7.0 Example 3MRA Uncertainty Analysis for Benzene

Representing a typical application of 3MRA Version 1.0 and the supporting SuperMUSE hardware and software toolset, an evaluation of Benzene disposal in various land-based waste management units was conducted as an illustrative example of the system capability.

The example demonstrates a preliminary uncertainty analysis of Benzene disposal, using 3MRA that describes the relative importance of various exposure pathways in driving risk levels for both ecological and human receptors, incorporating aspects of multiple site-based assessments rolled-up into an overall national assessment, following the underlying science methodology of 3MRA described in Marin *et al*. (1999, 2003). The example covers landfills, waste piles, aerated tanks, surface impoundments, and land application units. The site-based data used in the analysis included the 201 national facilities in the 3MRA site-based database representing 419 site-WMU combinations.

Similar to the model runtime trial analysis discussed in Section 6.6, the uncertainty analysis discussed here was based on an interim 3MRA Version 1.0 (Developers Release - January, 2002) which was used for all simulations. Due to changes between this interim beta version and the final 3MRA Version 1.0 modeling system, the actual data presented is provisional, and is intended to serve only as in illustration of 3MRA modeling system outputs.

7.1 Benzene Disposal Simulation Design

In this example, the sampling-based simulation design employed two basic experiments. The first experiment represents an aggregated 1-dimenional analysis (Section 2.6.6) under the assumption of use of all input parameterizations that would be described as *variable and certain,* or, alternatively, an analysis that convolves empirical input uncertainty discussed in the second experiment within a hybrid dimension of uncertainty and variability (i.e., U+V). The second experiment represents a pseudo 2nd-order analysis (Figure 2-10) that addresses empirical uncertainty in use of probability distributions to describe individual sites used in the experiment (Sections 2.6.3 and 2.6.6), and also forms the ability to quantify output sampling error (OSE) in the 50th probability percentile of the estimate of variability by way of confidence intervals stated about the mean of the output distribution. The confidence interval is formed upon actual output data collected at each wastestream concentration (C_w) simulated (Section 2.5.3).

National Risk Assessment Problem Statement

As discussed in Sections 4.4.5 and 4.3.3 and in the document *3MRA Modeling System: Technology Design and Users Guide*, from the data generated in this first experiment, the ELP2 can be used to determine a single $C_{w_{exit}}$ value for any definable assessment profile (A, B, C, D, E, F, G) (Sections 4.6.1 and 4.6.2). In reviewing the entities of the 9-tuple (Section 4.4.5), recall the basic question that 3MRA is capable of answering:

At what waste stream concentration (C_w) will wastes, when placed in a nonhazardous waste management unit over the unit's life, result in:

- Fewer than A% of the people living within B distance of the facility with a risk/hazard of C or less, and
- Fewer than D% of the habitats within E distance of the facility with an ecological hazard less than F,
- At G% of facilities nationwide?

The terms A, D, and G above formulate the population protection criteria and embody the statement of site variability for the other selected decision variables B, C, E, and F. A probability (H) may be further assigned to separate empirical input uncertainty (e.g., sampling from inputs representing non-target populations or *constant but uncertain* inputs) from variability within the derived protection profile for selected percentiles (A, D) of the target population or subpopulations selected via the ELP2 (i.e., uncertainty in population protection for various population or subpopulation percentiles). Furthermore, a probability (I) can be assigned to the simulation-based empirical output uncertainty (i.e., OSE) associated with the derived protection profile for the designated percentiles of the target population or subpopulations. Terminology "A" to "I" is used for simplicity here, and represents a departure from the indexing employed in the delineation of the 3MRA science methodology (Marin *et al.* 1999, 2003).

A given risk assessment question is therefore defined by the general 9-tuple risk assessment profile described by:

- A; % human population protection,
- B; radial distance from the source for human concern,
- C; increased risk of cancer in humans,
- D; % ecological population protection,
- E; radial ring distance from the source for ecological concern,
- F; ecological risk hazard quotient,
- G; % national sites protected for the given population percentile A or D;
- H; empirical uncertainty probability; and
- I; confidence in the total uncertainty probability H.

7.1.1 Experiment A: Aggregated 1st-Order Total Uncertainty Analysis

The first experiment was a simulation of Benzene across all 419 waste management units in the existing 3MRA site database. Analyzing five source types (AT, SI, LAU, WP, and LF), five C_w's (which were appropriately selected within the 3MRA database based on historical experience with these source types, chemical properties, and known toxicity), and using an initial Monte Carlo random seed value of 11031, 100 iterations were conducted for each unique site-source-C_w combination, totaling 209,500 simulations. In this experiment, due to data storage limitations and pending automation of ELP2 processing for multiple, individual iterations (Section 6.1.4), the 100 iterations were aggregated during simulation within a single ELP1 database structure, resulting in the pooling of protected, and separately, unprotected populations across all iterations.

7.1.2 Experiment B: Pseudo 2nd-Order Analysis of Variability and Empirical Uncertainty

For the second experiment, the same selections were made, but only 10 national realizations were simulated. In this case, the ELP1 output (Figures 4-3 and 2-10) was segregated by iteration into separate databases during simulation. Here, the ELP2 could be used to analyze individual national iterations to determine a single average $C_{w_{exit}}$ value for any assessment profile (A, B, C, D, E, F, G), where H is effectively viewed as 50%, and, through additional uncertainty analysis, any combination of concerns represented by 9-tuple (A, B, C, D, E, F, G, H, I).

Had the second experiment been conducted with 100 segregated national realizations (Figure 2-10), the average of all $C_{w_{exit}}$ values calculated by realization would equal the single average $C_{w_{exit}}$ calculated in the first experiment (assuming the same seed is used).

7.1.3 Interpretation of Variability and Uncertainty in the Experiment

Previously discussed, quantification of the empirical uncertainty imposed in site-based, national roll-ups due to use of the non-target national and regional distributions can be handled in a pseudo 2-dimensional analysis (Section 2.6.6). This is in effect a separation of the associated dimension of uncertainty laid upon site-based variability expressed in the site-based database. In the case of model inputs representing non-targeted sampled populations (i.e., variables in regional and national databases), the aspect of “individual” versus “population” is important in interpreting modeling system output (Sections 2.1.1 and 2.6.3). Such inputs are more appropriately designated as *constant and uncertain* with respect to value selections made for each model run at a given site. Using the “pseudo” 2nd-order analysis (Figure 2-10), these inputs are effectively separated from sampled site-based data (i.e., the point-estimate inputs from the site-based database) that represent *variable and certain* quantities (though some SME is present in these point estimates).

Presumed to be actually present in the latter quantities, in both Experiments A and B, the dimension of variability in modeling system output associated with sampled site-based data actually represents a hybrid dimension of site-based variability convolved with some SME. Essentially, some uncertainty due to random error (RE) is, at the present time, included within the variability captured in these descriptions in a national assessment. Thus, any simulation design expressing these model inputs as pure variability even in the pseudo 2nd-order analysis would ignore some level of uncertainty present in the data.

For the most part, all variables currently described in 3MRA databases represent a hybrid probability space of total uncertainty, representing variability plus at least SME uncertainty, and, due to stochastic national and regional variables, some uncertainty due to sampling of non-target populations. Experiment A, a 1-dimensional analysis, convolves all of this uncertainty in a single, hybrid dimension of total uncertainty, otherwise represented as variability. Experiment B separates the dimension of empirical uncertainty associated with all probability distribution functions in the 3MRA database from the dimension of variability associated with all constant point-estimates in the site-based database that vary from site to site. The actual probability percentiles used in this analysis (e.g., for Experiment A: effectively 50%, for Experiment B: 50% and 95%) are, thus, an expression of "H" in the 9-tuple.

Output Sampling Error (OSE)

Discussed in Sections 2.5.3 and 2.6.6, where the estimate of the given population percentile of a normal random output variable is subject to empirical uncertainty, the confidence intervals constructed about the mean represent confidence stated in the 50th probability percentile of that estimate (i.e., "H"). Thus, actual population percentile estimates (e.g., 99% and 95% population percentiles analyzed herein; i.e., "A" and "D"), representing CDFs of the hybrid variability dimension in both Experiments A and B, are imprecise due to OSE. In Experiment A, OSE is completely ignored. In Experiment B, OSE is addressed in the analysis herein as a confidence interval about the 50th probability percentile (i.e., "H") of the estimate of the hybrid variability dimension CDF for "A" and "D". For Experiment B, OSE uncertainty in other probability percentiles (e.g., 95% probability; i.e., "H") associated with the pseudo 2nd-order analysis is not addressed in this analysis (see Section 2.5.3). The actual probability levels used in this analysis for constructing the confidence intervals (e.g., Experiment B: 98% confidence or probability level $\alpha = 0.02$) are, thus, an expression of "I" in the 9-tuple

7.1.4 Summary of Experiment A and B

In the Experiment A, output sampling error is ignored and variability is not separated from empirical uncertainty (a result of the aggregation of ELP1 risk summaries across national realizations). In the second, Experiment B, empirical input uncertainty is separated from variability and OSE is addressed as described previously. In both experiments, ISE is ignored and SME is convolved within variability CDFs.

The first experiment can be defined by the 8-tuple (A, B, C, D, E, F, G, H) for H = 50%, and the second experiment can be described by the 9-tuple (A, B, C, D, E, F, G, H, I).

For purposes of further discussion and comparative analysis, two different assessment exposure profiles (see Sections 4.6.1and 4.6.2) were examined using the associated ELP1 databases generated by each simulation experiment:

- Experiment A:
  - (95%, 500m, 1x10^{-6}, 95%, 1000m, 1, 50%, 95%)$_{ABCDEFGH}$, and
  - (99%, 2000m, 1x10^{-6}, 99%, 2000m, 1, 50%, 95%)$_{ABCDEFGH}$.

- Experiment B:
  - (95%, 500m, 1x10^{-6}, 95%, 1000m, 1, 95%, 50% and 95%, 98%)$_{ABCDEFGHI}$, and
  - (99%, 2000m, 1x10^{-6}, 99%, 2000m, 1, 95%, 50% and 95%, 98%)$_{ABCDEFGHI}$.

For experiment B, the last element of the 9-tuple "I" is constructed as a 98% confidence interval about median CDF H=50%.

The aggregated ELP1 for MySQL databases (Section 6.4.3) and the ELP2Vis tool (Section 6.4.4) were used to construct the analysis. Since there is no applicable human hazard risk criteria considered for Benzene in 3MRA, the analysis here looks only at human cancer risk (i.e., ELP1 RTemplate risk summary table; see Table 6-8b) and ecological hazard risk (i.e., ELP1 ETemplate risk summary table; see Table 6-8d).

7.2 Benzene Disposal Uncertainty Analysis

The presentation of results for both experiments are summarized in Table 7-1, where Experiment A represents data associated with 100 national iterations or realizations, and Experiment B represents data associated with 10 national iterations. Example graphics are presented for the landfill WMU for Experiment B (Figures 7-1, 7-2, and 7-3). For this example, since data for Experiment A are relatively indistinguishable visually from the median probability percentile (i.e., "H") as represented in graphics for Experiment B, similar graphics are not presented separately for Experiment A. However, Experiment A is graphically represented in example ELP2Vis output shown in Figures 6-9, 6-10, and 6-12, discussed in Section 6.4.4.

As shown in Figure 7-1, waste stream exit levels for the landfill source were calculated for the two assessment profiles (95%, 500m, 1x10^{-6}, 95%, 1000m, 1, 95%, 50%, 98%)$_{ABCDEFGHI}$ and (99%, 2000m, 1x10^{-6}, 99%, 2000m, 1, 95%, 50%, 98%)$_{ABCDEFGHI}$, based on the sum of all ingestion and inhalation pathways. Data are based on individual calculations completed for each of 10 iterations simulated across 56 sites. For each iteration, the ELP2Vis was used to provide values for actual % site protection at the five C_w's evaluated; average % site protection values were then determined at these C_w's, along with the 98% confidence levels (Zar, 1999).

Using a log-linear interpolation scheme, the exit levels at the 95% site protection level were next derived for the average of the 10 national iterations, along with the associated confidence intervals and minimum and maximum values observed. Actual exit level values are presented in Table 7-1 for each profile examined. Log-linear interpolation represents the current policy approach, but alternative schemes (e.g., linear) could also be investigated to provide insight between individual C_w pairs simulated. The approach of using log-linear interpolation between C_w's imparts significant conservatism in assigning exit levels between C_w's. Sensitivity analysis planned for 3MRA described in Section 9 will be able to better evaluate the effect and appropriateness of this policy decision approach.

For all Benzene analyses described in Table 7-1, human cancer risk was the determinant concern at all associated waste concentration levels, for all source types. Not shown in Figure 7-1, for ecological concerns, all sites (100%) were protected at the lowest C_w evaluated for landfills (0.001 ug/g). Therefore, subsequent 9-tuple designations described in the following materials omit the 3 associated profile designations for ecological concerns (i.e., omit D, E, and F).

7.2.1 Pseudo 2nd-Order Total Uncertainty Analysis Based on Confidence Intervals

Based on 10 iterations, representing a total of 2800 actual simulations, an average landfill $C_{w_{exit}}$ of 138 ppm and 184 ppm was derived for the (95%, 500m, $1x10^{-6}$, 95%, 50%)$_{ABCGH}$ and (99%, 2000m, $1x10^{-6}$, 95%, 50%)$_{ABCGH}$ profiles, respectively. For the (95%, 500m, $1x10^{-6}$, 95%, 50%, 98%)$_{ABCGHI}$ profile, upper and lower 98% confidence intervals ranged between 179 and 108 ppm, respectively, where a maximum observed value of 233 ppm, and a minimum observed value of 29 ppm were noted in Experiment B. Based on the aggregated 1-dimensinal simulation Experiment A for 100 iterations (totaling 28,000 simulations), an average $C_{w_{exit}}$ of 135 ppm and 195 ppm was derived for the (95%, 500m, $1x10^{-6}$, 95%, 50%)$_{ABCGH}$ and (99%, 2000m, $1x10^{-6}$, 95%, 50%)$_{ABCGH}$ profiles, respectively. These values were relatively close estimates to those values found using only 10 iterations, with 98%, and 106% recovery, respectively (Table 7-1).

The pseudo 2nd-order analysis landfill exit levels for Benzene are depicted graphically in Figure 7-1 for both profiles considered. We note that a lower population protection level (95%) specified at a closer distance to the facility (500m) yielded significantly lower exit level thresholds for hazardous waste.

In summary of the 50% probability percentile of variability, Experiment B allowed for estimation of output sampling uncertainty "I", in the statement of the 50% probability "H" in predicting % sites protection for Benzene at each C_w. While Experiment B addresses similar empirical uncertainty ("H"), and confidence "I" associated with OSE, Experiment A retains less OSE, though not quantified, in the statement of the 50% probability "H" in predicting % sites protection for Benzene at each C_w. Experiment A generally allowed for examination of trends in average $C_{w_{exit}}$ for more extensive coverage of the input parameter space.

7.2.2 Pseudo 2nd-Order Total Uncertainty Analysis Based on CDFs of 95% Probability

For simple comparison in properly addressing empirical uncertainty in the national risk assessment, Figure 7-2 presents the exact same analysis shown in Figure 7-1 for the profile (99%, 2000m, $1x10^{-6}$, 95%, 50% and 95%)$_{ABCGH}$, but also presents the profile CDF for (99%, 2000m, $1x10^{-6}$, 95%, 95%)$_{ABCGH}$. The conclusion, as an exit level, that one would reach in establishing a suitable protection level with 95% probability of being met versus 50% probability (ignoring for now OSE), are quite different. In this analysis, due to the small sample size (n_s = 10), there is still significant OSE not addressed in the 95% percentile of probability, which is very near to the minimum value observed. In a more thorough analysis, the minimum CDF would fall further below the 95% probability percentile CDF on the graphic shown in Figure 7-2.

7.2.3 Analysis of All Source Types

In comparison to the analysis completed for disposal of Benzene in landfills, for land application units, a higher population protection level profile (99%, 2000m, $1x10^{-6}$, 95%, $50\%)_{ABCGH}$, specified at a greater distance from the facility (2000m), had a lower exit level threshold, i.e., 3.0 ppm versus 3.5 ppm determined for the (95%, 500m, $1x10^{-6}$, 95%, $50\%)_{ABCGH}$ profile. Differences between exit levels based on 10 national iterations versus 100 iterations were similarly small for land application units and surface impoundments. The differences were relatively much larger, however, for waste piles and aerated tanks. In both these cases, an overall significantly lower exit level (28 to 55% recovery) was determined with more intensive simulation based on 100 iterations. For aerated tanks, the average exit level derived from 100 iterations actually fell below the minimum simulation value seen during the first 10 iterations.

Comparing waste management unit types, using data for 100 national iterations and the (95%, 500m, $1x10^{-6}$, 95%, $50\%)_{ABCGH}$ profile, average exit levels were lowest for surface impoundments (0.19 ppm), followed by aerated tanks (2.0 ppm), land application units (3.1 ppm), waste piles (9.2 ppm), and landfills (135 ppm). While far more simulation is needed to properly evaluate the uncertainty and sensitivity of 3MRA predictions, from this example ecological and human health risk-based analysis, one can envision the potential future application of supplementary cost-benefit analyses. By also addressing external economic factors, one can ultimately determine the most cost-effective strategies for both the pretreatment of hazardous wastes, and the subsequent optimal disposal as a nonhazardous waste.

7.2.4 Dominant Exposure Pathway Analysis

The exposure pathways that drive human cancer risks were also examined for the (95%, 500m, $1x10^{-6}$, 95%, $50\%)_{ABCGH}$ profile for disposal of Benzene in landfills. Shown in Figure 7-3, the sum of all inhalation pathways dominated the sum of all ingestion pathways, for all C_w's examined. At the $1x10^{-6}$ increased cancer risk level, shower inhalation of contaminated groundwater was roughly equivalent, though slightly smaller in its impact on total inhalation risk, to ambient outdoor air inhalation concerns. At a slightly lower cancer risk threshold ($5x10^{-7}$), shower inhalation risk exceeded air inhalation risk. At a slightly higher cancer risk threshold ($5x10^{-6}$), total contaminated groundwater ingestion and shower inhalation was the limiting pathway, with a C_w of 960 ppm.

Compared to specific inhalation pathways, water and crop ingestion contributed significant, but relatively smaller risks to total cancer risk from all pathways. Fish, milk, beef, and soil ingestion played relatively insignificant roles. Figure 7-3 shows, in general, the effect that different cancer risk criteria would have on determination of exit level values for Benzene disposal. For all pathways shown, a maximum value of 1000 ppm was simulated for landfills, but extrapolation beyond this level was not conducted. For values shown at 1000 ppm, the actual C_w's will be > 1000 ppm at the identified cancer risk, and > 1000 ppm at higher cancer risk thresholds.

7.3 Efficacy of the Integrated SuperMUSE Approach for 3MRA

As a result of employing the overall 3MRA Version 1.0 and Version 1.x tool set capabilities in this preliminary analysis of Benzene disposal, the following is concluded.

The SuperMUSE computing cluster offers great potential to the analyst and decision-maker for conducting extensive uncertainty and sensitivity analysis tasking involving “embarrassingly parallel” model simulations (Section 5), in both Windows or Linux environs. The supporting Java toolset developed for parallel computing represents a critical component of exploiting for capabilities of such systems. Fairly small, easy to write, and well suited for this application, the Java toolset readily handled the tasks of machine and job management over the distributed computing system. For 3MRA, added runtime costs were negligible compared to stand-alone PC execution, while the benefits delivered represented powerful, efficient model evaluation capabilities.

The toolset is generally applicable to similar evaluation efforts for other models, where only a Model Tasker, which essentially parallelizes a model user interface, would need to be developed. Alternatively, integration of any model into FRAMES 2.0 could be used as a path to apply SuperMUSE and the supporting software tools directly. As the example for Benzene disposal showed, 3MRA, together with SuperMUSE capabilities, provides a powerful, integrated, probabilistic risk assessment technology for protection of both ecological and human health, and assessment of alternative strategies for hazardous waste identification and management.

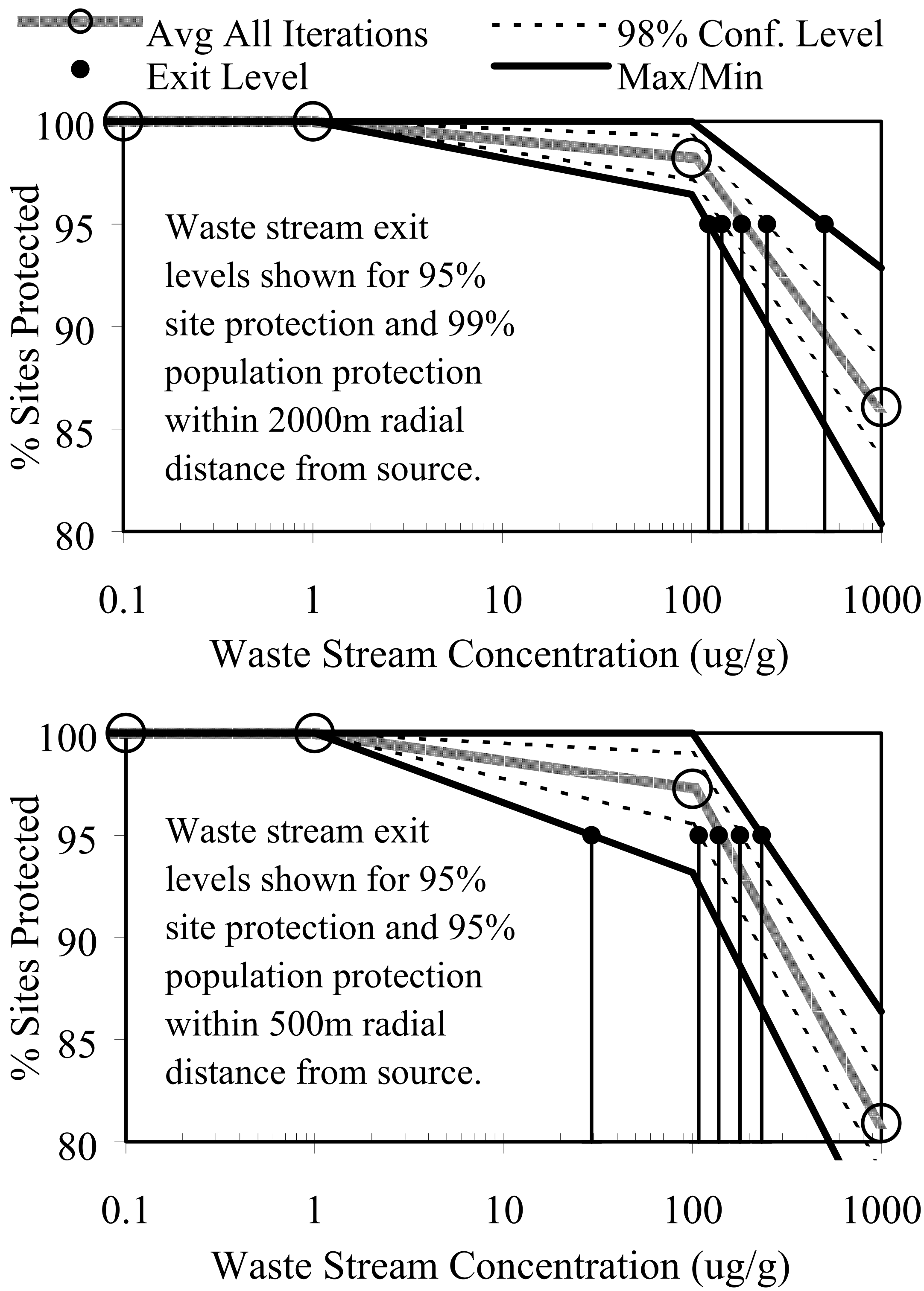

Figure 7-1. Benzene Disposal in Landfills: Uncertainty for Sum of All Ingestion and Inhalation Pathways – Pseudo 2nd Order Analysis for 50% Uncertainty (H) and 98% Associated Confidence (I) Due to OSE.
(10 Iterations at 56 Sites)

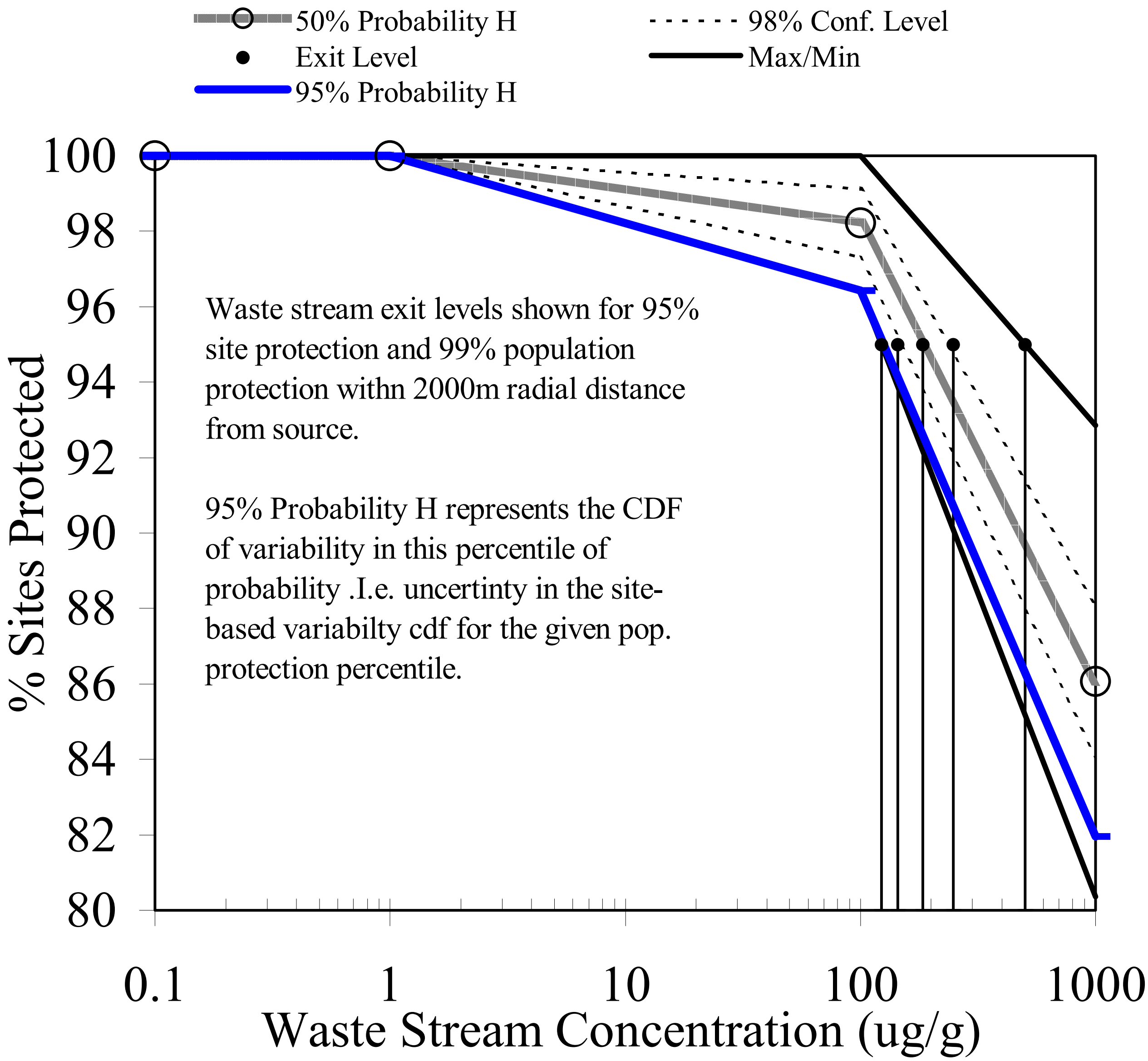

Figure 7-2. Benzene Disposal in Landfills: Uncertainty for Sum of All Ingestion and Inhalation Pathways – Pseudo 2nd Order Analysis for 50% and 95% Uncertainty (H) and 98% Associated Confidence (I) in 50% Uncertainty (H), Due to OSE.
(10 Iterations at 56 Sites)

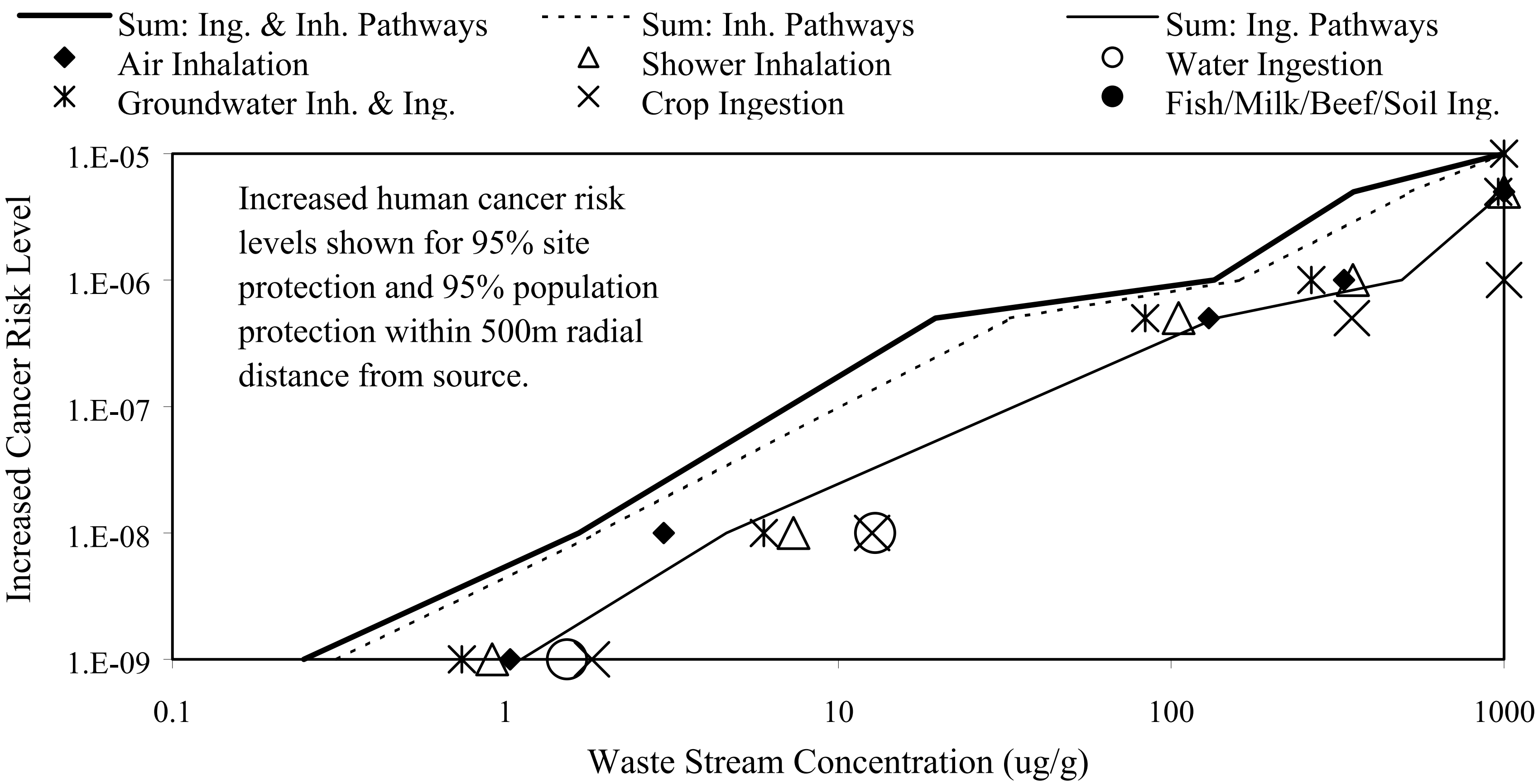

Figure 7-3. Benzene Disposal in Landfills: Exposure Pathway Analysis for Increased Human Cancer Risk.
(10 Iterations at 56 Sites)

Table 7-1. Benzene Disposal: Uncertainty Analysis for Summation of All Ingestion and Inhalation Pathways[a, b].

# Iterations Simulated at Each Site	Source Type	Surface Impoundment		Aerated Tank		Land Application Unit		Waste Pile		Landfill	
	# Sites Evaluated	137		137		28		61		56	
10	Total Simulations	6850		6850		1400		3050		2800	
	Radial Distance (m)	500[c]	2000	500[c]	2000	500[c]	2000	500[c]	2000	500[c]	2000
	% Sites Protected	95%	95%	95%	95%	95%	95%	95%	95%	95%	95%
	% Population Protected	95%	99%	95%	99%	95%	99%	95%	99%	95%	99%
	Maximum Value (ppm)	0.36	0.38	8.5	11	7.4	5.0	145	183	233	501
	Upper 98% C.L. (ppm)[d]	0.24	0.32	4.8	6.8	4.5	3.8	65	138	179	249
	Avg. Exit Level (ppm)	0.19	0.26	3.5	4.7	3.5	3.0	17	79	138	184
	Lower 98% C.L. (ppm)[d]	0.15	0.22	2.8	3.6	2.6	2.3	6.6	26	108	144
	Minimum Value (ppm)	0.12	0.18	2.4	2.6	1.4	1.4	2.1	11	29	123
100	Avg. Exit Level (ppm)	0.19	0.27	2.0	2.4	3.1	3.1	9.2	22	135	195
	Relative Difference[e]	100%	103%	55%	51%	89%	102%	54%	28%	98%	106%

[a] Scenario considered all human receptors/cohorts and an increased cancer risk of 1×10^{6}. Cancer risk was determinant for all sources. There is no applicable human hazard risk.

[b] Evaluated ecological receptors by ring and habitat groups (terrestrial, aquatic, wetland). No concerns observed for ecological hazard quotient = 1.0, for all waste concentrations considered.

[c] For ecological population concerns, radial distance was 1000 meters.

[d] C.L. indicates normal distribution confidence limit on average exit level (significance level $\alpha = 0.02$).

[e] Ratio of average waste stream exit levels calculated for 100 iterations and 10 iterations.