10.0 UNCERTAINTY AND SENSITIVITY ANALYSIS

10.1 Introduction

An analysis of the uncertainty associated with the EEMs presented in Chapters 3 through 8 was performed and the results are presented in this chapter. Every method that is used to estimate air pollutant emissions, whether it is an emission factor or a more complex emissions model, carries a certain level of uncertainty. There are two sources of uncertainty associated with EEMs:

- Uncertainty of the EEM itself: this refers to the ability of the method to accurately predict real-world emissions. In other words, if each value for all of the parameters in the method are precisely known, how accurate is the EEM (in terms of precision and bias) in predicting actual emissions?

- Uncertainty in the values of the EEM variables: in many cases, the values for the EEM parameters will not be precisely known and must be estimated. In addition, where the parameter may have a measured value, there is variability associated with this value. Often a sensitivity analysis is performed in order to gain an understanding of which variables have the largest impact on the predicted result (i.e., which contribute the most to the variability in the prediction).

Ideally, an analysis of uncertainty would address both sources and present the results as a combined result. However, in order to analyze method uncertainty (as described under the first bullet), field data are needed for comparison against the EEM-predicted results. These data are very rarely available and were not available for use in this uncertainty analysis. Limited EEM predictions compared against field data have shown that the EEMs can be expected to yield conservatively-biased (i.e., high) predictions within a factor of 3 to 10 (see Table A-7 in Appendix D).

A description of the approach and results obtained for the uncertainty analysis of EEM variables is given in the sections that follow. A sensitivity analysis is also performed for each EEM in order to determine which variable(s) contribute the most to the variability in the predicted results.

10.2 Approach

Monte Carlo simulations of each EEM were performed using a commercially-available software (Crystal Ball Version 4.0). Monte Carlo simulation is an efficient technique for analyzing real-world problems that have a large number of possible outcomes based on the potential values of associated variables. In a Monte Carlo simulation, random numbers for each variable are generated that conform to the real-world potential values. A large number of EEM trials are run (e.g., 10,000) using these randomly-generated values. Based on the results of this large number of trial simulations, a distribution and summary statistics are derived. These statistics can be used to gain an understanding of the variability associated with the EEM projections (e.g., mean, coefficient of variation, 95% confidence limits).

In order to perform the uncertainty/sensitivity analysis, assumptions had to be derived for an example application. The same set of assumptions (e.g., soil properties and benzene concentration level) were used during the analysis of each EEM. It was assumed that there was a need to develop an emission rate for benzene from soil remediation activities. The soil had been contaminated with gasoline and moderate levels of benzene were present (10 ppm). No other physical data were available for the soil (e.g., moisture content, bulk density, temperature) which is common during these analyses. However, it was assumed that the remediation would occur during the summer months (ambient temperature of 25 degrees C) and that the soil was a fine-textured clay.

For each EEM, a spreadsheet was developed that contained the equation(s) for estimating emissions and the associated variables. For each variable, assumptions were assigned that described the range and distribution of potential values (e.g., normal, uniform, triangular). These assumptions are summarized in Table 10-1. Most of the information used to develop the variable distributions were taken directly from the text of this report. For example, the percentage of benzene that is anticipated to volatilize during thermal desorption was assumed to be 99.50% based on information given in Chapter 3. Further, based on the same information and engineering judgement, it was assumed that the minimum percentage of benzene volatilized would be 99.00% and that the maximum would be 99.99%. Using the minimum, maximum, and likeliest values, a triangular distribution was developed for input to the Monte Carlo simulations.

Using the assumptions listed in Table 10-1 and the equations given in Chapters 3 through 8, Monte Carlo simulations were run for each EEM to develop distributions of the potential emission rates. Along with the distributions of potential emission rates, charts depicting the sensitivity of the EEM to the associated variables were developed.

10.3 Results

A summary of the uncertainty/sensitivity analysis is shown in Table 10-2. Monte Carlo modeling results are given in Appendix G. For each EEM, a point estimate of the emission rate is given. This value was derived by using the appropriate equation given in Chapters 3 through 8 and the mean or most likely values for the associated variables given in Table 10-1.

The mean of each Monte Carlo distribution is shown in Table 10-2 along with 95% confidence limits for the potential emission rate. In the final column, the variables which had the largest influence on the EEM predictions are listed along with the contribution to variance associated with each.

For excavation/removal, the total emission rate was influenced most by the soil bulk density variable. This variable is used to determine the air-filled porosity parameter (E_a) which, in turn, is used during the estimation of both the emission rate from the pore space and the emission rate from diffusion. These results signify the importance of gathering and using site-specific data whenever possible. Based on the 95% confidence limits, the total emission rate could vary by a factor of more than 5.

For thermal desorption, the emission rate was shown to vary by a factor of about

8. The variability was driven almost exclusively by the uncertainty in the estimate of control efficiency.

For soil vapor extraction, the vapor extraction rate was only independent variable, and therefore was the only variable that contributed to quantifiable uncertainty in the emission rate estimate. The 95% confidence limits show that the range in potential emissions could span a factor of about 2.

The analysis for in-situ biodegradation revealed that again the bulk density of the soil contributed the most to variability in the emission rate. However, the estimate of the number of pore volumes extracted per day was also a high contributor. Potential emissions varied by a factor of nearly 8.

For ex-situ biodegradation, the EEM was shown to be most sensitive to the estimate given for V (the fraction of benzene volatilized). This situation is likely to persist, as there is scant data of this type available. Potential surrogate data for use here include from studies of VOC volatilization from sewage treatment plants and sewer systems.

As with thermal desorption, the variability in predicted emissions for incineration is driven by estimates of control efficiency. Specific vendor estimates or guarantees would likely improve upon the assumptions used here. Often a minimum control efficiency can be guaranteed (e.g., >99.90%) that would be high enough to tighten the assumed distribution. This would result in lower variability of the projected emissions.

Details of the Monte Carlo simulations are given in Appendix G. Each EEM begins with a print-out of the spreadsheet used to build the emission projections (forecasts). Charts that display the sensitivity of the EEM to each variable are shown. Figures are also shown that depict the distributions of each forecast (e.g., emission rates) and assumptions.

10.4 References

Brady, N.C., *The Nature and Properties of Soils*, MacMillan Publishing Co., New York, NY, 1984.

Fleischer, E.J., et. al., "Evaluating the Subsurface Fate of Organic Chemicals of Concern Using the SESOIL Environmental Fate Model", *Proceedings of the Third Eastern Regional Groundwater Conference*, National Well Water Association, Springfield, MA, July 29-31, 1986.

Pechan, personal communication from staff of Weston, Inc., 1996.

Table 10-1
Scenario Development for the Uncertainty/Sensitivity Analysis

Variable	Value	Comments
Benzene concentration (C)	10 ppm	Based on hypothetical representative sampling of the site. The distribution is assumed to be normal with a mean of 10 and a standard deviation of 1.0.
Soil moisture content (Mfrac)	15%	Mid-point of the typical range for clay soils [clay soil is characteristic of the site (Brady, 1984)]. Distribution is uniform with 12% as the minimum and 18% as the maximum.
Ambient temperature (Ta)	298K	Assumed that the remediation takes place during the summer months.
Soil temperature (Ts)	293K	The soil temperature will be about 5 degrees cooler than the assumed ambient temperature of 298K. Based on data from Brady (1984).
Soil bulk density (beta)	1.5 g/cm^3	Soil assumed to be moderately compacted and finely-textured (Brady, 1984). The distribution is uniform with a minimum of 1.0 and a maximum of 2.0.
Particle density (p)	2.65 g/cm^3	Assumed from information given in Chapter 3. Uniform distribution around a 2.65 g/cm^3 mean and a +/- 5% error.
Volatilized fraction during thermal desorption (V)	99.50%	From information presented in Chapter 2. Triangular distribution with a minimum of 99.00%, a maximum of 99.99%, and a likeliest value of 99.50%.
Soil feed rate into the thermal desorber (F)	27,200 kg/hr	Assumed from information given in Chapter 2. Uniform distribution around a mean of 27,200 kg/hr and a +/- 10% error.
Vapor extraction rate during soil vapor extraction (Q)	85 m^3/min	Assumed from information given in Chapter 5. Uniform distribution around a 85 m^3/min mean and a +/- 30% error.
Pore volumes per day for in-situ bioremediation (pv)	1.0	Based on information given in Chapter 5. Distribution is triangular with a minimum of 0.3, a maximum of 2.0, and the likeliest value of 1.0.
Fraction volatilized during continuous ex-situ bioremediation (V)	0.60 vol/vol	Based on limited data soil/water partitioning (Fleischer, et al., 1986). End-points of the uniform distribution derived from an error estimate of +/- 30%.
Mass feed rate of soil into the continuous ex-situ bioreactor (Mr)	600 kg/hr	Assumed based on information provided in Chapter 6. Distribution is uniform with 600 kg/hr the mid-point and the end points determined from a +/- 10% error estimate.
Mass feed rate of soil into the thermal incinerator (Mw)	4,500 kg/hr	Assumed based on information from Pechan (1996). Distribution is uniform with 4,500 kg/hr as the mid-point and end-points determined from a +/- error assumption of 10%.
Control efficiency (CE) during thermal desorption and thermal oxidation processes	99.50%	Based on engineering judgement. Distribution is assumed to be triangular with a minimum of 99.00%, a maximum of 99.99%, and a most likeliest value of 99.50%.
Contaminated area	2500 m^2	Assumed.
Contaminated depth	5 m	Assumed.

Table 10-2.
Uncertainty/Senstivity Analysis Results

EEM No.	Remediation Process	Predicted Benzene Emissions, g/sec (g/hr)			EEM Parameters Contributing the Most to Emissions Variability (% Contribution to Variance)
		Point Estimate of Emissions	Monte Carlo Predictions		
			Mean	95% Confidence Limits	
1	Excavation/Removal: Emissions from Pore Space Emissions from Diffusion Total Emissions	 0.59 3.26 3.85	 0.98 3.19 4.17	 0.16 - 2.71 1.10 - 5.23 1.41 - 7.38	ER pore space: excavation rate (Q) = 50%; bulk density (beta) = 32%; exchange constant (ExC) = 17%. ER diffusion: bulk density (beta) = 90% ER total: bulk density (beta) = 85% excavation rate (Q) = 6%
2	Thermal Desorption	1.35	1.36	0.32 - 2.54	control efficiency (CE) = 93%
3	Soil Vapor Extraction	0.47	0.47	0.33 - 0.60	vapor extraction rate (Q) = 100% (this is the only independent variable)
4	In-Situ Biodegradation	0.017	0.018	0.005 - 0.039	bulk density (beta) = 58%; pore volumes extracted per day (pv) = 40%
5	Ex-Situ Biodegradation	3.72	3.60	1.80 - 5.82	fraction volatilized (V) = 89%; benzene concentration (C) = 6%
6	Incineration	0.23	0.23	0.052 - 0.42	control efficiency (CE) = 93%