

APPENDIX C

EXAMPLE CALCULATIONS

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SAMPLE CALCULATIONS FOR EXCAVATION (Section 3)

A site has approximately 10,000 m³ of soil contaminated with chloroform, 1,1,1-trichloroethane, and trichloroethylene in concentrations of 0.1, 10, and 1.0 ppm (μg/g), respectively. The distribution of the contamination within the soil is not accurately known. The soil's bulk density averages 1.5 g/cm³. Removal of all contaminants is expected to take 20 days of continual operation (1.728x10⁶ sec).

First estimate the total emissions potential for the site using Equations 3-1 and 3-2 from page 3-12:

$$M_{\text{Chloro}} = (10,000 \text{ m}^3)(0.1 \text{ } \mu\text{g/g})(1.5 \text{ g/cm}^3)(1 \text{ g/} \mu\text{g cm}^3/\text{m}^3) = 1,500 \text{ g}$$

$$ER_{\text{Chloro}} = M/t_{\text{sv}} = 1,500 \text{ g} / 1.728 \times 10^6 \text{ sec} = 8.7 \times 10^{-4} \text{ g/sec};$$

$$ER_{\text{TCE}} = (10,000)(1.0)(1.5)(1) / (1.728 \times 10^6) = 8.7 \times 10^{-3} \text{ g/sec};$$

$$ER_{\text{TCA}} = (10,000)(10)(1.5)(1) / (1.728 \times 10^6) = 8.7 \times 10^{-2} \text{ g/sec}.$$

These represent the average long-term emission rate if 100% of the contamination were volatilized and stripped from the soil.

The calculations using the excavation model and the default values given in the report are shown below for chloroform. First, the excavation rate is calculated from the known information: $Q = 10,000 \text{ m}^3 / 1.73 \times 10^6 \text{ sec} = 0.0058 \text{ m}^3/\text{sec}$. Next, the concentration must be converted from ppmw to g/cm³ using Equation 3-6:

$$Cs = (0.1 \text{ } \mu\text{g/g})(1.5 \text{ g/cm}^3)(10^{-6} \text{ g/} \mu\text{g}) = 1.5 \times 10^{-7} \text{ g/cm}^3$$

Now, the pore space and diffusion emissions can be calculated using Equations 3-3 and 3-4 from page 3-12:

$$ER_{\text{PS}} = (35)(100)(10^6)(0.44)(0.0058)(0.33) / (62,361)(298) = 0.16 \text{ g/sec}$$

$$\begin{aligned} ER_{\text{DIFF}} &= (1.5 \times 10^{-7})(10,000)(290) / (0.44 / 0.613 * 0.15) + (3.14 * 60 / 0.0269 * 0.613)^{0.5} \\ &= 0.4350 / 4.785 + (11,425)^{0.5} = 0.0039 \text{ g/sec}. \end{aligned}$$

The value, ER_{PS} , must be compared to the total mass of contamination present in the soil using Equation 3-7 on page 3-14:

$$ER_{\text{PS}} * t_{\text{sv}} = (0.16 \text{ g/sec})(1.728 \times 10^6 \text{ sec}) = 2.8 \times 10^5 \text{ g}$$

This value (2.8x10⁵ g) is > 0.33 M (0.33 * 1,500 = 500 g), so Equation 3-4 is giving a value that is far too conservative. Therefore, ER_{PS} should be calculated using Equation 3-8:

EMISSIONS FROM EXCAVATION
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(Continued)

$$ER_{PS} = M * 0.33/t_{sv} = (1,500 \text{ g})(0.33) / (1.728 \times 10^6 \text{ sec}) = 2.9 \times 10^{-4} \text{ g/sec}$$

The total emission rate of chloroform is thus:

$$ER = ER_{PS} + ER_{DIFF} = 0.00029 + 0.0039 = 0.0042 \text{ g/sec}$$

This is somewhat greater than the 8.7×10^{-4} g/s rate found from Equation 3-1. Equation 3-1, however, predicts the average emission rate if all contamination in the soil were to volatilize. However, 100% of the VOCs will not volatilize and be stripped from the soil, so it is reasonable that the emission rate estimate exceeds the average emission potential.

More accurate estimates could be obtained using compound-specific and site-specific input values rather than the default values. For example, the vapor pressure of chloroform is 208 mm Hg versus the default value of 35 mm Hg, and the molecular weight of chloroform is 119.38 g/mol versus the default value of 100 g/mol.

SAMPLE CALCULATIONS FOR THERMAL DESORPTION (Section 4)

A site to be remediated contains soil with the following levels of contamination:

Benzene	1.0 $\mu\text{g/g}$
Toluene	24.0 $\mu\text{g/g}$
Xylene	110.0 $\mu\text{g/g}$
Ethyl Benzene	20.0 $\mu\text{g/g}$

The full-scale desorption unit has a capacity of 7.5 tons per hour, and the percent volatilized is 99.00 for the other compounds of interest (i.e., equals the default value for BTEX). A fume incinerator with a 98% control efficiency will be used. Note that 1 $\mu\text{g/g}$ = 1 mg/kg.

To find the emission rate using the equation on page 4-18, the first thing to do is to get the input values into the proper units. The mass treatment rate of 7.5 tons/hr = 6820 kg/hr. Thus:

$$E_{\text{Benz.}} = (1.0 \text{ mg/kg} / 1,000 \text{ mg/g})(6,820 \text{ kg/hr})(99.00/100)(1-98/100) = 0.135 \text{ g/hr} \\ = (0.135 \text{ g/hr}) / (3,600 \text{ sec/hr}) = 3.8 \times 10^{-5} \text{ g/sec};$$

$$E_{\text{Tol.}} = (24/1,000)(6,820)(99.00/100)(1-98/100) = 3.24 \text{ g/hr} = 9.0 \times 10^{-4} \text{ g/sec};$$

$$E_{\text{Xyl.}} = (110/1,000)(6,820)(99.00/100)(1-98/100) = 14.8 \text{ g/hr} = 4.1 \times 10^{-3} \text{ g/sec}; \text{ and}$$

$$E_{\text{Ethyl Benz.}} = (20/1,000)(6,820)(99.00/100)(1-98/100) = 2.70 \text{ g/hr} = 7.5 \times 10^{-4} \text{ g/sec}.$$

SAMPLE CALCULATIONS FOR SOIL VAPOR EXTRACTION (Section 5)

A contaminated site to be remediated contains soil contaminated to the following extent:

Benzene:	100 ppm	(100 $\mu\text{g/g}$)
Toluene:	300 ppm	(300 $\mu\text{g/g}$)
Carbon Tetrachloride:	50 ppb	(0.050 $\mu\text{g/g}$)
Naphthalene:	800 ppb	(0.800 $\mu\text{g/g}$)

The site is a 200 m² field behind a factory. The water table is 30 m below the surface at this location. The entire volume of soil down to the water table is assumed to be contaminated. A vendor has quoted an estimate of five months to complete the clean-up. No physical data on the type of soil is known.

The uncontrolled stack emission rates are calculated with the equation on page 5-12. Use of this equation requires knowledge of the vapor extraction rate; for this scenario, a medium-sized SVE system of 85 m³/min may be assumed. One further needs the concentration of the extracted vapors. The saturated vapor concentrations can be calculated using the equation on page 5-17 or can be obtained from the following reference: Eklund and Albert, 1993*. The saturated vapor concentrations given in this reference are:

benzene	$4.00 \times 10^8 \mu\text{g/m}^3$
toluene	$1.49 \times 10^8 \mu\text{g/m}^3$
carbon tetrachloride	$9.34 \times 10^8 \mu\text{g/m}^3$
naphthalene	$1.58 \times 10^5 \mu\text{g/m}^3$

These values all assume that the soil is saturated with each contaminant. Given the low concentrations present in the soil, the extracted vapor will actually be well below saturation and the estimates will be quite conservative.

Putting the values given above into a mass balance equation for air emissions yields:

$$ER_{\text{benz}} = (4.00 \times 10^8 \mu\text{g/m}^3)(10^{-6} \text{ g}/\mu\text{g})(85 \text{ m}^3/\text{min}) / (60 \text{ sec}/\text{min}) = 570 \text{ g/sec}$$

$$ER_{\text{tolu}} = (1.49 \times 10^8)(10^{-6})(85) / (60) = 210 \text{ g/sec}$$

$$ER_{\text{CCl}_4} = (9.34 \times 10^8)(10^{-6})(85) / (60) = 1,300 \text{ g/sec}$$

$$ER_{\text{naph}} = (1.58 \times 10^5)(10^{-6})(85) / (60) = 0.22 \text{ g/sec.}$$

* Eklund, B. and C. Albert. Models for Estimating Air Emission Rates from Superfund Remedial Actions. EPA-451/R-93-001 (NTIS PB93-186807). March 1993.

EMISSIONS FROM IN-SITU BIOTREATMENT SYSTEMS (Section 6)

Assume the same scenario as given above for soil vapor extraction: A contaminated site to be remediated contains soil contaminated to the following extent:

Benzene:	100 ppm	(100 $\mu\text{g/g}$)
Toluene:	300 ppm	(300 $\mu\text{g/g}$)
Carbon Tetrachloride:	50 ppb	(0.050 $\mu\text{g/g}$)
Naphthalene:	800 ppb	(0.800 $\mu\text{g/g}$)

The site is a 200 m² field behind a factory. The water table is 30 m below the surface at this location. The entire volume of soil down to the water table is assumed to be contaminated. A vendor has quoted an estimate of five months to complete the clean-up. No physical data on the type of soil is known. During a pilot-scale test of the suitability of bioventing, the off-gas was found to have a concentration of roughly $1 \times 10^4 \mu\text{g/m}^3$ for benzene and toluene, and $1 \times 10^5 \mu\text{g/m}^3$ for carbon tetrachloride. No naphthalene was detected ($\text{DL} = 1 \times 10^6 \mu\text{g/m}^3$).

The extraction rate for the soil venting is calculated using the 2nd equation given on page 6-8. The volume of contaminated soil is $200 \text{ m}^2 * 30 \text{ m} = 6,000 \text{ m}^3$. The air filled porosity can be assumed to be 0.44 (see Table 3-4). Using these input values, the extraction rate can be calculated:

$$Q (\text{m}^3/\text{min}) = (1.0/1440 \text{ min})(6,000 \text{ m}^3)(0.44) = 1.83 \text{ m}^3/\text{min}$$

Using the available information, the emissions can be calculated as follows:

$$\begin{aligned} \text{ER}_{\text{benz}} &= (1 \times 10^4 \mu\text{g/m}^3)(10^{-6} \text{ g}/\mu\text{g})(1.83 \text{ m}^3/\text{min}) / (60 \text{ sec}/\text{min}) = 3.05 \times 10^{-4} \text{ g/sec} \\ \text{ER}_{\text{tolu}} &= (1 \times 10^4)(10^{-6})(1.83) / (60) = 3.05 \times 10^{-4} \text{ g/sec} \\ \text{ER}_{\text{CCl}_4} &= (1 \times 10^5)(10^{-6})(1.83) / (60) = 3.05 \times 10^{-3} \text{ g/sec} \\ \text{ER}_{\text{naph}} &= (1 \times 10^{-6})(10^{-6})(1.83) / (60) = < 1 \times 10^{-12} \text{ g/sec.} \end{aligned}$$

EMISSIONS FROM EX-SITU BIOTREATMENT SYSTEMS (Section 7)

Consider a site with a contaminated lagoon. The lagoon holds 500,000 L with an area of 100 m². The sludge beneath it is contaminated to a depth of about 3 m. The contaminants present in the sediments are benzene and chlorobenzene. The overlying water is considered to be uncontaminated. The concentrations are 10 µg/g benzene and 20 µg/g chlorobenzene in the sludge (µg/g = mg/kg). The bulk density of the sediments was measured and is 2.0 g/cm³. Therefore, the 300 m³ of contaminated sludge would weigh 600,000 kg. A batch biotreatment system will be used with a treatment rate of 2,000 kg batches treated for one day (86,400 sec) each. The Henry's Law constants for both compounds are in the 10⁻³ range, and V is assumed to be 20%.

Using the equation for batch treatment, the emission rates are estimated to be:

$$ER_{\text{BENZ}} = (10 \text{ mg/kg} / 1,000 \text{ mg/g})(2,000 \text{ kg})(20/100) / 86,400 \text{ sec} = 4.6 \times 10^{-5} \text{ g/sec; and}$$

$$ER_{\text{CHL}} = (20/1,000)(2,000)(20/100) / 86,400 = 9.3 \times 10^{-5} \text{ g/sec.}$$

EMISSIONS FROM THERMAL DESTRUCTION (Section 8)

Consider the following remediation scenario. The soil in a hypothetical site has been tested, and it contains:

PCBs	2 %
1,2,4-Trichlorobenzene	2800 ppb

The contractor will use a rotary kiln incinerator with a feed rate of 6000 kg/hr. An ultimate analysis of the soil shows it to contain: 1.0% S, 0.5% Cl, 0.15% Ba, and 0.08% Pb. The device burns propane, which is assumed to not contribute measurably to the emissions of any of the above compounds. The exit gas flow rate is not known. A scrubber will be used to control emissions of acid gases, and the vendor indicates that control efficiencies of 95% for SO₂ and 99% for HCl can readily be achieved.

First, find the concentration of organic contaminants in the waste feed in the specified units of g/kg (note that 1% = 10,000 ppm, 1,000 ppb = 1 ppm, and ppm = μg/g):

$$C_{\text{PCB}} = (20,000 \mu\text{g/g})(10^{-6} \text{ g}/\mu\text{g})(1,000 \text{ g/kg}) = 20 \text{ g/kg};$$

$$C_{\text{TCB}} = (2.8)(10^{-6})(1,000) = 0.0025 \text{ g/kg}.$$

Next calculate the organic emissions using the 1st equation on page 8-13 and a DRE for PCBs of 99.9999%, and a DRE for TCB of 99.99%.

$$\begin{aligned} \text{ER}_{\text{PCB}} &= (1 - 99.9999/100)(6,000 \text{ kg/hr})(20 \text{ g/kg}) = 0.12 \text{ g/hr} \\ &= (0.12 \text{ g/hr}) / (3,600 \text{ sec/hr}) = 3.3 \times 10^{-5} \text{ g/s; and} \end{aligned}$$

$$\text{ER}_{\text{TCB}} = (1 - 99.99/100)(6,000)(0.0025) = 0.0015 \text{ g/hr} = 4.2 \times 10^{-7} \text{ g/s}.$$

The uncontrolled metals emission rates are found using the second equation on page 8-13 (the controlled emissions may be significantly lower). First, find the concentration of contaminants in the waste feed in the specified units of g/kg (note that 1% = 10,000 ppm and ppm = μg/g):

$$C_{\text{Ba}} = (1,500 \mu\text{g/g})(10^{-6} \text{ g}/\mu\text{g})(1,000 \text{ g/kg}) = 1.5 \text{ g/kg; and}$$

$$C_{\text{Pb}} = (800)(10^{-6})(1,000) = 0.8 \text{ g/kg}.$$

The partitioning factor for both metals is 100% (from EPA, 1989); that is, the metals can be expected to be present in the gas-phase. The emission rates are then:

$$\begin{aligned} E_{\text{Ba}} &= (1.5 \text{ g/kg})(6,000 \text{ kg/hr})(100/100) = 9,000 \text{ g/hr} \\ &= (9,000 \text{ g/hr}) / (3,600 \text{ sec/hr}) = 2.5 \text{ g/sec; and} \end{aligned}$$

$$E_{\text{Pb}} = (0.8)(6,000)(100/100) = 4,800 \text{ g/hr} = 1.3 \text{ g/sec}$$

EMISSIONS FROM THERMAL DESTRUCTION

(Section 8)

(Continued)

For acid gases, again the first step is to convert the concentration of the element in the waste to the proper units:

$$C_{\text{Cl}} = (5,000 \mu\text{g/g})(10^{-6} \text{ g}/\mu\text{g})(1,000 \text{ g/kg}) = 5.0 \text{ g/kg}; \text{ and}$$
$$C_{\text{S}} = (10,000)(10^{-6})(1,000) = 10 \text{ g/kg}.$$

Their stoichiometric ratios are 1.028 (g HCl / g Cl) for HCl and 1.998 (g SO₂ / g S) for SO₂;

$$E_{\text{HCl}} = (5 \text{ g/kg})(1.028)(6,000 \text{ kg/hr})(1-99/100) = 308 \text{ g/hr}$$
$$= (308 \text{ g/hr}) / (3,600 \text{ sec/hr}) = 0.086 \text{ g/sec}; \text{ and}$$

$$E_{\text{SO}_2} = (10)(1.998)(6,000)(1-95/100) = 5,990 \text{ g/hr} = 1.7 \text{ g/sec}.$$