and compared to the total mass of contaminants present in the soil:

$$M = C * S_V * 10^6 cm^3/m^3 \qquad \text{(Eq. 5)}$$

where: M = Total mass of contaminant in a given volume of soil (g).

If Equation 3 gives a value that exceeds one-third of M, then the following equation should be substituted for Equation 3:

$$ER_{PS} = M * 0.33/t_{SV} \qquad \text{(Eq. 6)}$$

where: t_{SV} = Time to excavate a given volume, S_v, of soil (sec).

Average Emission Rate (Simplified Model)

The average emission rate from excavation is again equal to the sum of emission rates from the soil pore space and from diffusion:

$$ER = ER_{PS} + ER_{Diff} \qquad \text{(Eq. 2)}$$

Table 1

Input Variables for Emission Equations

Default Variable	Definition	Units	Default Value
P	Vapor pressure	mm Hg	35
MW	Molecular weight	g/g-mol	100
R	Gas constant	mm Hg-cm^3/g-mol °K	62,361
T	Temperature	Degrees Kelvin	298
E_a	Air-filled porosity	Dimensionless	0.440
S_V	Volume of soil moved	m^3	150
Q	Excavation rate	m^3/sec	0.042
10^6	Conversion factor	cm^3/m^3	--
ExC	Soil-gas to atmosphere exchange constant	Dimensionless	0.33
C	Concentration in soil	g/cm^3	1.35×10^{-4}
10,000	Conversion factor	cm^2/m^2	--
SA	Emitting surface area	m^2	290
K_{eq}	Equilibrium coefficient	Dimensionless	0.613
k_g	Gas-phase mass transfer coefficient	cm/sec	0.15
π	Pi	Dimensionless	3.14
t	Time[a]	sec	60
D_e	Effective diffusivity in air	cm^2/sec	0.0269
0.98	Conversion factor	g/mm Hg-m^3	--
1.22×10^6	Conversion factor	cm^2-sec-mmHg/g	--
1.79×10^9	Conversion factor	sec^2-cm-mmHg/g	--

Table 1 (Continued)

Default Variable	Definition	Units	Default Value
M	Total mass of contaminant	g	--
C'	Concentration in soil	ug/g	100
Other Variables Required to Calculate Certain Variables Listed Above			
t_{SV}	Time to excavate a given volume of soil	sec	--
ß	Bulk density	g/cm^3	1.5
ρ	Particle density	g/cm^3	2.65
D_a	Diffusivity in air	cm^2/sec	0.1
U	Wind speed	m/sec	2.0
μ_a	Viscosity of air	g/cm-sec	1.81×10^{-4}
ρ_a	Density of air	g/cm^3	0.0012
d_e	Diameter of excavation	m	24

[a]See Page 11 of Appendix A for discussion of time term.

$$ER_{PS} = P * Q * 0.91 \qquad \text{(Eq. 7)}$$

$$ER_{Diff} = \frac{(C)(10{,}000)(SA)}{\left(1.22\text{x}10^{6}\ \frac{C}{P}\right) + \left(1.79\text{x}10^{9}\ \frac{C}{P}\right)^{\frac{1}{2}}} \qquad \text{(Eq. 8)}$$

Variables are defined in Table 1. The derivation of these equations is presented in Appendix A (Equation 7 equals Equation A-13 in Appendix A and Equation 8 equals Equation A-20). Assuming a typical bulk density of undisturbed soil, C can be modified to a soil concentration term: $C' = C * 1cm^3/1.5g * 10^6$ ug/g; where: C' = Concentration of species i in soil (ug/g). The emission rate obtained using Equation 7 should be compared to the total mass of contaminant present in the volume of soil excavated - M. If Equation 7 gives a value that exceeds ⅓ of M, then Equation 6 should be substituted for Equation 7.

Worst-Case Emission Rate

The worst-case (i.e. maximum) instantaneous emission rate, ER_{MAX}, for contaminated soil occurs when the exposed surface area is at a maximum and immediately after a bucket load of soil is dumped onto the storage pile. This emission rate can be approximated by considering the case where a pure chemical is exposed to the atmosphere. This emission rate can be determined from Equation 6 (there is no need to consider pore space gas concentrations and diffusion since the pure chemical is already exposed to the atmosphere). Set the time term, t, equal to zero and replace the K_{eq} term with the equivalent expression: $P*MW*E_a/R*T*C$. Equation 6 then reduces to:

$$ER_{MAX} = \frac{(k_g)(P)(MW)(SA)(10{,}000)}{RT} \qquad \text{(Eq. 9)}$$

ESTIMATION OF AMBIENT AIR CONCENTRATIONS

Estimates of short-term, worst-case ambient concentrations should be obtained by using site specific release parameters in the EPA's TSCREEN model[3]. Estimates of long term concentrations should be obtained by using EPA's Industrial Source Complex (ISCLT) model. Here, for simplicity, the annual average estimates are derived by multiplying the short term estimate obtained from the TSCREEN model, by a conversion factor to account for variations of wind direction over time. This approach results in a higher estimate of the annual average concentration than if the ISCLT model, with site specific data, is used.

Table 2 presents three excavation scenarios that vary in excavation rate and physical dimensions. The scenarios were developed based on a review of the existig literature[5] and field experience. The worst-case, short-term downwind dispersion of emitted gases from each of these scenarios for an emission rate of 1 gram per second, is illustrated in Figure 2. Of the variables listed in Table 2, only the physical dimensions of the excavation pit and storage pile factor into the estimated downwind dispersion. Two additional curves in Figure 2 indicate the downwind dispersion for excavation areas of larger dimensions (500 m^2 and 1,000 m^2, respectively). The curves were calculated according to the following assumptions: 1) the combined emission rate for the excavation pit and storage pile is 1 gram per second; 2) the excavation pit and storage pile are sufficiently close to one another so that the size of the area emission source is equal to the combined horizontal areas of the pit and storage pile; 3) a flat terrain without any structures near the excavation site was assumed; and 4) downwash was not applicable. The emission source and the receptors were assumed to be at ground level. Downwind concentration estimates for emission rates other than 1 gram per second can be extrapolated from Figure 2 by multiplying the indicated y-axis value (dispersion factor) for the applicable downwind distance by the actual emission rate.

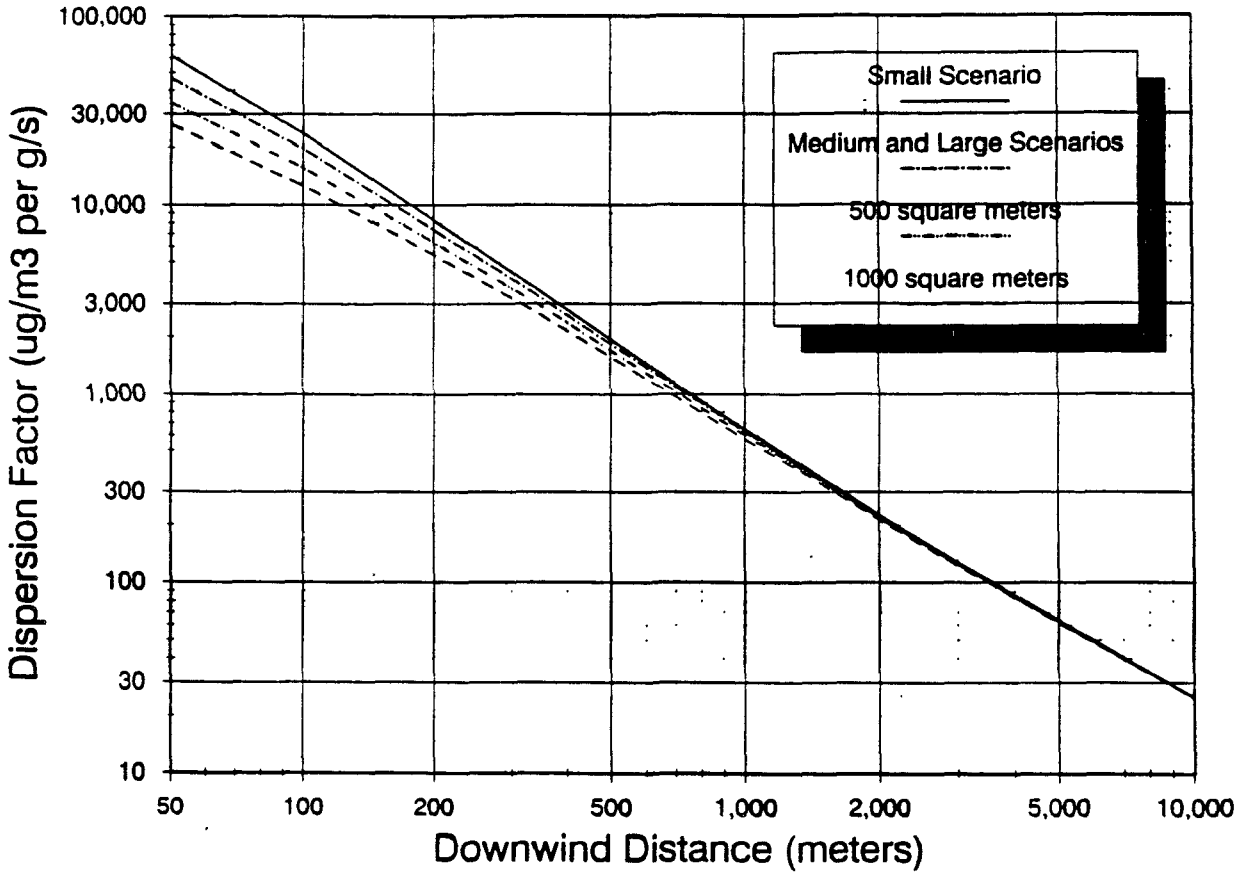

Figure 2. One-Hour Average Downwind Dispersion Factor Versus Distance for Excavation With No Air Controls

Table 2.

Example Scenarios for Excavation of Contaminated Soil

Parameter	Units	Scenario		
		Small	Medium	Large
Soil Moved Per Scoop	m^3	1	2	4
No. Scoops Per Hour	#/hr	50	75	60
Total Volume of Soil Moved	m^3/hr	50	150	240
Excavation Pit:				
Dimensions	m	10x5x1	10x15x1	10x12x2
Area	m^2	50	150	120
Storage Pile:				
Dimensions	m	5x5x2	5x10x3	8x10x3
Area	m^2	65	140	188

Figure 2 can be used to estimate the maximum hourly ambient air concentration for an emission rate of 1 gram per second at selected distances downwind from an excavation pit. If the excavation rate is not known, a medium rate scenario should be assumed. The dispersion factor, in micrograms/m^3 per g/sec, obtained from Figure 2 can be substituted into Equation 10 to estimate the maximum hourly ambient concentration and into Equation 11 to estimate the annual average ambient air concentration for a given downwind distance. Since TSCREEN provides maximum short-term estimates, the factor of 0.05 in Equation 11 is used to convert the short-term estimate to a maximum annual average estimate. A conservative factor of 0.05 assumes that the wind blows downwind 5% of the time over one year and that the terrain is relatively flat. This assumption has been recently revised by EPA; it is still under review by EPA, however, and is subject to further change.

$$C_m = (ER)(F) \qquad \text{(Eq. 10)}$$

$$C_a = (ER)(F)(0.05) \qquad \text{(Eq. 11)}$$

where:
C_m = Maximum hourly ambient air concentration($\mu g/m^3$);
C_a = Annual average ambient air concentration ($\mu g/m^3$);
ER = Emission rate (g/sec); and
F = Dispersion Factor from Figure 2 ($\mu g/m^3/g/sec$).

ESTIMATION OF HEALTH EFFECTS

Cancer Effects Due to Long-Term Exposure

Potential cancer effects resulting from long-term exposure to substances emitted to the air can be evaluated using inhalation unit risk factors. Inhalation unit risk factors are a measure of the cancer risk for each $\mu g/m^3$ of concentration in the ambient air. They are available on EPA's Integrated Risk Information System (IRIS), the Agency's preferred source of toxicity information. User Support can be contacted at (513) 569-7254. Table 3 provides inhalation unit risk factors listed in IRIS as of January 1991 for selected organic compounds.

The next best source of inhalation unit risk factors is EPA's Health Effects Assessment Summary Tables (HEAST) which are updated quarterly.[5]

Equation 12 can be used to estimate the cancer risk at a specified distance downwind of the excavation area. Cancer risk is a measure of the increased probability of developing cancer in a lifetime as a result of the exposure in question. Equation 12 assumes continuous exposure (24 hours/day, 365 days/year for 70 years) to the estimated annual average concentration in air.

$$R = (C_a)(IUR) \qquad \text{(Eq. 12)}$$

R is the cancer risk from long-term exposure to a specific VOC in air, dimensionless; C_a is the annual average ambient concentration estimated from Equation 11, $\mu g/m^3$; IUR is the inhalation unit risk factor, $(\mu g/m^3)^{-1}$ obtained from Table 3.

If the source operates for less than 70 years, multiply C_a by x/70, where x is the expected operating time of the source in years before using Equation 12. If more than one VOC is present, the cancer risks for each VOC can be summed to derive the total cancer risk at a specified distance downwind of the source.

Non-Cancer Effects Due to Long-Term Exposure

Non-cancer effects can be evaluated by using chronic inhalation reference concentrations (RfCs). An inhalation RfC is the an estimate (with uncertainty spanning perhaps an order of magnitude) of continuous exposure to the human population that is likely to be without appreciable risk of deleterious effects during a lifetime. RfCs for a limited number of compounds are available in IRIS and HEAST.

Table 3.

Long-Term and Short-Term Health-Based Action Levels for Ambient Air

No.	Chemical	CAS Number	Carcinogenicity[a]	Chronic Toxicity[a]	Long-Term Action Levels			Short-Term Action Levels[d]
					Risk-Specific Concentrations for Carcinogencity	RfC-Based Concentrations for Non-Carcinogenic Effects (µg/m³)	Concentrations Based on Occupational Exposure[d]	
			Inhalation Unit Risk 1/(µg/m³)	Inhalation RfC (mg/m³)	10-6 70-year Risk (µg/m³)		Lowest OEL/1000 (µg/m³)	Lowest OEL/100 (µg/m³)
1	Acetaldehyde	75-07-0	–	–	–	–	180	1,800
2	Acetic Acid	64-19-7	–	–	–	–	25	250
3	Acetic anhydride	108-24-7	–	–	–	–	20	200
4	Acetone	67-64-1	–	(4e-01)[b]	–	400	1,780	17,800
5	Acetonitrile	75-05-8	–	5e-02	–	50	67	670
6	Acrolein	107-02-8	ND[c,e]	1e-04[c]	–	0.1	0.23	2.30
7	Acrylic acid	79-10-7	–	3e-04	–	0.3	5.90	59
8	Acrylonitrile	107-13-1	6.8e-05	–	1.5e-02[c]	–	4.30	43
9	Allyl alcohol	107-18-6	–	(2e-02)[b]	–	20	4.80	48
10	Allyl chloride	107-05-1	ND[c,e]	1e-03	–	1	3.00	30
11	Aniline	62-53-3	(1.6e-06)[b]	–	6.3e-01	–	7.60	76
12	Anthracene	120-12-7	–	(1e+00)[b]	–	1,000	0.20	2.00
13	Benzaldehyde	100-52-7	–	(4e-01)[b]	–	400	–	–
14	Benzene	71-43-2	8.3e-06	–	1.2e-01[c]	–	0.30	3.00
15	Benzoic acid	65-85-0	–	(1e+01)[b]	–	10,000	–	–
16	Benzyl alcohol	100-51-6	–	(1e+00)[b]	–	1,000	–	–
17	Benzyl chloride	100-44-7	–	–	–	–	5	50
18	Bromoform	75-25-2	1.1e-06[c]	(7e-02)[b]	9.1e-01	70	5	50
19	1,3-Butadiene	106-99-0	2.8e-04	–	3.6e-03	–	22	220
20	n-Butane	106-97-8	–	–	–	–	1,900	19 000
21	2-Butanol	15892-23-6	–	–	–	–	303	3,030
22	n-Butanol	71-36-3	–	(4e-01)[b]	–	400	152	1,520
23	n-Butyl-Acetate	123-86-4	–	–	–	–	710	7,100
24	Tert-Butyl-Alcohol	75-65-0	–	–	–	–	300	3,000
25	Carbon disulfide	75-15-0	–	1e-02	–	10	12	120

Table 3.
(Continued)

No.	Chemical	CAS Number	Carcinogenicity[a]	Chronic Toxicity[a]	Long-Term Action Levels			Short-Term Action Levels[d]
					Risk-Specific Concentrations for Carcinogenicity	RfC-Based Concentrations for Non-Carcinogenic Effects ($\mu g/m^3$)	Concentrations Based on Occupational Exposure[d]	
			Inhalation Unit Risk $1/(\mu g/m^3)$	Inhalation RfC (mg/m^3)	10-6 70-year Risk ($\mu g/m^3$)		Lowest OEL/1000 ($\mu g/m^3$)	Lowest OEL/100 ($\mu g/m^3$)
26	Carbon Tetrachloride	56-23-5	1.5e-05	(2e-03)[b]	6.7e-02	2	12.60	126
27	Carbonyl Sulfide	463-58-1	--	--	--	--	--	--
28	Catechol	120-80-9	--	--	--	--	20	200
29	Chlorine	7782-50-5	--	--	--	--	1.5	15
30	Chlorobenzene	108-90-7	--	2e-02	--	20	46	460
31	Chlorodifluoromethane	75-45-6	--	--	--	--	3,540	35,400
32	Chloroform	67-66-3	2.3e-05	(4e-02)[b]	4.3e-02[c]	40	9.78	98
33	Chloromethyl methyl ether	107-30-2	ND	--	--	--	--	--
34	Chloropentafluoroethane	76-15-3	--	--	--	--	6,320	63,200
35	Chloroprene	126-94-8	--	1e-03[c]	--	1	35	350
36	m-Cresol	108-39-4	ND[e]	(2e-01)[b]	--	200	22	220
37	o-Cresol	95-48-7	ND[e]	(2e-01)[b]	--	200	22	220
38	p-Cresol	106-44-5	ND[e]	(2e-01)[b]	--	200	22	220
39	Cyanogen	460-19-5	--	(1e-01)[b]	--	100	20	200
40	Cyclohexane	110-82-7	--	--	--	--	1,030	10,300
41	Cyclohexanol	108-93-0	--	--	--	--	200	2,000
42	Cyclohexanone	108-94-1	--	--	--	--	100	1,000
43	Cyclohexene	110-83-8	--	--	--	--	1,010	10,100
44	Cyclopentane	287-92-3	--	--	--	--	1,720	17,200
45	Diazomethane	334-88-3	--	--	--	--	0.34	3.4
46	Dibutyl-O-Phthalate	84-74-2	--	(4e-01)[b]	--	400	5.00	50
47	o-Dichlorobenzene	95-50-1	--	2e-01	--	200	300	3,000
48	p-Dichlorobenzene	106-46-7	(6.9e-06)[b]	7e-01[c]	1.4e-01	700	450	4,500
49	Dichloroethylether	111-44-4	3.3e-04[c]	--	3.0e-03	--	29	290
50	Dichlorodifluoromethane	75-71-8	--	2e-01	--	200	4,950	49,500

Table 3.
(Continued)

No.	Chemical	CAS Number	Carcinogenicity[a]	Chronic Toxicity[a]	Long-Term Action Levels			Short-Term Action Levels[d]
					Risk-Specific Concentrations for Carcinogencity	RfC-Based Concentrations for Non-Carcinogenic Effects ($\mu g/m^3$)	Concentrations Based on Occupational Exposure[d]	
			Inhalation Unit Risk $1/(\mu g/m^3)$	Inhalation RfC (mg/m^3)	10-6 70-year Risk ($\mu g/m^3$)		Lowest OEL/1000 ($\mu g/m^3$)	Lowest OEL/100 ($\mu g/m^3$)
51	1,1-Dichloroethane	75-34-3	ND[e]	5e-01	–	500	400	4,000
52	1,2-Dichloroethane	107-06-2	2.6e-05	–	3.8e-02[c]	–	4.00	40
53	1,1-Dichloroethylene	75-35-4	5e-05	(3e-02)[b]	2.0e-02	30	4.00	40
54	cis-1,2-dichloroethylene	156-59-2	–	(4e-02)[b]	–	40	790	7,900
55	trans-1,2-dichloroethylene	156-60-5	–	(7-02)[b]	–	70	790	7,900
56	Dichloromethane	75-09-2	4.7e-07	3e+00[c]	2.1e-00	3,000	174	1,740
57	Dichloromonofluoromethane	75-43-4	–	–	–	–	40	400
58	1,2-Dichloropropane	78-87-5	(1.9e-05)[b]	–	5.3e-02	–	347	3,470
59	1,3-Dichloropropene	542-75-6	3.7e-05[c]	2e-02[c]	2.7e-02	20	4.5	45
60	1,2-Dichloro-1,1,2,2-Tetrafluoroethane	76-14-2	–	–	–	–	6,990	69,900
61	Diethanolamine	111-42-2	–	–	–	–	13	130
62	Diethyl amine	109-89-7	–	–	–	–	30	300
63	N,N-Dimethylaniline	121-69-7	–	–	–	–	25	250
64	Diethyl ether	60-29-7	–	–	–	–	1,200	12,000
65	Dimethylamine	124-40-3	–	–	–	–	18	180
66	Dimethyl formamide	68-12-2	–	3e-02	–	30	30	300
67	1,1-Dimethyl hydrazine	57-14-7	(2.5e-03)[b]	–	4.0e-04	–	1	10
68	2,4-Dinitrophenol	51-28-5	–	(7e-03)[b]	–	7	–	–
69	1,4-Dioxane	123-91-1	(3.1e-06)[b]	–	3.2e-01	–	90	900
70	Diphenyl	92-52-4	–	–	–	–	1.00	10
71	Epichlorohydrin	106-89-8	1.2e-06[c]	3e-04[c]	8.3e-01	0.3	7.6	76
72	1,2-Epoxybutane	106-88-7	–	–	–	–	–	–
73	Ethanol	64-17-5	–	–	–	–	1,880	18,800
74	Ethyl acetate	141-78-6	–	(3.0e+00)[b]	–	3,000	1,400	14,000
75	Ethyl acrylate	140-88-5	(1.4e-05)[b]	–	7.1e-02	–	20	200

Table 3.
(Continued)

No.	Chemical	CAS Number	Carcinogenicity[a]	Chronic Toxicity[a]	Long-Term Action Levels			Short-Term Action Levels[d]
					Risk-Specific Concentrations for Carcinogenicity	RfC-Based Concentrations for Non-Carcinogenic Effects	Concentrations Based on Occupational Exposure[d]	
			Inhalation Unit Risk 1/(µg/m³)	Inhalation RfC (mg/m³)	10-6 70-year Risk (µg/m³)	(µg/m³)	Lowest OEL/1000 (µg/m³)	Lowest OEL/100 (µg/m³)
76	Ethyl amine	75-04-7	–	–	–	–	18	180
77	Ethylbenzene	100-41-4	–	1e-00	–	1,000	434	4,340
78	Ethyl bromide	74-96-4	–	–	–	–	22	220
79	Ethyl carbamate	51-79-6	–	–	–	–	–	–
80	Ethyl chloride	75-00-3	–	1e+01	–	10,000	2,600	26,000
81	Ethylenediamine	107-15-3	–	(7.0e-02)[b]	–	70	25	250
82	Ethylene dibromide	106-93-4	2.2e-04[c]	–	4.5e-03	–	–	–
83	Ethylene glycol	107-21-1	–	(7.0e+00)[b]	–	7,000	125	1,250
84	Ethylene imine	151-56-4	–	–	–	–	0.88	8.80
85	Ethylene oxide	75-21-8	1.0e-04	–	1.0e-02	–	1.80	18
86	Formaldehyde	50-00-0	1.3e-05	–	7.7e-02	–	0.37	3.70
87	Formic Acid	64-18-6	–	(7e+00)	–	7,000	9.00	90
88	Furan	110-00-9	–	(4.0e-03)[b]	–	4	–	–
89	Glycerol	56-81-5	–	–	–	–	5.00	50
90	n-Heptane	142-82-5	–	–	–	–	1,600	16,000
91	n-Hexane	110-54-3	–	2e-01	–	200	176	1,760
92	Hydrazine	302-01-2	4.9e-03[c]	–	2.0e-04	–	0.13	1.3
93	Hydrochloric acid	7647-01-0	–	–	–	–	7.5	75
94	Hydrogen cyanide	74-90-8	–	–	–	–	11	110
95	Hydrogen Sulfide	7783-06-4	–	9e-04[c]	–	0.9	14	140
96	Isobutanol	78-83-1	–	1e+00	–	1,000	150	1,500
97	Isobutyl acetate	110-19-0	–	–	–	–	700	7,000
98	Isopropyl alcohol	67-63-0	–	–	–	–	980	9,800
99	Isopropyl amine	75-31-0	–	–	–	–	12	120
100	Isopropylbenzene	98-82-8	–	9e-03[c]	–	9	245	2,450

Table 3.
(Continued)

No.	Chemical	CAS Number	Carcinogenicity[a]	Chronic Toxicity[a]	Long-Term Action Levels			Short-Term Action Levels[d]
					Risk-Specific Concentrations for Carcinogenicity	RfC-Based Concentrations for Non-Carcinogenic Effects (µg/m³)	Concentrations Based on Occupational Exposure[d]	
			Inhalation Unit Risk 1/(µg/m³)	Inhalation RfC (mg/m³)	10-6 70-year Risk (µg/m³)		Lowest OEL/1000 (µg/m³)	Lowest OEL/100 (µg/m³)
101	Methanol	67-56-1	–	(2e+00)[b]	–	2,000	260	2,600
102	Methyl acetate	79-20-9	–	(4e+00)[b]	–	4,000	606	6,060
103	Methyl acrylate	96-33-3	–	(1e-01)[b]	–	100	35	350
104	Methyl amine	74-89-5	-	–	–	–	12	120
105	Methyl bromide	74-83-9	–	(6e-03)[b]	–	6	19	190
106	Methyl-tert-butyl-ether	1634-04-4	–	–	–	–	–	–
107	Methyl chloride	74-87-3	1.8e-06	–	5.5e-01	–	103	1,030
108	Methylcyclohexane	108-87-2	–	–	–	–	1,600	16,000
109	Methyl-ethyl-ketone	78-93-3	ND	3e-01	–	300	590	5,900
110	Methyl formate	107-31-3	–	–	–	–	246	2,460
111	Methyl hydrazine	60-34-4	(3.1e-04)[b]	–	3.2e-03	–	0.019	0.19
112	Methyl iodide	74-88-4	–	–	–	–	10	100
113	Methyl-Isobutyl-Ketone	108-10-1	–	8e-02	–	80	205	2,050
114	Methyl isocyanate	624-83-9	–	–	–	–	0.047	0.47
115	Methyl-Isopropyl-Ketone	563-80-4	–	–	–	–	705	7,050
116	Methyl mercaptan	74-93-1	–	–	–	–	0.98	10
117	Methyl methacrylate	80-62-6	–	(3e-01)[b]	–	300	410	4,100
118	Methyl-n-Propyl-ketone	107-87-9	–	–	–	–	700	7,000
119	Alpha-methyl-styrene	98-83-9	–	(2e-01)[b]	–	200	240	2,400
120	Monoethanolamine	141-43-5	–	–	–	–	7.50	75
121	Morpholine	110-91-8	–	–	–	–	70	700
122	Naphthalene	91-20-3	–	(1e-02)[b]	–	10	50	500
123	2-Nitropropane	79-46-9	2.7e-03	2e-02[c]	3.7e-04	20	35	350
124	N-Nitrosodimethylamine	62-75-9	1.4e-02[c]	–	7.1e-05	–	–	–
125	N-Nitrosomorpholine	59-89-2	–	–	–	–	–	–

Table 3.
(Continued)

No.	Chemical	CAS Number	Carcinogenicity[a]	Chronic Toxicity[a]	Long-Term Action Levels			Short-Term Action Levels[d]
					Risk-Specific Concentrations for Carcinogencity	RfC-Based Concentrations for Non-Carcinogenic Effects ($\mu g/m^3$)	Concentrations Based on Occupational Exposure[d]	
			Inhalation Unit Risk $1/(\mu g/m^3)$	Inhalation RfC (mg/m^3)	10-6 70-year Risk ($\mu g/m^3$)		Lowest OEL/1000 ($\mu g/m^3$)	Lowest OEL/100 ($\mu g/m^3$)
126	n-Nonane	111-84-2	--	--	--	--	1,050	10,500
127	n-Octane	111-65-9	--	--	--	--	1,400	14,000
128	n-Pentane	109-66-0	--	--	--	--	1,770	17,700
129	Phenanthrene	85-01-9	--	--	--	--	0.20	.2
130	Phenol	108-95-2	--	(2e+00)[b]	--	2,000	19	190
131	Phosgene	75-44-5	--	--	--	--	0.4	4
132	Phosphine	7803-51-2	--	3e-05	--	0.03	0.4	4
133	Phthalic anhydride	85-44-9	--	(7e+00)[b]	--	7,000	6.00	60
134	Propane	74-98-6	--	--	--	--	1,800	18,000
135	1,2-Propanediol	57-55-6	--	6e+00	--	6,000	--	--
136	1-Propanol	71-23-8	--	--	--	--	492	4,920
137	beta-Propiolactone	57-57-8	--	--	--	--	1.5	15
138	Propionaldehyde	123-38-7	--	--	--	--	--	--
139	Propionic acid	79-09-4	--	--	--	--	30	300
140	n-Propyl-Acetate	109-60-4	--	--	--	--	835	8,350
141	Propylene oxide	75-56-9	3.7e-06	3e-02	2.7e-01	30	48	480
142	1,2-Propylenimine	75-55-8	--	--	--	--	5	50
143	Pyridine	110-86-1	--	4e-03	--	4	15	150
144	Quinone	106-51-4	--	--	--	--	0.4	4
145	Styrene	100-42-5	5.7e-07	(7e-01)[b]	1.8e+00	700	213	2,130
146	1,1,1,2-Tetrachloro-2,2-Difluoroethane	76-11-9	--	--	--	--	4,170	41,700
147	1,1,2,2-Tetrachloroethane	79-34-5	5.8e-05	--	1.7e-02	--	6.90	69
148	Tetrachloroethylene	127-18-4	5.2e-07	(4e-02)[b]	1.9e+00	40	170	1,700
149	Tetrahydrofuran	109-99-9	--	--	--	--	590	5,900
150	Toluene	108-88-3	--	2e+00[c]	--	2,000	375	3,750

Table 3.
(Continued)

No.	Chemical	* CAS Number	Carcinogenicity[a]	Chronic Toxicity[a]	Long-Term Action Levels			Short-Term Action Levels[d]
					Risk-Specific Concentrations for Carcinogencity	RfC-Based Concentrations for Non-Carcinogenic Effects (µg/m³)	Concentrations Based on Occupational Exposure[d]	
			Inhalation Unit Risk 1/(µg/m³)	Inhalation RfC (mg/m³)	10-6 70-year Risk (µg/m³)		Lowest OEL/1000 (µg/m³)	Lowest OEL/100 (µg/m³)
151	p-Toluidine	106-49-0	(5.4e-05)[b]	–	1.9e-02	–	8.80	88
152	1,1,1-Trichloroethane	71-55-6	–	1.0e+00	–	1,000	1,900	19,000
153	1,1,2-Trichloroethane	79-00-5	1.6e-05	(1.0e-02)[b]	6.3e-02	10	45	450
154	Trichloroethylene	79-01-6	1.7e-6	–	5.9e-01	–	269	2,690
155	Trichlorofluoromethane	75-69-4	–	7.0e-01	–	700	5,620	56,200
156	1,2,3-Trichloropropane	96-18-4	–	(2.0e-02)[b]	–	20	60	600
157	1,1,2-Trichloro-1,2,2-Trifluoroethane	76-13-1	–	(2.7e+01)[b]	–	27,000	7,600	76,000
158	Triethylamine	121-44-8	–	–	–	–	40	400
159	Trifluorobromomethane	75-63-8	–	–	–	–	6,090	60,900
160	1,2,3-Trimethylbenzene	526-73-8	–	–	–	–	123	1,230
161	1,2,4-Trimethylbenzene	95-63-6	–	–	–	–	123	1,230
162	1,3,5-Trimethylbenzene	108-67-8	–	–	–	–	123	1,230
163	Vinyl acetate	108-05-4	–	2e-01	–	200	30	300
164	Vinyl bromide	593-60-2	3.2e-05	–	3.1e-02	–	20	200
165	Vinyl-chloride	75-01-4	8.4e-05	–	1.2e-02	–	2.60	26
166	m-Xylene	108-38-3	–	7.0e-01	–	700	434	4,340
167	o-Xylene	95-47-6	–	7.0e-01	–	700	434	4,340
168	p-Xylene	106-42-3	–	3.0e-01	–	300	434	4,340

INSTRUCTIONS ON USE:

Read short-term action level directly from last column. For the three columns of long-term action levels, use the 10-6 risk data, if available, then the RfC data; use the OEL/1000 if no other data exists.

[a] EPA does not necessarily endorse the use of oral slope factors or oral RfDs to derive inhalation values. These are intended to serve as screening levels only and do not represent EPA guidance.
[b] Derived based on oral slope factor (or oral RfD).
[c] Verified, available on IRIS or Workgroup concurrence on final database file, and IRIS input pending.
[d] EPA does not necessarily endorse the use of occupational exposure limits to derive short- and long-term action levels for ambient air. These are intended to serve as screening levels only and do not represent EPA guidance. Intended changes for OEL values are included, where applicable.
[e] EPA Class C or D carcinogen.

If inhalation RfCs were not available from either IRIS or HEAST, then chronic oral reference dose (RfD) data (in mg/kg/day) were multiplied by 70 kg (average body weight of an adult), then divided by 20 m^3/day (average adult inhalation rate), and finally multiplied by 1000 $\mu g/mg$ to derive a value in $\mu g/m^3$.

Ambient air action levels based on extrapolated oral data should be used cautiously. Before extrapolating data an array of factors should be assessed on a compound by compound basis to determine the feasibility of route-to-route extrapolations. Important factors include the absorption, distribution, metabolism and excretion of the compound; portal of entry effects; acute and chronic toxicities, and other information.

For compounds lacking RfC or RfD values, action levels were based on occupational exposure levels recommended by the Occupational Safety and Health Administration (OSHA)[6] and the American Conference of Governmental Industrial Hygienists (ACGIH)[7]. The action levels were estimated by using the lower of the OSHA Permissible Exposure Limit-Time Weighted Average (PEL-TWA) level (or ceiling value) or the ACGIH Threshold Limit Value - Time Weighted Average (TLV-TWA) level (or ceiling value). The lower value was divided by 1000 to compensate for differences between occupational and residential exposures.

Long-term ambient air action level concentrations for non-carcinogens based on RfCs, extrapolated RfDs and occupational exposure levels for 168 compounds are also listed in Table 3. The action levels are in units of $\mu g/m^3$ to facilitate comparison to the ambient air concentrations estimated from Equation 11.

Short-Term Exposure

The short term (one hour) action levels, in $\mu g/m^3$, are presented in the last column of Table 3. The listed values were obtained by dividing the lowest of (1) the OSHA PEL-TWA or (2) the ACGIH TLV-TWA (or ceiling limits if 8-hour averages are not available) by 100. Division by 100 accounts for variations in human sensitivity (occupational levels are designed to protect healthy adult workers) and for uncertainties in using occupational exposure levels to derive ambient air action levels.

The occupational exposure levels on which the short-term action levels are based are subject to change. To check the values in Table 3 (or to derive values for compounds not listed in Table 3), determine the current OSHA PEL-TWA values by consulting 29 CFR Section 1910 and the most recent edition of the ACGIH publication entitled Threshold Limit Values and Biological Exposure Indices.

The short-term action levels listed in Table 3 can be compared directly with the estimated maximum hourly ambient air concentrations obtained by using Equation 10 and Figure 2. Use of the short term action levels should consider that no EPA accepted method exists to determine the short-term concentrations of airborne chemicals acceptable for community exposure.

EXAMPLE

The following steps illustrate the use of the estimation procedures presented in this document. The goal is to estimate the maximum hourly and annual average ambient air concentrations at the nearest receptor to an excavation area and compare these values to the action level concentrations listed in Table 3.

Step 1 For this example, assume a site that has approximately 10,000 m^3 of soil contaminated with chloroform, 1,1,1-trichloroethane, and trichloroethylene at concentrations in the soil of 0.1, 10, and 1.0 ug/g, respectively. The volume of contaminated soil is not known with any certainty. The bulk density of the soil at the site averages about 1.5 g/cm^3. The rate of excavation has not yet been determined, nor has the need for air emission controls, so a medium excavation rate of 150 m^3/hour and no air emission controls is assumed. The removal is expected to be in continual operation for 20 days (1.728×10^6 seconds). The nearest off-site downwind receptor is 400 meters away.

Step 2 Estimate the total emissions potential for the site. Using Equation 1, the average long-term emission rate of chloroform would be:

$$ER = \frac{(10{,}000)(0.1)(1.5)(1)}{(1.728 \times 10^6)} = 8.68 \times 10^{-4}$$

The average long-term emission rate for 1,1,1-trichloroethane is 8.68×10^{-2} g/sec, and for trichloroethylene is 8.68×10^{-3} g/sec.

Step 3 Estimate the emission rate of each compound. The data are plugged into Equations 7 and 8 along with the assumed excavation rate of 0.042 m^3/sec. For chloroform, the emission rate would be:

$$ER_{PS} = (208)(0.042)(0.98) = 8.56 \text{ g/sec}$$

$$ER_{DIFF} = \frac{(1.5 \times 10^{-7})(10{,}000)(290)}{\left[(1.22 \times 10^6)\left(\frac{1.5 \times 10^{-7}}{208}\right)\right] + \left[(1.79 \times 10^9)\left(\frac{1.5 \times 10^{-7}}{208}\right)\right]^{1/2}}$$

Step 4 Compare the results of the emissions from the pore space gas to the total mass of the contaminant present in the soil. For chloroform for one hour's excavation (i.e., 150 m^3):

$$C_{TOT} = (1.50 \times 10^{-7})(150)(10^6) = 22.5 \text{ g}$$

$$E_{PS} = (8.56 \text{ g/sec})(3600 \text{ sec}) = 30{,}820 \text{ g.}$$

Since ER_{PS} overpredicts, use Equation 6 instead of Equation 7.

$$ER_{PS} = (22.5 \text{ g})(0.33)/(3600 \text{ sec}) = 2.08 \times 10^{-3} \text{ g/sec}$$

The overall emission rates for all three compounds are given below. In all cases, Equation 6 was used in place of Equation 7.

Step 5 Compare the estimated emission rates from Step 3 and 4 to those from Step 2. The comparison is:

Compound	Equation 1 Emission Rate (g/sec)	Equation 6 Emission Rate (g/sec)
Chloroform	0.000868	0.38
1,1,1-Trichloroethane	0.0868	3.1
Trichloroethylene	0.00868	0.74

Given the excavation is not to be performed continuously over the twenty day period, it is expected that the short-term emission rates exceed the long-term emission rates. Each rate will be used to calculate the downwind risk over the appropriate time period.

Step 6 Estimate the downwind ambient air concentrations. From Figure 2, the maximum hourly ambient air concentration at a distance of 400 meters is approximately 2800 ug/m^3 per g/sec emission rate. This corresponds to an annual average dispersion factor of 140 ug/m^3 per g/s (2900 x 0.05 = 140). The ambient air concentrations estimated from Equations 10 and 11 are presented in Table 4. Using Equation 10, the hourly average ambient air concentration for chloroform would be:

$$C_m = (0.38)(2800) = 1100 \text{ ug/m}^3$$

Using Equation 11, the annual average air ambient concentration for chloroform would be:

$$C_a = (0.000868)(140) = 0.12 \text{ ug/m}^3$$

Step 7 Compare the downwind concentrations to the action level ambient air concentrations. The short-term and long-term action levels from Table 3 for the compounds of interest are presented in Table 5. Of the estimated maximum hourly ambient concentrations, only chloroform exceeds the applicable action levels. The estimated value is about one order of magnitude greater than the action level. The annual average ambient concentrations show exceedances of the long-term action levels for both chloroform and trichloroethylene, by a factor of 2 to 3.

Step 8 Document the results of the air pathway analysis and define a future course of action. Based on these screening level results, a more rigorous analysis of the air impacts is warranted. This would most likely involve refining the emission rate, dispersion, and health risk estimates. The emission rate estimate could be improved by using the actual or proposed operating conditions or by making field measurements at the excavation site. The dispersion estimates could be improved by using a less conservative model (e.g. EPA's Industrial Source Complex model) and site-specific meteorological conditions. The health risk estimate could be improved by using the expected operational lifetime of the SVE system rather than assuming a 70-year exposure. If the more rigorous analysis still indicates that adverse air impacts may occur, then the addition of air emission controls or altering the operating conditions to control emissions (e.g. limiting the excavation rate and the total exposed surface area) should be considered.

CONCLUSIONS

The procedures presented here are not intended to negate the need for rigorous analyses that consider site specific meteorological conditions and the health effects of the specific compounds involved. Although the procedures are based on what is typical and reasonable for cleaning up Superfund sites, the underlying assumptions need to be kept in mind. Emission models assume steady-state conditions, dispersion models assume Gaussian distribution of the plume contaminant concentration, and many of the health levels are not endorsed by the Environmental Protection Agency. EPA's Regional Toxicologist should be contacted for general toxicological information and technical guidance on evaluation of chemicals without established toxicity values.

Table 4.

Estimated Emission Rates and Ambient Air Concentrations

	Soil Concentration For Example Problem (g/cm^3)	Emission Rate (g/s)	Ambient Concentrations ($\mu g/m^3$)	
			Maximum Hourly	Annual Average
Chloroform	1.5×10^{-7}	Long Term: 8.7×10^{-4} Short Term: 0.38	1100	0.12
1,1,1-Trichloroethane	1.5×10^{-5}	Long Term: 8.7×10^{-2} Short Term: 3.1	9000	12
Trichloroethylene	1.5×10^{-6}	Long Term: 8.7×10^{-3} Short Term: 0.74	2100	1.2

Table 5.

Action Level Concentrations

	Table 3 Action Levels $\mu g/m^3$	
	Short-Term	Long-Term
Chloroform	98	0.043[1]
1,1,1-Trichloroethane	19,000	1,000[2]
Trichloroethylene	2,690	0.59[1]

[1]Based on 10^{-6}, 70-year risk.
[2]Based on reference dose concentrations (RfCs).

ACKNOWLEDGEMENTS

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APPENDIX A

MODEL DERIVATION

APPENDIX A

MODEL DERIVATION

Derivation of a Screening Model for VOC Emissions From Soils Handling Activities

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Screening Model for VOC Emissions from Soils Handling Activities
APPENDIX A - MODEL DERIVATION

A.1 INTRODUCTION

Background information about the modeling problem is presented in this appendix followed by a presentation of an emission model for estimating VOC emissions from the excavation of contaminated soil. A simplified version of the model is developed, then the models are evaluated.

Objective

Develop simple predictive model for estimating VOC emissions from soils handling activities, such as excavation.

Intended Use

The model will be used for assessing potential emissions during remediation of Superfund sites. At a minimum, the model should provide an emission factor to estimate emissions per unit time or unit operation. Ideally, it should also be appropriate for evaluating the effect of different remediation scenarios, e.g. starting waste concentrations, excavation rates, and control efficiencies.

Requirements

1. Model should be conservative, since the data may be used in some cases for health risk assessment.

2. Model should require as few input parameters as is feasible for ease of use.

Assumptions

1. During excavation, the surface area of soil in contact with the atmosphere is greatly increased. This results in up to one-third of the soil gas being released to the atmosphere. In dry soils containing very low levels of VOCs, most of the contaminants are present in the soil pore spaces, thus the percentage of the VOCs emitted is relatively high.

2. Once the soil has been dumped into place, the organic liquid to soil gas equilibrium is quickly re-established. The emissions can be estimated by a modification of the RTI landtreatment model.[1]

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[1]p. 5-14 and 5-15 of EPA-450/3-87-026, Review Draft, November 1989.

3. The freshly dumped soil is soon covered by relatively deep layers of subsequently excavated soil. These layers of soil result in longer-term emissions from the deeper layers being diffusion controlled, i.e., low. Therefore, the significant period for emissions is during excavation and the first six minutes or so afterwards. Subsequent (i.e. t > 6 min) emissions from this material are assumed to be zero.

4. The total exposed surface area of contaminated soil is assumed to remain constant. New material is exposed at the same rate that previously exposed material is covered.

5. The emissions from the pit are approximately equivalent to the emissions from the pile of excavated soil. The emissions from the soil in the backhoe bucket are negligible.

6. Wet soils are assumed to have relatively low levels of VOC emissions, even if the soil VOC concentrations are high. Wet soils may have little air-filled porosity and therefore the rate of diffusion of VOCs through wet soils is relatively low.

Possible Excavation Scenarios

Two general scenarios are followed during excavations at waste sites.

1. Soil is excavated using a backhoe and placed into a short-term storage pile. The soil is later picked up from the pile and dumped directly into transport vehicles (e.g. trucks or railcars) that are subsequently covered to minimize further emissions. Overall, each m^3 of soil is excavated and dumped two times.

2. Soil is excavated using a backhoe and placed into a temporary storage pile. The soil is moved from the pile using a front-end loader (and/or backhoe) to a staging area where a large storage pile is established. The pile is typically covered to minimize leaching and air emissions. The soil is eventually re-excavated and dumped into transport vehicles (e.g. trucks or railcars) that are subsequently covered to minimize further emissions. Alternatively, the soil may be re-excavated and fed to an on-site treatment system. Overall, each m^3 of soil is excavated and dumped three times.

It is rarely feasible or efficient to dig soil and immediately transfer the soil directly to transport vehicles or treatment systems. The excavation scenario and the emission equations shown below are designed to predict the emissions from a single soil handling event. To predict the total emissions from excavation, the equations must be sequentially applied to each event where the soil is handled (i.e., two or three times in most cases). The values for certain input parameters to the equations, such as the concentration of the contaminant in the soil and the bulk density of the soil, will be

altered by the act of excavation and a separate (different) value will be required for these parameters when modeling each soil handling event of the overall excavation process.

Details of Excavation Scenario

Soil is excavated for 50 min/hour[2]. Each scoop of soil contains 2 m^3 of material and has dimensions of 1m x 2m x 1m. The cycle time is 40 seconds[3], so 75 scoops are moved per hour (= 150 m^3 of soil moved per hour). The excavation pit, after one hour of operation, has dimensions of 10m x 15m x 1m.

Each scoop of dumped soil is assumed to maintain its 1x2x1 dimensions, so that the pile of dumped soil is equivalent to a series of stacked blocks. After one hour, a pile 5m x 10m x 3m high is established. The total exposed surface area of the pile is 140 m^2 and the bottom of the pit has another 150 m^2 of exposed area (the sides of the excavation pit are assumed to be clean overburden). The exposed surface areas are assumed to remain constant during further hours of operation with any additional area being covered with some type of impermeable cover that acts as a barrier to further emissions.

A.2 DERIVATION OF EMISSION MODELS

The models are based on adding the emissions resulting from the release of soil-gas (pore space gas) to the atmosphere when excavation soil is dumped onto a storage pile to the emissions resulting from diffusion from contaminated soil present in the excavation pit and in the storage pile. A discussion of the input parameters and typical input values are given in Sections A.4 and A.5. Limitations of the models are also given in those sections.

Pore-Space Gas Model

The general form of the equation used to estimate the emission rate from the pore space gas for any given compound is the ideal gas law:

$$P\,V = nR\,T \qquad \text{(Eq. A-1)}$$

where:

P	=	Vapor pressure of compound i (mm Hg);
V	=	Volume (cm^3);
n	=	Number of moles of gas;

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[2]Page 8-35 of the Excavation Handbook by H.K. Church (MCGraw-Hill, 1981) states that excavation equipment can be assumed to be in use for 30 to 50 minutes per hour.

[3]Page 12-38, op cit, gives a cycle time of 0.67 minutes for a 25 foot hoist distance and a 90° angle of swing return.

R	=	Gas constant; and
T	=	Temperature (°K).

The mass of contaminants present in the pore space of soil can be determined as follows. First substitute M_{PS}/MW for n and then solve for M_{PS}:

$$M_{PS} = \frac{P\ V\ MW}{R\ T} \qquad \text{(Eq. A-2)}$$

where:	M_{PS}	=	Mass of pore space contaminants (g); and
	MW	=	Molecular weight of species i (g/g-mole).

Then substitute soil volume and air-filled porosity terms for V to account for the volume of air within a given volume of soil. Air-filled porosity is the fraction of the total soil volume that is air. A factor of 10^6 to convert from cm^3 to m^3 is also needed:

$$M_{PS} = \frac{P\ MW}{RT}\ (10^6)(E_a)(S_V) \qquad \text{(Eq. A-3)}$$

where:	E_a	=	Air-filled porosity (dimensionless);
	10^6	=	Conversion factor (cm^3/m^3);
	S_V	=	Volume of soil moved (m^3); and
	R	=	Gas constant, 62,361 (mm Hg - cm^3/g-mole °K).

To derive an emission rate, Equation A-3 must be modified to account for the rate at which soil is being moved and to account for the percentage of soil gas that is released or exchanged with the atmosphere:

$$ER_{PS} = \frac{P\ MW}{RT}\ (10^6)(E_a)(Q)(ExC) \qquad \text{(Eq. A-4)}$$

where:	ER_{PS}	=	Average emission rate from the pore space gas (g/sec);
	ExC	=	Soil gas to atmosphere exchange constant (%/100); and
	Q	=	Excavation rate (m^3/sec).

The excavation rate term, Q, is equal to S_V divided by the total time period in seconds over which the given volume of soil is being moved. Equation A-4 assumes that the instantaneous emission rate is equivalent throughout the excavation cycle, whereas the emissions from each scoop of soil are probably due primarily to two emission puffs: one when the backhoe bucket enters the soil and initially disturbs the soil and the second, larger puff, when the bucket dumps the soil onto the storage pile. Equation A-4 also assumes that the pore space is saturated with the contaminant vapor.

Diffusion Model

The general form of the equation used to estimate the emission rate from the contaminated soil in the excavation pit and in the storage pile is the RTI landtreatment model:

$$EF = \frac{M_o}{l}\left[\frac{1}{\left(\frac{E_a}{K_{eq}\,k_g}\right) + \left(\frac{\pi\,t}{D_e\,K_{eq}}\right)^{\frac{1}{2}}}\right] e^{-t/tb} \qquad \text{(Eq. A-5)}$$

where:

EF	=	Emission flux through the soil at some time t (g/cm^2-sec);
M_o	=	Initial loading of contaminant in soil (g/cm^2);
l	=	Depth to which contaminant is mixed in soil (cm);
K_{eq}	=	Weight fraction of VOC in air space (dimensionless);
k_g	=	Gas-phase mass transfer coefficient (cm/sec);
D_e	=	Effective diffusivity (cm^2/sec);
t	=	Time since start of excavation of soil of interest (sec); and
t_b	=	Time constant for biological decay of contaminant i (sec).

Several modifications to the model were made to make it applicable to excavation. First, the biological expoential decay term ($e^{-t/tb}$) was set equal to one since the timeframes of interest are very short. Second, the initial loading term (M_o) and the depth to which the waste is mixed term (l) were combined into a waste loading term, designated C. Third, a factor of 10,000 was added to convert the emission units from mass per cm^2 to mass per m^2. Fourth, a term was added to account for the surface area of the emitting soil. The resulting equation is:

$$ER_{Diff} = \frac{(C)(10{,}000)}{\left(\frac{E_a}{K_{eq}\,k_g}\right) + \left(\frac{\pi\,t}{D_e\,K_{eq}}\right)^{\frac{1}{2}}}\,[SA] \qquad \text{(Eq. A-6)}$$

where:

ER_{Diff}	=	Instantaneous emission rate from diffusion through the soil (g/sec);
C	=	Soil concentration of species of interest (g/cm^3);
10,000	=	Conversion factor (cm^2/m^2); and
SA	=	Surface area of emission source (m^2).

The surface area term, SA, includes the area of the exposed contaminated soil for both the excavation pit and the storage pile. It is assumed that the surface area of the emission source remains constant, i.e., excavation was already underway before the particular soil being modeled was handled and excavated soil is moved off-site or covered to reduce emissions at the same rate that new soil is being uncovered and excavated. To model the case where no contaminanted soil is initially exposed, the surface area term in Equation A-6 can be divided by a factor of two to yield an average amount of exposed surface area.

A.3 EMISSION MODELS

The overall emission rate equation is formed by adding Equations A-4 and A-6. Note that the timeframes of the two equations as shown are not equivalent. Equation A-4 describes the emissions over the course of excavating and dumping one scoop of soil (40 seconds in the assumed scenario), while Equation A-6 gives an instantaneous emission rate at some time t since the contaminated material was first exposed to the air. An average value for t is discussed in Section A.4 and the timeframe of the two models are reconciled so that they yield an average emission rate.

The general form of the emission models for estimating an "average" emission rate for the excavation of contaminated soil is given as Equation A-7 and a worst-case emission rate is given as Equation A-8. It is a simple matter to modify either of these equations to calculate an emission flux (i.e., rate per area) or total emissions for a given period of time.

Emission Rate

An emission rate in g/sec for excavation was derived in the previous section and is:

$$ER = \frac{P\ MW}{RT}(10^6)(E_a)(Q)(ExC) + \frac{(C)(10{,}000)}{\left(\frac{E_a}{K_{eq}k_g}\right) + \left(\frac{\pi\ t}{D_e\ K_{eq}}\right)^{\frac{1}{2}}}(SA) \qquad \text{(Eq. A-7)}$$

Worst-Case Emission Rates

The worst-case (i.e., maximum) instantaneous emission rate, ER_{MAX}, for contaminated soil occurs when the exposed surface area is at a maximum and immediately after a bucket load of soil is dumped onto the storage pile. This emission rate can be approximated by considering the case where a pure chemical is exposed to the atmosphere. This emission rate can be determined from Equation A-6 (there is no need to consider pore space gas concentrations and diffusion since the pure chemical is already exposed to the atmosphere). Set the time term, t, equal to zero and replace the K_{eq} term with the equivalent expression: $P*MW*E_a/R*T*C$. Equation A-6 then reduces to:

$$ER_{MAX} = \frac{(k_g)(P)(MW)(SA)(10{,}000)}{RT} \qquad \text{(Eq. A-8)}$$

A.4 SIMPLIFIED EMISSION MODELS

The first half of Equation A-7 is simplified first, followed by simplification of the second half of Equation A-7.

Simplified Pore-Space Gas Model

The first half of Equation A-7 can be simplified as follows. Assume the following:

R	=	62,361;
MW	=	100;
T	=	298;
ExC[4]	=	0.33.

Substituting these values into the first half of Equation A-7 yields an emission rate for pore space gas, ER_{PS}, of:

$$ER_{PS} = \frac{P\ MW}{RT}(10^6)(E_a)(Q)(ExC) = \frac{(P)(E_a)(Q)(100)(10^6)(0.33)}{(62{,}361)(298)} \qquad \text{(Eq. A-9)}$$

$$ER_{PS} = \left(\frac{5.4\ g/m^3}{mm\ Hg}\right) * P * E_a * Q * 0.33 \qquad \text{(Eq. A-10)}$$

[4]Assume ExC = 0.33 for dry, sandy soils and ExC = 0.10 for wet soils or those with a high clay content.

Vapor pressures for most VOCs of interest are available in tabluated physical constants in Appendix B. These values are for 25°C, but P can be estimated at other temperatures[5]. According to SEAMs, the air-filled porosity (E_a) can be assumed to be:

E_a	Soil Conditions
0.35	Wet, or compacted soil
0.55	Dry, uncompacted soil

E_a can be assumed to be 0.05 for sludges, tarry wastes, and saturated soils. Alternatively, E_a can be calculated as follows:

$$E_a = 1 - \left[\frac{\beta + (\beta)(M_{FRAC})}{p}\right] \qquad \text{(Eq. A-11)}$$

where:
- β = Bulk density of soil (g/cm^3);
- M_{FRAC} = Moisture fraction in soil (Wt.% Moisture/100); and
- p = Particle density (g/cm^3).

Default values are as follows. Bulk density (β) usually is in the range of 1.0 to 2.0 and can be assumed to be about 1.5 for uncompacted soils prior to excavation. After excavation, the bulk density is lower and a value of 1.2 may be assumed. Particle density (p) is typically about 2.65 ± 5% for soils. These default values yield an E_a for dry soil of 0.43 before excavation and 0.55 after excavation.

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[5]Vapor pressure can be roughly estimated at temperatures other than 25°C by the following equation:

$$P = P^o e^{\left(\frac{-21T_B}{1.987}\left(\frac{1}{T} - \frac{1}{T_o}\right)\right)} \qquad \text{(Eq. A-12)}$$

where:
- P = Vapor pressure of compound i at temperature T (mmHg);
- P^o = Vapor pressure of compound i at temperature T_o (mmHg);
- T_B = Normal boiling point of compound i (°K);
- T = Temperature (°K);
- T_o = Reference Temperature (°K) - Usually 298°K;
- 1.987 = Gas constant (cal/g-mol °K); and
- 21 = Heat of vaporization constant (cal/g-mol °K).

Using the SEAMS value for E_a (0.55), Equation A-10 for dry soil then reduces down to:

$$ER_{PS} = P * Q * 0.98 \text{ g/mmHg-m}^3 \qquad \text{(Eq. A-13)}$$

Equation A-13 is the simple screening model. If desired, it can be further reduced. Using the excavation scenario described above, Q can be assumed to be 150 m^3/3600 sec. Equation A-13 for dry soil then reduces down to:

$$ER_{PS} = (0.04 \text{ g/mm Hg})*P \qquad \text{(Eq. A-14)}$$

Simplified Landtreatment Model

The second half of Equation A-7 can be simplified as follows. The following equations[6,7] can be used to describe the terms K_{eq} and D_e, which appear in Equation A-7:

$$K_{eq} = \frac{P \text{ MW } E_a}{RT \text{ C}} \qquad \text{(Eq. A-15)}$$

$$D_e = \frac{D_a (E_a)^{3.33}}{(E_T)^2} \qquad \text{(Eq. A-16)}$$

where: D_a = Diffusivity in air of species i (cm^2/sec); and
E_T = Total porosity (dimensionless).

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[6]The equation shown for calculating K_{eq} assumes that the contaminant is an oily waste. For dilute aqueous wastes, K_{eq} = H/RT, where H = Henry's Law constant in mm Hg-cm^3/g-mol.

[7]Strictly speaking, the concentration term, C, in Equations A-15 and A-7 should be adjusted to account for the mass of contaminant lost with the pore-space gas. This adjustment has not been included in the model for the sake of simplicity.

K_{eq} represents the relative saturation of the soil-gas with respect to a given compound and cannot realistically exceed 1. Calculated values of K_{eq} using Equation A-15 will exceed 1 if the soil-gas is below saturation with respect to that compound. If the output of Equation A-15 is $K_{eq} > 1$, then a value of $K_{eq} = 1$ should be used in all equations having a K_{eq} term. Alternatively, K_{eq} could be determined by field measurements of the pore space concentration in the soil ratioed to the total concentration of the contaminant in the soil.

E_T can be calculated by Equation A-11 if the moisture fractir is set to zero.

Assume the following:

R	=	62,361;
MW	=	100;
T	=	298;
D_a	=	0.1;
E_a	=	0.55;
E_T	=	0.625;

Substitute these values into Equations A-15 and A-16 to yield:

$$K_{eq} = \frac{P}{C\ 332{,}200} \qquad \text{(Eq. A-17)}$$

$$D_e = 0.035 \qquad \text{(Eq. A-18)}$$

The second half of Equation A-7 can then be simplified by inserting Equations A-17 and A-18, and by assuming that $E_a = 0.55$ and that $k_g = 0.15$. Equation A-7 then reduces to:

$$ER_{Diff} = \frac{(C)(10{,}000)}{\left(1.22\text{x}10^6 \frac{C}{P}\right) + \left(2.98\text{x}10^7 \frac{C\ t}{P}\right)^{\frac{1}{2}}} (SA) \qquad \text{(Eq. A-19)}$$

Equation A-19 provides an instantaneous emission rate at time = t. It is assumed that emissions from freshly excavated soil are significant for a period of 360 seconds, after which the soil is covered by subsequent layers of excavated material. The emission rate versus time over this 360 second period for a given scoop of soil will generally exhibit an exponential decay. The exact shape of this decay curve will vary as

the input parameters such as vapor pressure and air-filled porosity vary. Therefore, it is necessary to determine at what time t the instantaneous emission rate approximates the average emission rate over the 360 second period. This can be done by calculating the instantaneous emission rates at t = 0 second, t = 15 seconds, t = 30 seconds, and so on. The emission rate is calculated for every 15 second period up to t=360 and the results plotted. The average emission rate is calculated by summing the instantaneous emission rates and dividing the sum by the number of data points (in this example, 24). The value for the average emission rate is then found on the plot of emission rate versus time, and the corresponding time found on the x-axis. This time t is then used in Equation A-19. For the typical case, the instantaneous rate at t = 60 seconds is a good approximation of the overall emission rate for the first 360 seconds. Using this value Equation A-19 yields the simple screening equation:

$$ER_{Diff} = \frac{(C)(10{,}000)}{\left(1.22 \times 10^{6} \frac{C}{P}\right) + \left(1.79 \times 10^{9} \frac{C}{P}\right)^{\frac{1}{2}}} (SA) \qquad \text{(Eq. A-20)}$$

Equation A-20 assumes that the emission flux arising from diffusion is equal for both the excavation pit and the excavated soil in the storage pile. Equation A-20 will overpredict emissions if $K_{eq} > 1$. P at temperatures other than 25°C can be estimated using Equation A-12. From the excavation scenario described earlier, SA can be assumed to be 290 m^2.

Assuming a typical bulk density of undisturbed soil, C can be modified to a weight basis as follows:

$$C' = C * \frac{1\ cm^3}{1.5\ g} * 10^6\ \mu g/g \qquad \text{(Eq. A-21)}$$

where: C' = Concentration of species in soil (μg/g).

The overall emission rate is determined by adding Equations A-13 and A-20. This estimated value should be checked to see whether or not it exceeds the total mass of contaminants present in the soil that is moved, which is equal to the theoretical maximum emissions (not considering emissions from the un-excavated soil in the pit). To do this, the emission rate should be multiplied by 3,600 seconds to get the total emissions over a reasonably long period of time, one hour. The mass of contaminants present in the soil can be determined by:

$$C_{TOT} = C * S_V * 10^6\ cm^3/m^3 \qquad \text{(Eq. A-22)}$$

where: C_{TOT} = Total starting mass of contaminant in excavated soil (g).

Equations A-4 and A-13 are based on the assumption that the soil pore gas is saturated with the compound of interest. If this is not the case, then Equations A-4 or A-13 may overpredict the emission rate. The output from Equations A-4 or A-13 should be multiplied by the duration of excavation and compared to the total mass of

contaminants present in the soil. If Equations A-4 or A-13 gives a value that exceeds one-third of C_{TOT}, then they should be replaced with the following equation:

$$ER_{PS} = C_{TOT} * 0.33/t_{sv} \qquad \text{(Eq. A-23)}$$

where: t_{sv} = Time to excavate a given volume of soil (sec).

A.5 MODEL EVALUATION

The emission model was evaluated to determine the sensitivity of the model to various input parameters. All the independent variables in Equation A-7 are listed in Table A-1. For each variable a typical value is given along with the range of values likely to be encountered at Superfund site excavations. The uncertainty associated with measuring each variable is also estimated in Table A-1. The range of physical properties was based on n-butane being the lightest VOC likely to be encountered at a site and naphthalene being the heaviest compound likely to be of concern. Typical physical property values were based on C6 to C8 compounds (e.g. benzene to xylene). The soil volume term was kept constant to show the variability in surface area for a given volume of soil. The gas-phase mass transfer coefficient (k_g) was estimated using the correlations given with the RTI landtreatment model and the following input values:

Parameter	Units	Minimum Value	Maximum Value	Typical Value
Wind Speed	m/sec	1.0	4.47	2.0
Viscosity of air	g/cm-sec	1.81×10^{-4}		
Density of air	g/cm^3	1.2×10^{-3}		
Diffusity in air	cm^2/sec	0.25	0.059	0.1
Diameter of excavation	m	24		

The minimum and maximum values for the independent input parameters from Table A-1 were combined to generate a best-case and worst-case set of emission scenarios. These are shown in Table A-2 along with the case using the typical input parameters. As seen in Table A-2, the three cases shown differ greatly in the estimated average emission rate.

To identify which parameters had the greatest effect on the overall emissions, a set of calculations were performed using the base or typical case as the starting point. The effect of each parameter was examined by substituting the minimum and maximum value for each into the base case conditions. The results of this first-order sensitivity analysis are shown in Table A-3. The two independent variables having the largest effect on the overall emission rate are the starting concentration of the contaminant in the soil and the vapor pressure of the contaminant. Note that temperature has a small effect, but that emissions are inversely proportional to temperature. This is, of course, contrary to the overall effect of temperature on emissions: emissions increase as temperature increases. This seeming anomaly is due to

Table A-1.
Input Parameters for Emission Equations

Equation Parameter	Units	Typical Input Values			Typical Uncertainty (±%)	Comments
		Minimum	Maximum	Typical		
Independent Variables						
Concentration	ug/Kg (ppbw)	50	5,000,000	100,000	50	
Bulk Density	g/cm3 (dry)	1.0	2.0	1.35	10	
Moisture	%	5.0	25	10	5	
Particle Density	g/cm3	2.55	2.8	2.65	5	
Temperature	K	273	313	298	2	
Da	cm2/sec	0.059	0.25	0.1	25	Varies w/temperature
P	mm Hg	0.053	1820	35	300	Varies w/temperature
MW	g/gmol	41	166	100	1	
R	mm Hg-cm3/gmol-K	62361	62361	62361	1	
pi	--	3.14	3.14	3.14	1	
kg	cm/sec	0.062	0.52	0.15	25	
t	sec	60	60	60	25	
Q	m3/sec	0.042	0.042	0.042	30	
Surface Area	m2	290	435	290	50	
Exchange Constant	%	1	50	33	200	
Dependent Variables						
C	g/cm3	5.00×10^{8}	0.010	1.35×10^{-4}		
Ea	vol/vol	0.588	0.107	0.440		
Et	vol/vol	0.608	0.286	0.491		
De	cm2/sec	0.0273	0.0018	0.0296		
Keq	g/g	1.50	0.166	0.613		
Keq	g/g (max)	1				Keq cannot exceed one

Table A-2.
Emission Scenarios

Parameter	Units	Typical Input Values			Emission Scenarios		
		Minimum	Maximum	Typical	Best Case	Worst Case	Typical Case
Concentration	ug/Kg (ppbw)	50	5,000,000	100,000	50	5000000	1000
Bulk Density	g/cm3 (dry)	1.0	2.0	1.35	2.0	1.0	1.35
Moisture	%	5.0	25	10	25	5.0	10
Particle Density	g/cm3	2.55	2.8	2.65	2.55	2.8	2.65
Temperature	K	273	313	298	273	313	298
C	g/cm3	5.00×10^{-8}	1.00×10^{2}	1.35×10^{-4}	1.00×10^{-7}	5.00×10^{-3}	1.35×10^{-4}
Ea	vol/vol				0.020	0.625	0.440
Et	vol/vol				0.216	0.643	0.491
Da	cm2/sec	0.059	0.25	0.1	0.059	0.25	0.1
P	mm Hg	0.053	1820	35	0.053	1820	35
MW	g/gmol	41	166	100	166	41	100
R	mm Hg-cm3/gmol-K	62361	62361	62361	62361	62361	62361
pi	--	3.14	3.14	3.14	3.14	3.14	3.14
Kg	cm/sec	0.062	0.52	0.15	0.062	0.52	0.15
De	cm2/sec				3×10^{-6}	0.1265	0.0269
Keq	g/g				0.101	0.478	0.613
Keq	g/g (max)						
t	sec	60	60	60	60	60	60
Excavation Rate	m3/sec	0.042	0.042	0.042	0.042	0.042	0.042
Surface Area	m2	290	435	290	290	435	290
Exchange Constant	%	1	50	33	1	50	33
Emission Rate	g/sec				1.51×10^{-5}	422	4.65

Notes: 1. Use Keq(max) if Keq is >1.

Table A-3.
Results of Sensitivity Analysis

Equation Parameter	Units	Typical Input Values			Change in Emission vs Base Case	
		Minimum	Maximum	Typical	Minimum Value (± %)	Maximum Value (± %)
Independent Variables						
Concentration	ug/Kg (ppbw)	50	5,000,000	100,000	-99.9	348
Bulk Density	g/cm3 (dry)	1.0	2.0	1.35	21.9	-66.4
Moisture	%	5.0	25	10	10.7	-29.1
Particle Density	g/cm3	2.55	2.8	2.65	-6.1	8.4
Temperature	K	273	313	298	5.8	-3.1
Da	cm2/sec	0.059	0.25	0.1	-16.9	41.0
P	mm Hg	0.053	1820	35	-98.5	38.0
MW	g/gmol	41	166	100	-42.7	38.0
R	mm Hg-cm3/gmol-K	62361	62361	62361	NA	NA
pi	--	3.14	3.14	3.14	NA	NA
kg	cm/sec	0.062	0.52	0.15	-4.3	2.4
t	sec	1	3600	60	1688	-65.4
Excavation Rate	m3/sec	0.042	0.042	0.042	NA	NA
Surface Area	m2	290	435	290	0.0	37.7
Exchange Constant	%	1	50	33	-23.8	12.6
Dependent Variables						
C	g/cm3	1.00×10^{-7}	5.00×10^{-3}	1.35×10^{-4}	-99.9	302
Ea	vol/vol	0.020	0.625	0.440	-98.8	89.0
Et	vol/vol	0.216	0.643	0.491	87.1	-17.3
De	cm2/sec	3.00×10^{-6}	0.1265	0.0269	-74.7	80.4
Keq	--	1.00×10^{-4}	1	0.613	-75.3	21.8

main effect of temperature being to increase the vapor pressure and diffusivity terms. If these terms are not corrected for temperature, then the model will become less accurate as the temperature deviation from 25°C increases.

Equation A-7 requires the input of the time after the start of excavation (t). It was assumed earlier that the emission rate at t=60 seconds was equal to the average emission rate over t=0 to t=360 seconds. It was further assumed that after 360 seconds, the excavated soil would be covered with additional layers of soil and the diffusion of further material (emissions) would be minimal. The effect of time (t) was examined by substituting a range of times into the base case conditions. The results of these trials are given in Table A-4 and depicted in Figure A-1 and A-2.

The effect of the initial soil concentration of the contaminant on the predicted emission rate was examined by using the same base case assumptions and varying the concentration from 1 ppbw to 10,000 ppmw. These results are shown in Table A-5 and are plotted in Figure A-3. As the concentration increases, the percentage of the total mass of material emitted decreases. Also, the relative contribution of pore-space gas to the total emissions also decreases. The effect of vapor pressure (and molecular weight) was examined by inserting the values for vapor pressure and molecular weight for several common organic species into the base case. All compounds were assumed to be present at 100 ppmw in the soil. These results are shown in Table A-6.

A final check of the models was made by comparing model predictions to field data (Eklund, et al. Field Measurement of VOC Emissions From Soils Handling Operations at Superfund Sites. EPA Contract No. 68-02-4392, Work Assignment 64. September 1990). Comparisons of both the detailed (Equation A-7) and simple models (Equations A-13 and A-20) to field data are shown in Table A-7. Total emissions for twenty minute sampling periods are shown for two different field sites. The detailed model using site-specific input data agrees with the field measurements within a factor of five in all but two cases. The simplified model shows equally good agreement.

The equations presented here are a first attempt to model emissions from soils handling operations. The equations are limited by a lack of laboratory or field data to define certain key relationships between the variables. For example, the excavation rate and the total exposed area are assumed in the equations to have a direct linear relationship with the emission rate. No data, however, exist to support this assumption. Similarly, the effects of temperature, scoop size, and surface area to volume ratio on emissions have not been investigated. Another limiting assumption is that 33% of the pore space gas is exchanged with the atmosphere. This value is arbitrary and was selected since it fit reasonably well with the very limited field data that are available.

Measurements of emission rates from dynamic processes such as excavation are very difficult to perform and are of limited accuracy. Limitations exist for dispersion models used in indirect approaches (e.g., transect) and in the sampling and analytical precision when attempting to determine emission rates using a mass balance approach. Emerging measurement technologies, such as remote optical sensing, may allow more detailed evaluation of the effect of these parameters in the future.

Table A-4.

Effect of Time (t) on Emissions

Time (sec)	Diffusion Emission Rate (mg/sec)	Total Emission Rate (mg/sec)
0	81.9	83.1
5	11.0	12.1
10	8.09	9.23
20	5.89	7.03
30	4.87	6.01
40	4.25	5.39
50	3.83	4.96
60	3.51	4.65
90	2.89	4.02
120	2.51	3.65
180	2.06	3.20
240	1.79	2.93
300	1.61	2.74
360	1.47	2.61
420	1.36	2.50
480	1.28	2.41
540	1.20	2.34
600	1.14	2.28
1200	0.81	1.95
1800	0.66	1.80
2400	0.58	1.71
3000	0.51	1.65
3600	0.47	1.61

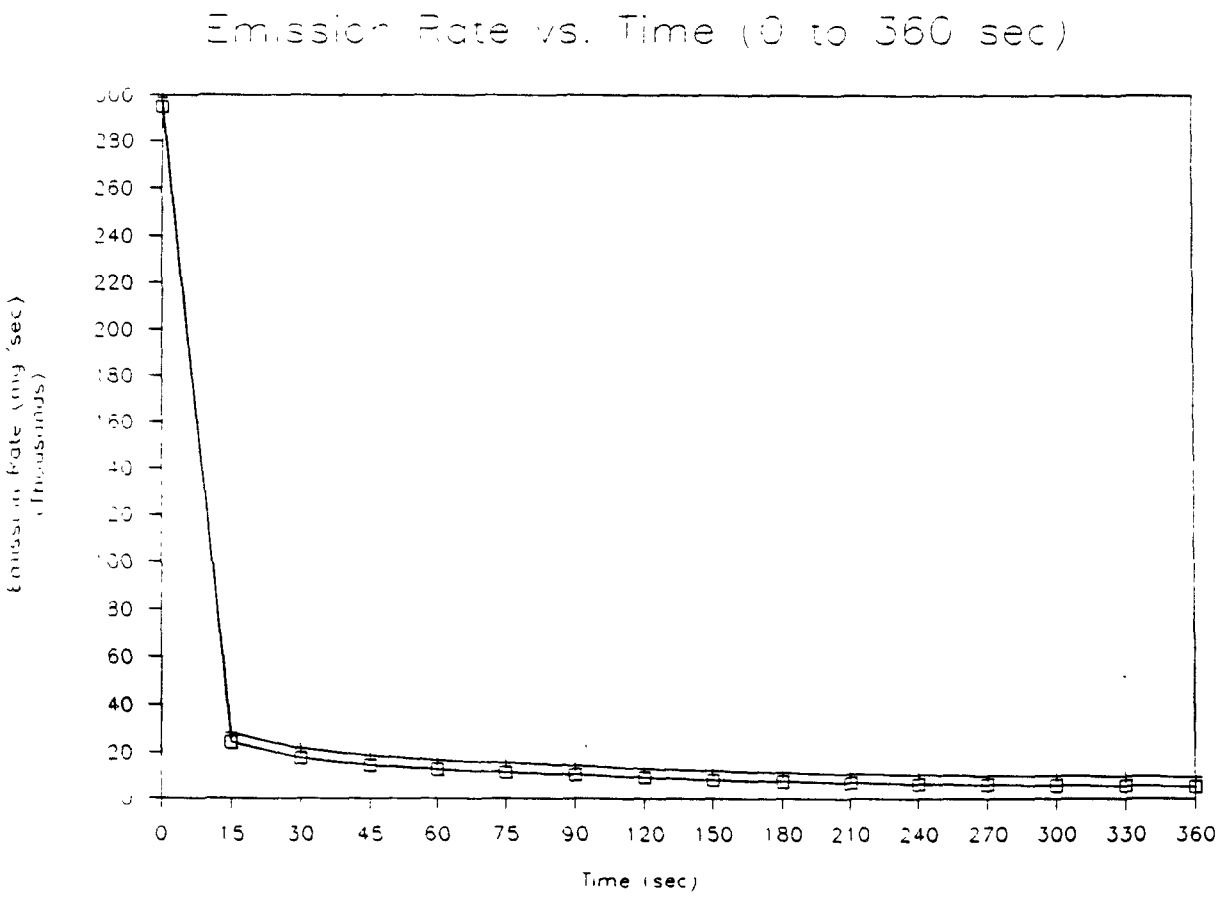

Figure A-1. Emission Rate vs. Time for Base Case Conditions for 0 to 360 seconds.

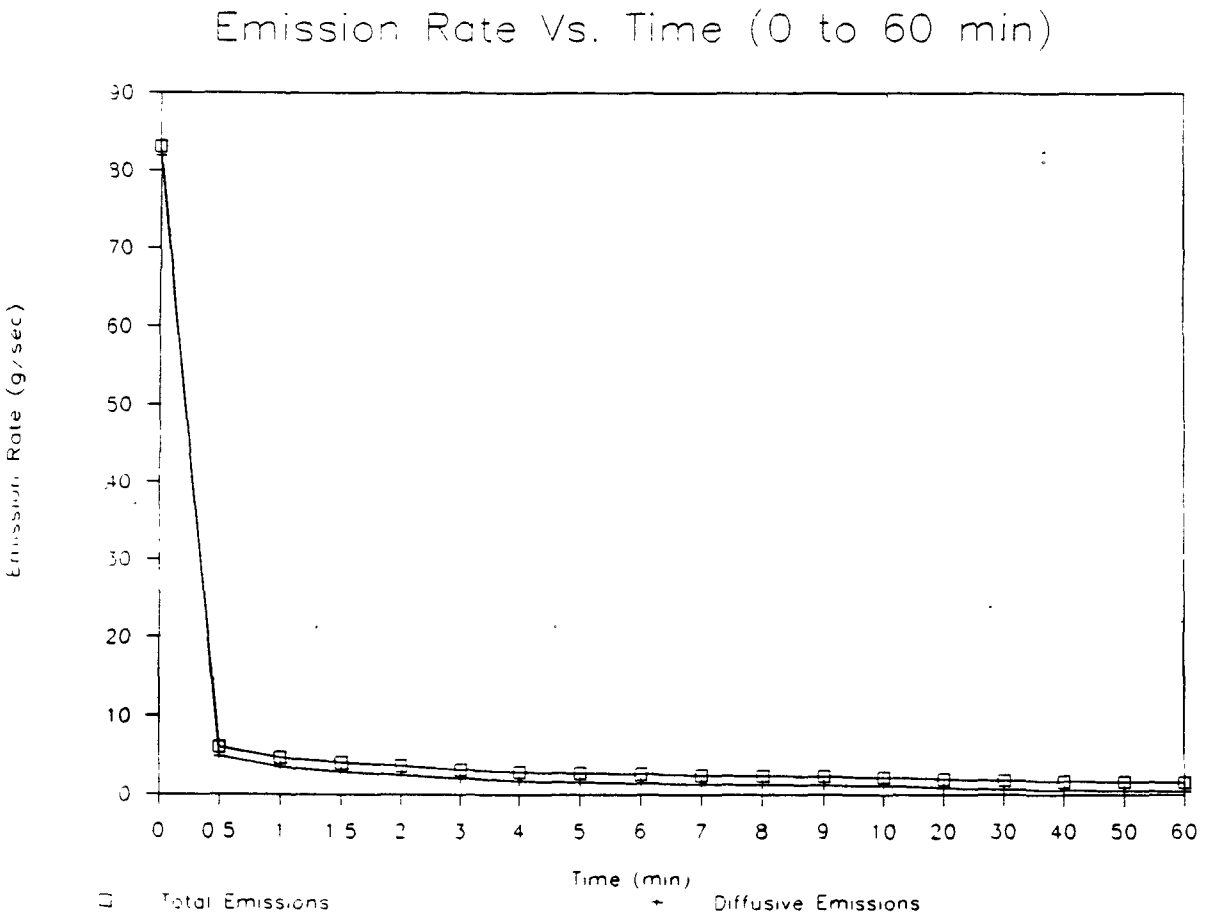

Figure A-2. Emision Rate vs. Time for Base Case Conditions for 0 to 60 Minutes.

Table A-5.

Effect of Conc. (C) on Emissions

Conc (ug/Kg)	Log Conc (ug/Kg)	Pore Gas Emission Rate (g/sec)	Diffusive Emission Rate (g/sec)	Total Emission Rate (g/sec)	Emissions* Vs. Total Mass (%)
1	1	1.88×10^{-5}	4.52×10^{-5}	6.40×10^{-5}	114
10	2	1.88×10^{-4}	4.52×10^{-4}	6.40×10^{-4}	114
100	3	1.87×10^{-3}	4.52×10^{-3}	6.40×10^{-3}	114
1000	4	0.019	0.045	0.06	114
10000	5	0.188	1.14	1.33	236
100000	6	1.138	3.51	4.65	82.6
1000000	7	1.138	10.15	11.29	20.1
10000000	8	1.138	25.32	26.46	4.7

* Includes only mass of contaminants in excavated soil

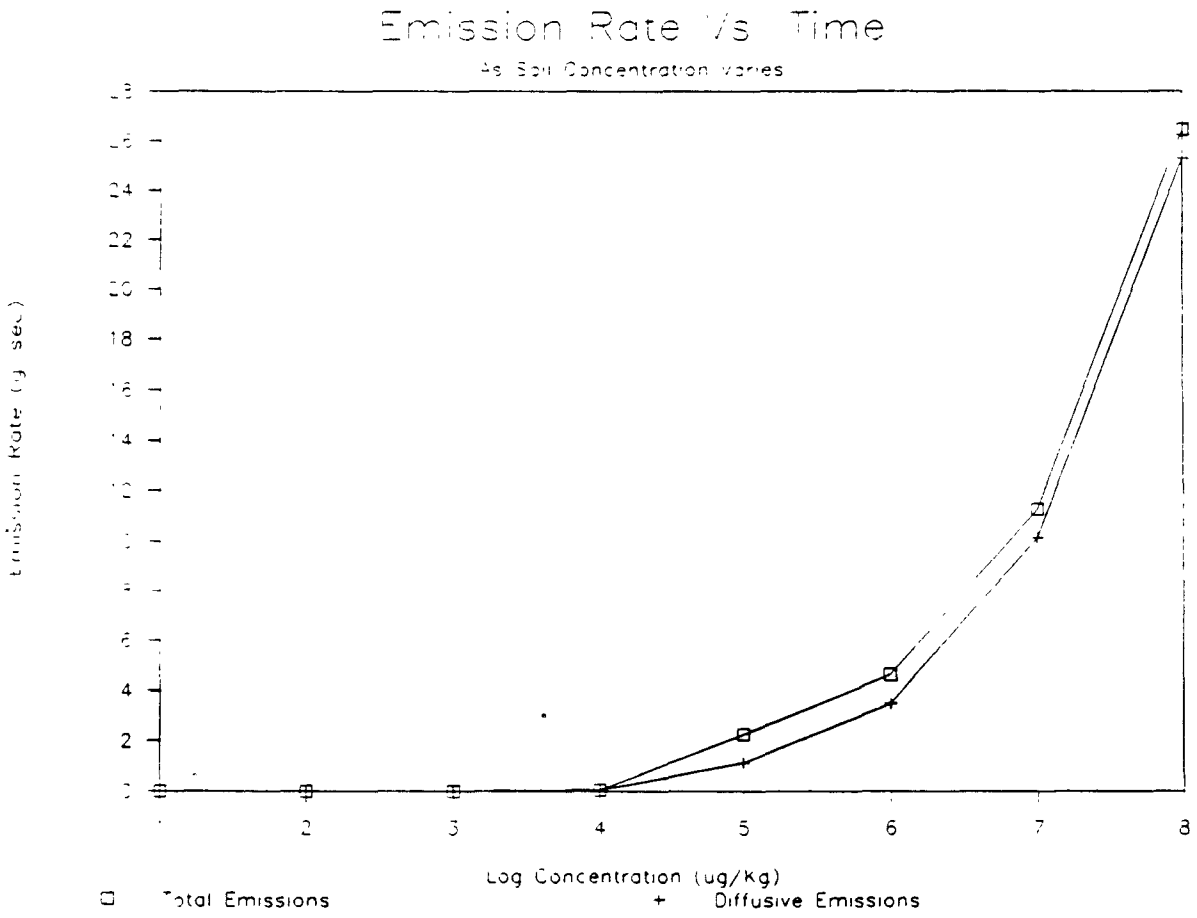

Figure A-3. Emission Rate vs. Time as Soil Concentration Increases.

Table A-6.

Effect of Molecular Weight (MW) + Vapor Pressure (P) on Emissions

Conc (ug/Kg)	Molecular Weight (g/g-mol)	Vapor Pressure (mm Hg)	Diffusive Emission Rate (g/sec)	Total Emission Rate (/sec)
Alkanes				
butane	58.12	1820	4.52	6.40 *
pentane	72.15	513	4.52	6.40 *
hexane	86.18	150	4.52	6.40 *
heptane	100.2	46	4.05	5.55
octane	114.23	17	2.57	3.21
nonane	128.26	4.3	1.30	1.48
Aromatics				
benzene	78.12	95.2	5.18	7.06
ethylbenzene	106.16	10	1.87	2.21
o-xylene	106.2	7.0	1.54	1.78

* Pore space emissions equal the total mass of contaminant present divided by 3.

Table A-7

Comparison of Model Predictions to Field Data

Site	Run #	Compound	FIELD RESULTS		MODEL PREDICTIONS				PREDICTIONS FOR SIMPLE MODELS			
			Mass of Contam. Present (g)	Total Emissions (g)	Pore Space Emissions - EPS - (g)	Diffusive Emissions - Ei - (g)	Total Emissions (g)	Accuracy (%)	Pore Space Emissions -EPS- (g)	Diffusive Emissions - Ei - (g)	Total Emissions (g)	Accuracy (%)
A	1	Xylenes	855	24	49	182	231	863	7 4	62	69	189
	2	Xylenes[a]	12	37	4.0	20.3	24	-34	7 0	20	27	-27
	3	Xylenes[a]	140	82	47	203	249	204	83	203	285	248
A	1	Ethylbenzene	53	6.6	21	32	52	692	3.1	32	35	432
	2	Ethylbenzene[a]	1.2	8.4	0.4	4.2	4.6	-46	3.0	4.2	7.1	-15
	4	Ethylbenzene[a]	14	14	4.6	42	46	230	35	42	76	443
B	2	Xylenes[a]	0 13	7.2	4.3	20	24	236	5.8	2.0	7.8	8.3
	3	Xylenes[a]	2.7	2.2	0.9	9 2	10	357	5.8	9	15	581
	4	Xylenes[a]	3.7	2.3	1.2	11	12	421	5.8	11	17	621

Accuracy = (Model - Field)/Field x 100

[a] Pore space emissions equal total mass of contaminant present divided by 3.

APPENDIX B

PHYSICAL AND CHEMICAL CONSTANTS FOR SELECTED COMPOUNDS

APPENDIX B - PHYSICAL PROPERTY DATA

No.	Organic Compound	CAS NO.	Formula	Molecular Weight (g/g-mol)	Vapor Pressure (mm Hg)[1]	Diffusivity in Air (cm^2/sec)
1	Acetaldehyde	75-07-0	C2H4O	44.00	760	0.1240
2	Acetic acid	64-19-7	C2H4O2	60.06	15.41	1.1300
3	Acetic anhydride	108-24-7	C4H6O3	102.09	5.266	0.2350
4	Acetone	67-64-1	C3H6O	58.08	266	0.1240
5	Acetonitrile	75-05-8	C2H3N	41.06	90	0.1280
6	Acrolein	107-02-8	C3H4O	56.1	244.2	0.1050
7	Acrylic acid	79-10-7	C3H4O2	72.1	5.2	0.0908
8	Acrylonitrile	107-13-1	C3H3N	53.06	114	0.1220
9	Allyl alcohol	107-18-6	C3H6O	58.08	23.3	0.1140
10	Allyl chloride	107-05-1	C3H5CL	76.53	368	
11	Aniline	62-53-3	C6H7N	93.13	1	0.0700
12	Anthracene	120-12-7	C14H10	178.23	1.3E-06	
13	Benzaldehyde	100-52-7	C7H6O	106.12	1	
14	Benzene	71-43-2	C6H6	78.12	95.2	0.0932
15	Benzoic acid	65-85-0	C7H6O2	122.12	0.00704	
16	Benzyl alcohol	100-51-6	C7H8O	108.14	0.15	
17	Benzyl chloride	100-44-7	C6H5CH2Cl	126.6	1.21	0.0750
18	Bromoform	75-25-2	CHBr3	252.77	5.6	
19	1,3-Butadiene	106-99-0	C4H6	54.09	2100.00	0.2490
20	N-Butane	106-97-8	C4H10	58.12	1820	0.2490
21	2-Butanol	15892-23-6	C4H10O	74.12	10	
22	N-Butanol	71-36-3	C4H10O	74.12	6.5	
23	N-Butyl-Acetate	123-86-4	C6H12O2	116.16	15	
24	Tert-Butyl-Alcohol	75-65-0	C4H10O	74.12	0.17	
25	Carbon disulfide	75-15-0	CS2	76.13	366	0.1040
26	Carbon tetrachloride	56-23-5	CCL4	153.82	113	0.0632
27	Carbonyl sulfide	463-58-1	COS	60.1	–	
28	Catechol	120-80-9	C6H4(OH)2	110.1	–	
29	Chlorine	7782-50-5	Cl2	70.9	–	
30	Chlorobenzene	108-90-7	C6H5CL	112.56	11.8	0.0730
31	Chlorodifluoromethane	75-45-6	CHCLF2	86.47	–	
32	Chloroform	67-66-3	CHCL3	119.38	208	0.0888
33	Chloromethyl methyl ether	107-30-2	C2H5Cl0	80.51	–	
34	Chloropentafluoroethane	76-15-3	C2CLF5	154.47	–	
35	Chloroprene	126-99-8	CH2CHCH2Cl	76.53	273	0.1040
36	M-Cresol	108-39-4	C7H8O	108.14	0.08	0.0740
37	O-Cresol	95-48-7	C7H8O	108.14	0.24	0.0740
38	P-Cresol	106-44-5	C7H8O	108.14	0.11	0.0740
39	Cyanogen	460-19-5	C2N2	52.04	3980	
40	Cyclohexane	110-82-7	C6H12	84.16	100	0.0839
41	Cyclohexanol	108-93-0	C6H12O	100.16	1.22	0.2140
42	Cyclohexanone	108-94-1	C6H10O	98.14	4.8	0.0784
43	Cyclohexene	110-83-8	C6H1O	82.15	–	

Appendix B. (Continued)

No.	Organic Compound	CAS NO.	Formula	Molecular Weight (g/g-mol)	Vapor Pressure (mm Hg)	Diffusivity in Air (cm^2/sec)
44	Cyclopentane	287-92-3	C5H10	70.13	317.44	
45	Diazomethane	334-88-3	CH2N2	42.04	–	
46	Dibutyl-O-Phthalate	84-74-2	C16H22O4	278.35	1.00E-05	0.0439
47	O-Dichlorobenzene	95-50-1	C6H4CL2	147.00	1	0.0690
48	P-Dichlorobenzene	106-46-7	C6H4CL2	147.00	1.2	0.0690
49	Dichloroethylether	111-44-4	C4H8Cl2O	143.02	1.4	
50	Dichlorodifluoromethane	75-71-8	CCL2F2	120.91	4870	
51	1,1-Dichloroethane	75-34-3	C2H4CL2	98.96	234	0.0919
52	1,2-Dichloroethane	107-06-2	C2H4CL2	98.96	80	0.0907
53	1,1-Dichloroethylene	75-35-4	C2H2CL2	96.94	600	0.1040
54	cis-1,2-Dichloroethylene	156-59-2	C2H2CL2	96.94	208	
55	trans-1,2-Dichloroethylene	156-60-5	C2H2CL2	96.94	324	
56	Dichloromethane	75-09-2	CH2CL2	84.93	362	
57	Dichloromonofluoromethane	75-43-4	CHCL2F	102.92	1360	
58	1,2-Dichloropropane	78-87-5	C3H6CL2	112.99	42	
59	1,3-Dichloropropene	542-75-6	C3H4Cl2	110.98	43	
60	1,2-Dichloro-1,1,2,2-Tetrafluoroethane	76-14-2	C2CL2F4	170.92	–	
61	Diethanolamine	111-42-2	C4H11NO2	105.14	–	
62	Diethyl amine	109-89-7	C4H11N	73.14	350@35C	
63	N,N-Dimethylaniline	121-69-7	C8H11N	121.18	–	
64	Diethyl ether	60-29-7	C4H10O	74.12	440@20C	0.0782
65	Dimethylamine	124-40-3	C2H7N	45.08	563 @ 0C	
66	Dimethyl formamide	68-12-2	C3H7NO	73.09	4.0	0.0939
67	1,1-Dimethyl hydrazine	57-14-7	C2H8N2	60.10	157	0.1060
68	2,4-Dinitrophenol	51-28-5	C6H4N2O5	184.11	53.8	
69	1,4-Dioxane	123-91-1	C4H8O2	88.11	37	0.2290
70	Diphenyl	92-52-4	C12H10	154.21	–	
71	Epichlorohydrin	106-89-8	C3H5ClO	92.53	17	0.0860
72	1,2-Epoxybutane	106-88-7	C4H8O	72.0	–	
73	Ethanol	64-17-5	C2H6O	46.07	50	0.1230
74	Ethyl acetate	141-78-6	C4H8O2	88.11	100	
75	Ethyl acrylate	140-88-5	C5H8O2	100.12	40	0.0770
76	Ethyl amine	75-04-7	C2H7N	45.08	1057	
77	Ethylbenzene	100-41-4	C8H10	106.16	10	0.0750
78	Ethyl Bromide	74-96-4	C2H5Br	108.97	–	
79	Ethyl carbamate	51-79-6	C3H7NO2	89.09	10	
80	Ethyl Chloride	75-00-3	C2H5Cl	64.51	1200	0.2710
81	Ethylenediamine	107-15-3	C2H8N2	60.10	10.7	
82	Ethylene dibromide	106-93-4	C2H4Br	187.88	14	
83	Ethylene glycol	107-21-1	C2H6O2	62.07	0.13	0.1080
84	Ethylene imine	151-56-4	C2H5N	43.07	–	
85	Ethylene oxide	75-21-8	C2H4O	44.06	1250	0.1040

Appendix B. (Continued)

No.	Organic Compound	CAS NO.	Formula	Molecular Weight (g/g-mol)	Vapor Pressure (mm Hg)[1]	Diffusivity in Air (cm^2/sec)
86	Formaldehyde	50-00-0	CH2O	30.03	3500	0.1780
87	Formic acid	64-18-6	CH2O2	46.03	42	0.0790
88	Furan	110-00-9	C4H4O	68.08	596	0.1040
89	Glycerol	56-81-5	C3H8O3	92.09	1.60E-04	
90	N-Heptane	142-82-5	C7H16	100.2	46	
91	N-Hexane	110-54-3	C6H14	86.18	150.3	0.2000
92	Hydrazine	302-01-2	H4N2	32.05	14.4	
93	Hydrochloric acid	7647-01-0	HCl	36.46	32,450	
94	Hydrogen cyanide	74-90-8	CHN	27.03	--	
95	Hydrogen sulfide	7783-06-4	H2S	34.08	15,200	0.1760
96	Isobutanol	78-83-1	C4H10O	74.12	10	0.0860
97	Isobutyl acetate	110-19-0	C6H12O2	116.16	--	
98	Isopropyl alcohol	67-63-0	C3H8O	60.1	42.8	0.0980
99	Isopropyl amine	75-31-0	C3H9N	59.11	460	
100	Isopropylbenzene	98-82-8	C9H12	120.19	10.9@40C	
101	Methanol	67-56-1	CH4O	32.04	114	0.1500
102	Methyl acetate	79-20-9	C3H6O2	74.08	235	0.1040
103	Methyl acrylate	96-33-3	C4H7O2	86.09	--	
104	Methyl amine	74-89-5	CH5N	31.06	770@ -6C	
105	Methyl bromide	74-83-9	CH3BR	94.94	--	
106	Methyl-tert-butyl-ether	1634-04-4	C5H12O	88.15	245	0.0806
107	Methyl chloride	74-87-3	CH3CL	50.49	3830	0.1260
108	Methylcyclohexane	108-87-2	C7H14	98.19	43	
109	Methyl-ethyl-ketone	78-93-3	C4H8O	72.11	100	0.0808
110	Methyl formate	107-31-3	C2H4O2	60.05	500	
111	Methyl hydrazine	60-34-4	CH6N2	46.07	49.6	
112	Methyl iodide	74-88-4	CH3I	141.94	91	
113	Methyl-Isobutyl-Ketone	108-10-1	C6H12O	100.16	19.31	
114	Methyl isocyanate	624-83-9	C2H3NO	57.05	348	
115	Methyl-Isopropyl-Ketone	563-80-4	C5H10O	86.13	15.7	0.0750
116	Methyl mercaptan	74-93-1	CH4S	48.1	--	
117	Methyl methacrylate	80-62-6	C5H8O2	100.10	39	0.0770
118	Methyl-N-Propyl-Ketone	107-87-9	C5H10O	86.13	--	
119	Alpha-Methyl-Styrene	98-83-9	C9H10	118.18	0.076	0.2640
120	Monoethanolamine	141-43-5	C2H7NO	61.08	--	
121	Morpholine	110-91-8	C4H9NO	87.12	10.08	
122	Naphthalene	91-20-3	C10H8	128.19	0.023	0.0590
123	2-Nitropropane	79-46-9	C3H7NO2	89.09	12.9	
124	N-Nitrosodimethylamine	62-75-9	C2H6N2O	74.08	--	
125	N-Nitrosomorpholine	59-89-2	C4H8N2O	116.11	--	
126	N-Nonane	111-84-2	C9H20	128.26	4.28	
127	N-Octane	111-65-9	C8H18	114.23	17	

Appendix B. (Continued)

No.	Organic Compound	CAS NO.	Formula	Molecular Weight (g/g-mol)	Vapor Pressure (mm Hg)[1]	Diffusivity in Air (cm^2/sec)
128	N-Pentane	109-66-0	C5H12	72.15	513	
129	Phenanthrene	85-01-8	C14H10	178.23	2.00E-04	
130	Phenol	108-95-2	C6H6O	94.11	0.0341	0.0820
131	Phosgene	75-44-5	CCl2O	98.92	1,394	0.1080
132	Phosphine	7803-51-2	H3P	34.00	2,000	
133	Phthalic anhydride	85-44-9	C8H4O3	148.11	0.0015	0.0710
134	Propane	74-98-6	C3H8	44.1	760	
135	1,2-Propanediol	57-55-6	C3H8O2	76.11	0.3	
136	1-Propanol	71-23-8	C3H8O	60.1	20.85	
137	beta-Propiolactone	57-57-8	C3H4O2	72.06	3.4	
138	Propionaldehyde	123-38-7	C3H6O	58.08	300	
139	Propionic acid	79-09-4	C3H6O2	74.08	10	
140	N-Propyl-Acetate	109-60-4	C5H10O2	102.12	35	
141	Propylene oxide	75-56-9	C3H6O	58.08	524.5	0.1040
142	1,2-Propylenimine	75-55-8	C3H7N	54.1	112	
143	Pyridine	110-86-1	C5H5N	79.1	20	0.0910
144	Quinone	106-51-4	C6H4O2	108.09	--	
145	Styrene	100-42-5	C8H8	104.15	7.3	0.0710
146	1,1,1,2-Tetrachloro-2,2-Difluoroethane	76-11-9	C2CL4F2	203.83	--	
147	1,1,2,2,-Tetrachloroethane	79-34-5	C2H2CL4	167.85	6.5	
148	Tetrachloroethylene	127-18-4	C2CL4	165.83	19	0.0720
149	Tetrahydrofuran	109-99-9	C4H8O	72.11	72.1	0.0980
150	Toluene	108-88-3	C7H8	92.14	30	0.0870
151	P-Toluidine	106-49-0	C7H9N	107.16	0.3	
152	1,1,1-Trichloroethane	71-55-6	C2H3CL3	133.41	123	0.0780
153	1,1,2-Trichloroethane	79-00-5	C2H3CL3	133.41	25	0.0792
154	Trichloroethylene	79-01-6	C2HCL3	131.4	75	0.0790
155	Trichlorofluoromethane	75-69-4	CCL3F	137.37	667	
156	1,2,3-Trichloropropane	96-18-4	C3H5CL3	147.43	3.1	
157	1,1,2-Trichloro-1,2,2-Trifluoroethane	76-13-1	C2CL3F3	187.38	300	
158	Triethylamine	121-44-8	C6H15N	101.19	400	
159	Trifluorobromomethane	75-63-8	CBRF3	148.91	--	
160	1,2,3-Trimethylbenzene	526-73-8	C9H12	120.19	--	
161	1,2,4-Trimethylbenzene	95-63-6	C9H12	120.19	--	
162	1,3,5-Trimethylbenzene	108-67-8	C9H12	120.19	1.86	
163	Vinyl Acetate	108-05-4	C4H6O2	86.09	115	0.0850
164	Vinyl bromide	593-60-2	C2H3Br	107.0	895	
165	Vinyl-Chloride	75-01-4	C2H3CL	62.5	2660	0.0900
166	M-Xylene	108-38-3	C8H10	106.2	8	0.0700
167	O-Xylene	95-47-6	C8H10	106.2	7	0.0870
168	P-Xylene	106-42-3	C8H10	106.2	9.5	

[1] All vapor pressures are at 25°C unless otherwise indicated.