

## Two-Dimensional Monte Carlo Simulation and Beyond: A Comparison of Several Probabilistic Risk Assessment Methods Applied to a Superfund Site\*

Ted W. Simon

U.S. Environmental Protection Agency, Atlanta, GA\*\*

### ABSTRACT

Four different probabilistic risk assessment methods were compared using the data from the Sangamo Weston/Lake Hartwell Superfund site. These were one-dimensional Monte Carlo, two-dimensional Monte Carlo considering uncertainty in the concentration term, two-dimensional Monte Carlo considering uncertainty in ingestion rate, and microexposure event analysis. Estimated high-end risks ranged from  $2.0 \times 10^{-4}$  to  $3.3 \times 10^{-3}$ . Microexposure event analysis produced a lower risk estimate than any of the other methods due to incorporation of time-dependent changes in the concentration term.

**Key Words:** variability, uncertainty, two-dimensional Monte Carlo, microexposure event analysis, fish consumption, Superfund

### INTRODUCTION

Techniques have been developed for the separation of variability and uncertainty in Monte Carlo simulation. These techniques presently are being applied to environmental risk assessment (Burmester and Wilson, 1996; Goodrum *et al*, 1996; Hoffman and Hammonds, 1992, 1994; Price *et al*, 1996; Morgan and Henrion, 1990; USEPA, 1997a). The general goal of these various techniques is to determine the level of uncertainty associated with each of the many descriptors of risk. To date, no systematic comparison of the various

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\*\* U.S. Environmental Protection Agency, Region 4, Atlanta Federal Center, 61 Forsyth Street, SW, Atlanta, GA 30303-3104; Tel: (404) 562-8642; Fax: (404) 562-8566; E-mail: [simon.ted@epa.gov](mailto:simon.ted@epa.gov)

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methods has been attempted. This paper attempts such a comparison in terms of the details of the methods and the risk estimate each produces.

Consumption of contaminated fish was the pathway of concern at the Sangamo-Weston Superfund site in South Carolina. Compared to other Superfund sites, a large amount of site-specific data had been collected. In addition, a probabilistic risk assessment has already been presented as part of the baseline risk assessment (Bechtel, 1993).

Initially, risk estimates are developed using a deterministic approach for a reasonable maximum exposure (RME) estimate and a central tendency exposure (CTE) estimate. These estimates are compared with risk estimates at the 95th and 50th percentiles obtained from one-dimensional (1D) Monte Carlo analysis, from two-dimensional (2D) Monte Carlo analysis considering uncertainty in the concentration term, from 2D Monte Carlo analysis considering uncertainty in ingestion rate, and from microexposure event analysis.

## METHODS

### The Sangamo Weston Superfund Site

From 1955 until 1977, a capacitor manufacturing plant discharged untreated waste water into Town Creek near Pickens, South Carolina. Polychlorinated biphenyls (PCBs) migrated downstream into Twelve Mile Creek, a major tributary of Lake Hartwell. Located on the border of Georgia and South Carolina, Lake Hartwell occupies 56,000 acres and provides for public recreation, flood control, and hydropower generation. The U.S. Army Corps of Engineers impounded the lake between 1955 and 1963. Approximately 300,000 people visit the lake each year for recreation. Many of the lake visitors harvest and consume fish from the lake (Bechtel, 1993).

The PCB-contaminated sediment from the Sangamo-Weston facility was prevented from reaching the lake for a time by the dams of two small hydroelectric plants. Periodic flushing of the sediment behind the dams discharged the PCBs further downstream until approximately 730 acres of the lake bottom sediment in the Seneca River arm was contaminated. The PCBs entered the food chain and became concentrated in the fish living in Lake Hartwell. High levels of PCBs were detected in fish collected from Lake Hartwell in 1976.

### PCB Concentrations in Fish

In 1991, a large sampling effort was mounted to characterize PCB contamination in fish and other media in Lake Hartwell. PCBs were detected in fish tissue obtained from all parts of the lake. Sixty-four samples of fish tissue were obtained from the Seneca River arm. The territorial fish, such as largemouth bass, in the contaminated arm of the lake had higher concentrations of PCBs than territorial fish in the other portions of the lake. The concentrations in the migratory species, such as hybrid bass, tended to be similar in fish taken from all parts of the lake (Bechtel, 1993).

### Human Consumption of Fish from Lake Hartwell

Data from a 1992 survey by the South Carolina Wildlife and Marine Resources Department (SCWMRD) were used in the risk assessment to estimate human consumption rates of fish from Lake Hartwell. The survey obtained data from anglers regarding the number of fish meals consumed per month and the size of each meal (Bales, 1993). When anglers were in possession of fish, the lengths of the fish were measured and converted to weight using species-specific length-weight regression equations developed by SCWMRD. The dress-out percentage of the harvested fish was assumed to be 40% and the fish possessed by the anglers were assumed to be eaten in entirety at the next fish meal. Anglers were asked how many people would consume the fish and the calculated dress-out weight of the fish was assumed to be equally split among the consumers. Anglers were also questioned about their targeted fish species.

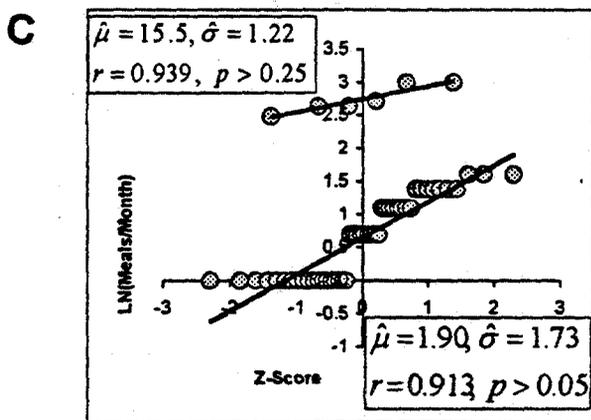
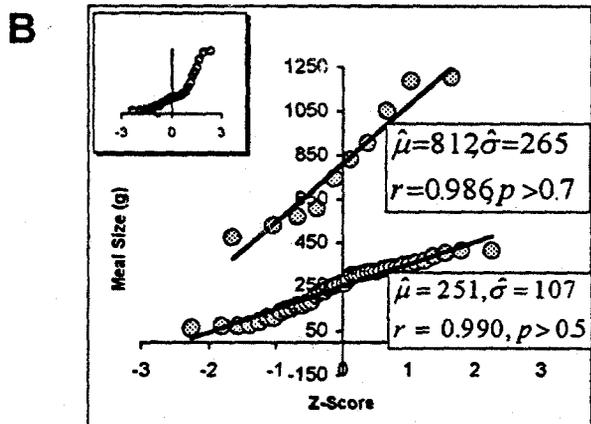
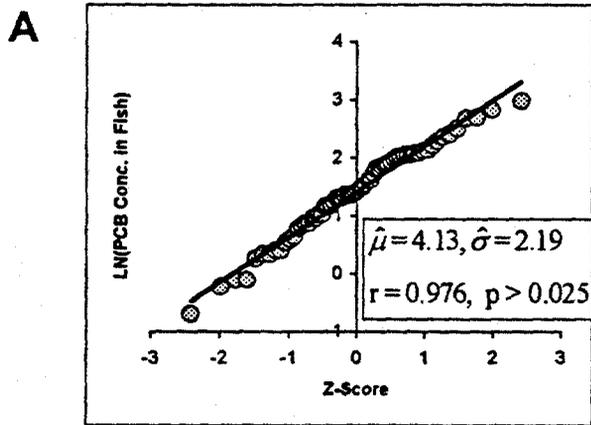
### Development of Distributions

Variability in the exposure factors was assumed to follow either a normal or a lognormal distribution. Parameters for input distributions were determined using probability plots (D'Agostino and Stevens, 1986). The probability plot correlation coefficient was used to test goodness-of-fit (Filliben, 1975). The probability plots for several exposure factors showed changes in their slopes (*e.g.*, Figure 1B). In such cases, two or more parametric distributions were used to represent the exposure factor, and a particular distribution was chosen randomly based on the proportion of that distribution in the entire sample. All data are available from the author.

The 64 samples of fish from the contaminated arm of the lake were used to determine a distribution of the concentration in fish tissue. The lognormal distribution was chosen as a candidate distribution because factors such as fish feeding rates, sediment deposition rates, bioaccumulative properties of PCBs, etc. would suggest that multiplicative processes contributed to the levels observed in fish. This choice was confirmed by the linearity of the probability plot (Figure 1A).

The long-term mean concentration of PCBs in the fish consumed will be different for each consumer and will depend on the number of fish meals and the preferred species of consumption. Data had been collected regarding the fish preferences and target species of fish consumers at the lake in addition to the frequency of fish meals. Fish preferences were determined for four groups of fish consumers — 1 meal per month, 2 meals per month, 3 to 5 meals per month, and more than 5 meals per month (Table 3). Based on these preferences, four sets of weighting factors were determined, one set for each of the four consumption groups (Table 3).

A triangular distribution with the arithmetic mean (AM) as the mode, the 5% lower confidence limit of the AM as the lower bound, and the 95% upper confidence limit of the AM as the upper bound was used to represent uncertainty in the mean PCB concentration in the fish consumed (Gilbert, 1987).



**Figure 1**  
 Probability plots to obtain parametric distributions of exposure factors. In all graphs, the values in the inset boxes indicate the GM, the GSD, the normal or lognormal correlation coefficient and the associated probability (Filliben, 1975). (A) Napierian logarithms of PCB concentrations in all fish. (B) Meal size in grams. The inset shows a break in the probability plot indicating multiple distributions. (C) Napierian logarithms of meal frequencies in meals/month.

## Two-Dimensional Monte Carlo Simulation and Beyond

The arithmetic mean represents the chronic average concentration in fish consumed.

The distribution for site-specific meal sizes was obtained from the creel survey (Figure 1B; Bales, 1993). Fish meal sizes for adults are described by two normal distributions (Table 2). Apparently, a small number of people eat large quantities of fish (>1 lb) at a sitting. Slightly less than 20% (10/52) of the population was assumed to eat large meals and their meal sizes were obtained from the higher distribution. Selection of the meal size distribution was random and followed the proportions obtained in the survey. Meal sizes were truncated at 64 and 1200 g, the minimum and maximum meal size values obtained from the creel survey. These values seemed reasonable upper and lower truncation bounds; 64 g is less than a quarter pound, and 1200 g, about 3 lbs, seems a very large meal.

The meal frequency of anglers consuming fish also occurred in two lognormal distributions. A small proportion of anglers (6/52) appeared to consume fish very frequently (~15 meals/month). The majority of the anglers (46/52) consumed fish less frequently (~2 meals/month) (Figure 1C). Selection of the exposure frequency distribution was random and followed these proportions. Meal frequencies were truncated at 0 and 31 meals/month. To obtain exposure frequency in meals per year, the number of meals per month was multiplied by 12.

Body weight was obtained from the EPA's Exposure Factors Handbook (USEPA, 1997c) as a weighted average of adult men and women, ages 20 to 65. Exposure Duration was also obtained from the Exposure Factors Handbook. The distributions used are shown in Table 2.

### Deterministic Risk Assessment

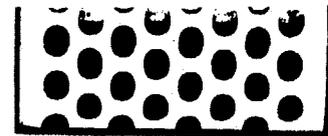
A deterministic risk assessment was performed using standard methods and exposure assumptions (USEPA, 1989; Table 1). Reasonable maximum exposure (RME) and central tendency exposure (CTE) risk estimates were obtained.

### One-Dimensional Monte Carlo

The distributions described above were used in a Monte Carlo simulation. Latin Hypercube sampling (LHS) was performed for 10,000 iterations and the results used to estimate various percentiles of risk using the standard risk equation and the cancer slope factor for PCBs (USEPA, 1989; USEPA, 1997b). The distribution used for concentration depended on the monthly meal frequency (Table 3).

Table 1. Values of variables used in the Deterministic Risk Assessment.

Variable	Symbol	RME Value	CTE Value	Source
Cancer Slope Factor	CSF	2.0 (mg/kg-day) <sup>-1</sup>	2.0 (mg/kg-day) <sup>-1</sup>	USEPA, 1997b
Concentration	C	7.0 mg/kg	7.0 mg/kg	95% UCL of the arithmetic mean of the concentration data (USEPA, 1992)
Ingestion Rate	IR <sub>Adult</sub>	357 g/meal	357 g/meal	Arithmetic mean of survey data (Bales, 1993)
Exposure Frequency	EF	46 meals/year	46 meals/year	Arithmetic mean of survey data (Bales, 1993); the survey presented the data in meals/month; the value here is the result of multiplying by 12 to obtain meals/year
Exposure Duration	ED <sub>Adult</sub>	30 year	9 year	Default value (USEPA, 1989, 1998)
Body Weight	BW <sub>Adult</sub>	70 kg	70 kg	Default value (USEPA, 1989, 1998)
Averaging Time	AT	25550 days	25550 days	Default value (USEPA, 1989, 1998)



**Table 2. Distributions of exposure factors used in the one-dimensional Monte Carlo simulation.**

Parameter	Units	Distribution	Mean or preferred		Minimum	Maximum	Source	
			value	Standard deviation				
Concentration in fish	mg/kg	Triangular	See Table 3 for values				Site-specific	
Ingestion rate	g/meal	Normal	(42/52)	251	107	64	1200	State report Bales, 1993
			(10/52)	812	265			
Exposure frequency	Meals/mo	Lognormal	(46/52)	1.90	1.73	0	31	State report Bales, 1993
			(6/52)	15.5	1.22			
Exposure duration	Years	Lognormal	4.4	2.9	1	70	USEPA, 1998	
Body Weight	kg	Normal	78.1	14.05	30	150	USEPA, 1998	

*Notes:* For Lognormal distributions, values given are the geometric mean and geometric standard deviation.

**Table 3. Weighting factors and triangular distribution parameters for uncertainty around PCB concentration in fish tissue.**

Fish species	5% LCL	Arithmetic mean	95% UCL	Weighting factors for concentration by meals per month			
				1	2	3-5	>5
All species	4.76	5.64	6.91	0.210	0.222	0.222	0.333
Largemouth Bass	5.77	6.86	8.52	0.474	0.444	0.500	0.167
Hybrid Bass	1.07	1.39	1.98	0	0.111	0.167	0
Catfish	4.45	5.66	7.85	0.316	0.111	0.111	0.5
Bluegill	2.70	3.41	4.86	0	0.111	0	0

Parameters of the weighted distributions			
Meals/month	5% LCL	Arithmetic mean	95% UCL
1	5.14	6.23	7.97
2	4.53	5.46	6.95
3-5	4.61	5.55	7.00
>5	3.73	5.12	7.88

#### Two-Dimensional Monte Carlo Simulation to Assess Uncertainty in Concentration

First, the concentration term was separated from the risk equation as follows:

$$\text{Risk} = \text{CSF} \cdot \left( \frac{\text{IR} \cdot \text{EF} \cdot \text{ED} \cdot 12 \frac{\text{months}}{\text{year}} \cdot 10^{-3} \frac{\text{kg}}{\text{g}}}{\text{BW} \cdot \text{AT}} \right) \cdot C \quad (1)$$

where IR = Ingestion Rate or Meal Size (g/meal)  
 EF = Exposure Frequency (meals/month)  
 ED = Exposure Duration (years)  
 BW = Body Weight (kg)  
 AT = Averaging Time (days)  
 C = Concentration (mg/kg)  
 CSF = Cancer Slope Factor (mg/kg-day)<sup>-1</sup>

## Two-Dimensional Monte Carlo Simulation and Beyond

LHS sampling was used to obtain a distribution of 1000 intake factors consisting of all exposure factors except concentration. Each of these 1000 intake factors represents the physiological parameters and fish consumption practices of an hypothetical receptor. The total number of meals for each hypothetical receptor was determined as the product of the exposure duration and the exposure frequency. Although the data were not collected in the creel survey, it was assumed that ingestion rate was correlated with body weight with a correlation coefficient of 0.65.

As previously mentioned, each hypothetical receptor was assumed to receive the average concentration in fish tissue over the long term. However, that average value was slightly different for each hypothetical receptor based on fish preferences and the total number of fish meals consumed. To estimate the uncertainty around the average concentration, a bootstrap procedure was used. The size of each bootstrap iteration was the total number of fish meals for that particular receptor. Weighting factors (Table 3) were used to select the species distribution from which an individual bootstrap datum was obtained. For each receptor, 500 bootstrap iterations were used to estimate the arithmetic mean, the 5% lower confidence limit of the mean and the 95% upper confidence limit of the mean for each receptor. These three values served to determine a triangular distribution for that particular receptor.

Variability in risk was determined by multiplying each of the 1000 intake factors by the corresponding arithmetic mean concentration for that particular hypothetical receptor. Uncertainty around this estimate of variability was determined first by multiplying each intake factor by 1000 values obtained by simple random sampling from the triangular distribution for concentration and second by multiplying each of these products by the cancer slope factor for PCBs.

### Two-Dimensional Monte Carlo Simulation to Assess Uncertainty in Ingestion Rate

Ingestion rate was considered as a fish consumption rate in g/day and was separated from the risk equation as follows:

$$\text{Risk} = \text{CSF} \cdot \left( \frac{C \cdot \text{ED} \cdot 10^{-3} \frac{\text{kg}}{\text{g}} \cdot 365 \frac{\text{days}}{\text{year}}}{\text{BW} \cdot \text{AT}} \right) \cdot \text{FCR} \quad (2)$$

where FCR = Fish Consumption Rate (g/day)  
ED = Exposure Duration (years)  
BW = Body Weight (kg)  
AT = Averaging Time (days)  
C = Concentration (mg/kg)  
CSF = Cancer Slope Factor (mg/kg-day)<sup>-1</sup>

Exposure frequency does not appear as a variable in this equation. Exposure frequency is embedded in the expression used for ingestion rate (Eq. 3).

A distribution of fish consumption rates in g/day was determined from the 52 lake-wide data in the creel survey using the following equation and the distributions given in Table 2:

$$\text{FCR g / day} = \frac{\text{IR g / meal} \cdot \text{EF meals / mo} \cdot 12 \text{ mo / year}}{365 \text{ days / year}} \quad (3)$$

The uncertainty in consumption rate was modeled using bounding estimates as a triangular distribution at each percentile of the fish consumption rate. The lower bound of the triangular distribution was obtained from national data on fish consumers in the southeast (Ruffle *et al.*, 1994). The upper bound was obtained from the Columbia River Native American subsistence fishing study (CRITFC, 1994). The mode was the fish consumption rate from the Lake Hartwell data (Figure 2).

The distribution for the concentration term was the same as that used in the one-dimensional Monte Carlo assessment, one of four triangular distributions determined by the number of meals per month that particular receptor consumed (Table 3).

LHS sampling was used to obtain a distribution of 1000 intake factors consisting of all exposure factors except ingestion rate. Each of these 1000 intake factors represents the physiological parameters and chronic average exposure concentration of an hypothetical receptor. One thousand random percentiles representing ingestion rate were obtained from the Uniform(0,1) distribution to correspond to each intake factor. These ingestion rate percentiles were correlated with body weight with a correlation coefficient of 0.65. To obtain a distribution of variability of risks, each intake factor was multiplied by the value from the FCR distribution from Lake Hartwell corresponding to the ingestion rate percentile and the cancer slope factor for PCBs.

The uncertainty around each of the risk values in this distribution was determined by multiplying the product of each intake factor and the cancer slope factor for PCBs by 1000 random values from the triangular distribution specified by the ingestion rate percentile. This multiplication yielded 1000 distributions of risk, each of which represented uncertainty around a specific risk value.

#### Microexposure Event Analysis

Microexposure event analysis (MEE) evaluates a receptor's long-term dose as the sum of individual exposure events (Price *et al.*, 1996). MEE permits modeling of time-dependent changes in exposure factors. The exposure duration is broken into a series of epochs to accommodate these time-dependent changes. Time steps of different sizes may be used with different exposure factors. The randomly selected value of each time-dependent exposure factor

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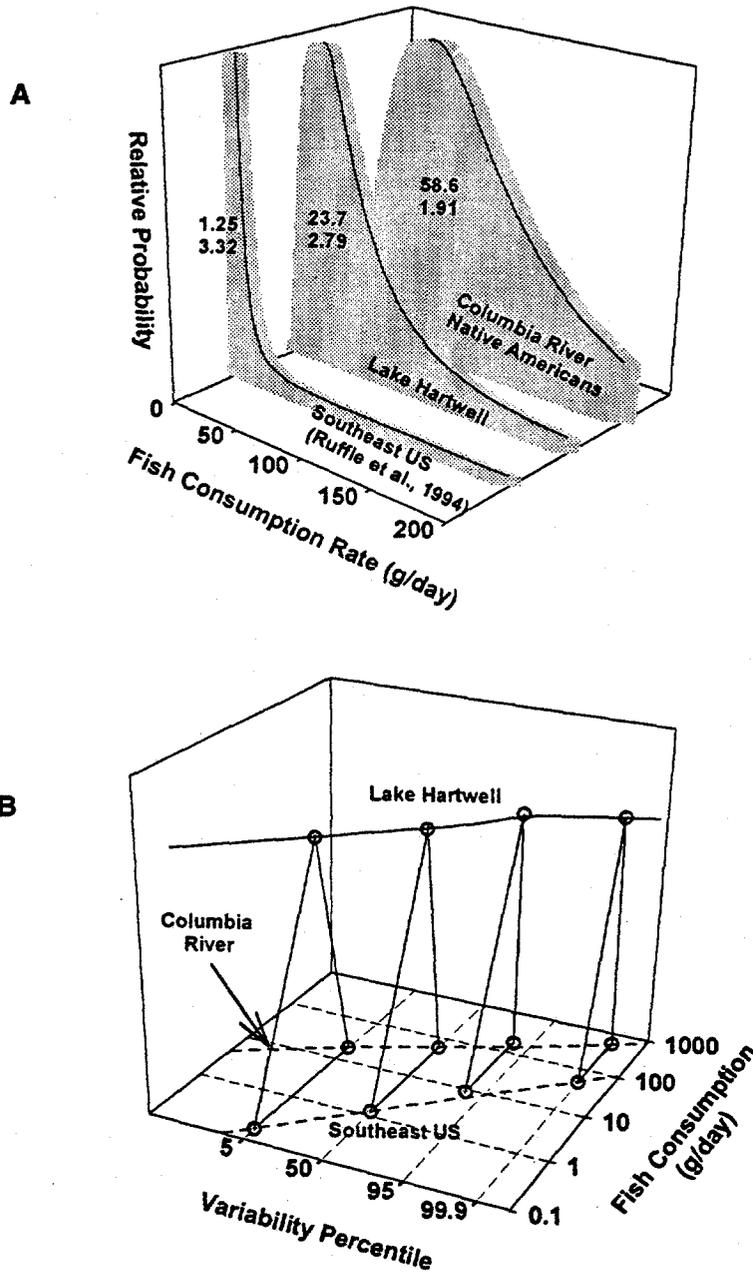


Figure 2. Variability and uncertainty in fish consumption rate. (A) Comparison of the distribution of Fish Consumption Rates at Lake Hartwell with the two distributions used as uncertainty bounds. The numbers shown with each distribution indicate the GM and GSD. (B) Triangular distributions showing uncertainty at selected percentiles of variability.

Table 4. Sensitivity Analysis for the Various Risk Assessment Methods

Exposure Factor	1D MC	2D Conc	2D IR	MEE
Exposure duration (ED)	0.7044	0.6323	0.6644	0.1456
Exposure frequency (EF)	0.4833	0.5269	0.5410	0.6357
Ingestion rate (IR)	0.3746	0.4331	0.3917	0.4926
Fish consumption rate (FCR)			0.6847	
Concentration	-0.1094	0.3321 (lower) 0.0754 (pref) -0.5744 (upper)	-0.1663	0.3997
Body weight	-0.1298	-0.1296	0.0372	-0.0450

represents the average value within that epoch. Two-dimensional analysis separating variability and uncertainty can also be incorporated into MEE.

The time-independent exposure factors were gender, age at the start of the simulation, and body weight percentile. These were chosen for each receptor at the beginning of an iteration. Time-dependent factors were exposure frequency, concentration, actual body weight and meal size. These changed throughout the simulated receptor's life by choosing different values for each epoch. Children below the age of 7 were assumed not to eat fish. Late childhood and adolescence (years 7 to 18) were considered a single epoch. Young adulthood (19 to 25) was another epoch. From age 25 on, the epochs were 5 years in length.

For each epoch, intake of PCBs was determined by summing the amounts consumed at each fish meal. Average body weight for that time period was chosen at random from a uniform distribution with limits 3% above and below the body weight during the previous epoch. The fluctuations were bounded by values 3 standard deviations from the mean for each epoch (Table 5). This procedure simulated normal fluctuations in weight. The selected body weight for the particular epoch was used to determine the dose for that epoch in mg/kg.

One feature of MEE distinct from the other risk assessment methods was the ability to model decreasing concentrations in fish tissue. EPA's Water Quality Analysis Simulation Program (WASP4) models time-dependent changes in chemical concentrations in water and sediment (Schnoor *et al.*, 1987). The Food and Gill Exchange of Toxic Substances program (FGETS) models uptake of chemicals into fish tissue (USEPA, 1991). WASP4 was used in conjunction with FGETS to predict concentrations of PCBs in fish tissue over time as

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part of the Sangamo-Weston Baseline Risk Assessment. The results of these simulations suggested that PCB levels in fish would increase within the first 3 years and then decline to negligible levels by 20 years (Bechtel, 1993; Figure 3A).

PCBs are a mixture of different congeners. Each congener may have a different environmental fate depending on circumstances. The mechanism of decreasing concentrations in fish tissue assumed both in the original risk assessment and here was decreased availability due to sediment deposition. The modeling efforts in the original risk assessment shows that clean sediment from upstream would cover the contaminated sediment on the bottom of the lake. In time, the contaminated sediment would not be available for contact by benthic macroinvertebrates and would not be transmitted to fish via the food chain.

The concentration-time profile was fit with an empirical equation originally used to describe chemical kinetics in excitable cells (Beeler and Reuter, 1977). This equation duplicates the modeling results from the Baseline Risk Assessment without representing the mechanism of decreasing concentration. The GM, the 10th percentile and the 90th percentile were fit for all times up to 30 years using the Marquardt-Levenberg algorithm (Figure 3A). The general form of this equation is

$$\text{Concentration} = \frac{Ae^{B(t+C)} + D(t+E)}{e^{F(t+C)} + F} \quad (4)$$

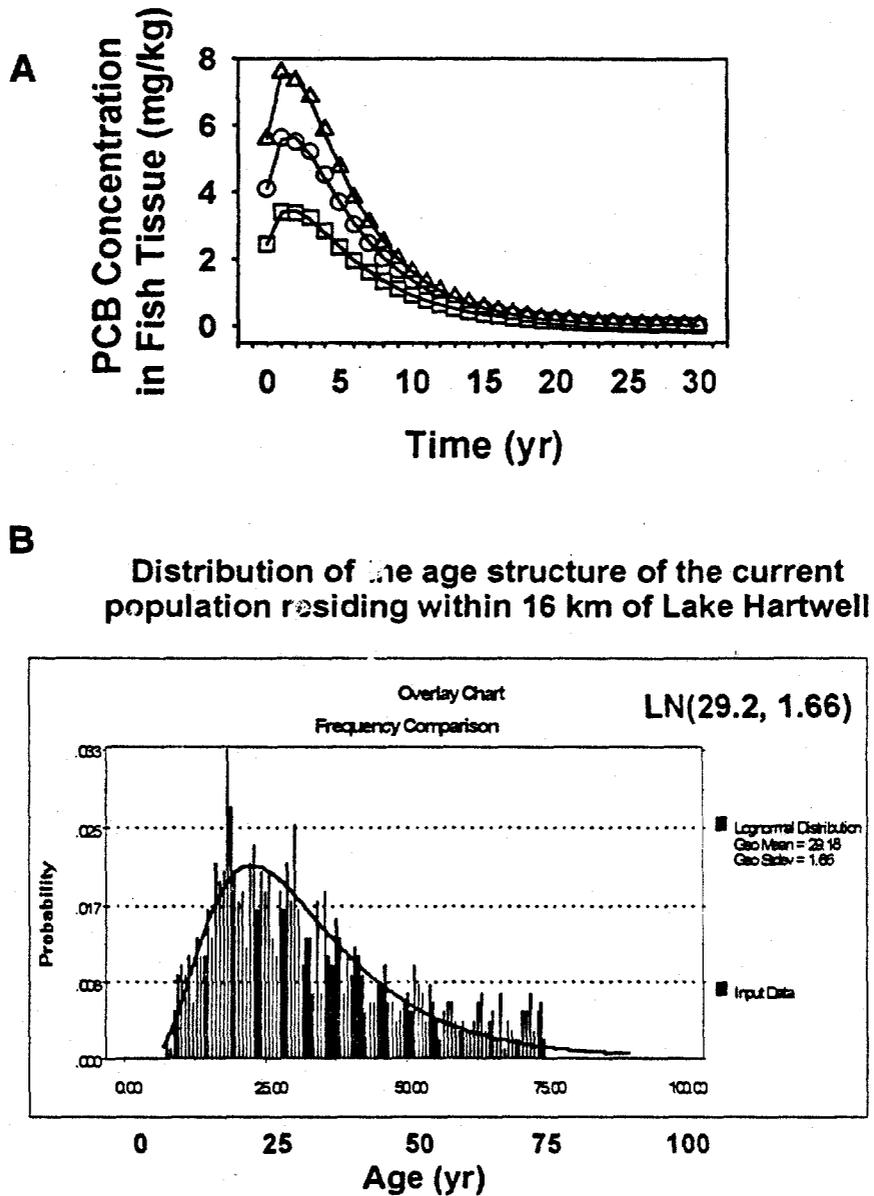
where  $t$  = time

$e$  = 2.7182... base of Napierian logarithms

A, B, C, D, E and F are constants

Variability in concentration at all times was described by a lognormal distribution during each epoch. The randomly selected value for concentration represents the average value for concentration during that epoch. Uncertainty in concentration was not considered quantitatively because the uncertainty regarding concentration is relatively low (e.g., Figure 4B).

At the end of each epoch, the question was asked whether that hypothetical receptor moved away or died and, hence, ceased to consume fish. Probabilities of moving away were determined from value for average total residence time (Table 14-154 in USEPA, 1997c) by a reverse cumulative distribution plot. The distribution of the age structure of the population (Figure 3B) was modeled as a mixture of uniform distributions of ages weighted by the proportion of that age group in the population (Table 4). Probabilities of dying were obtained from the reverse cumulative plot of the age structure of the population (Figure 3B). At the end of each epoch, exposure duration was determined by adding the previous residence tenure to the current duration of the iteration.



**Figure 3.** Parameters for MEE. (A) Change in PCB concentrations in fish tissue with time. The upper curve (triangles) shows the 90th percentile of concentration. The middle curve (circles) shows the geometric mean. The lower curve (squares) shows the 10th percentile. (B) Age structure of the population around Lake Hartwell.

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Doses for each time period in mg/kg were summed to obtain a lifetime total dose. This lifetime total dose was divided by 25550 days (70 years expressed in days) to obtain the lifetime average daily dose (LADD). The LADD was multiplied by the cancer slope factor for PCBs — 2.0 per (mg/kg-day) to obtain a value for lifetime cancer risk for the possible outcome.

Exposure frequency and meal size were treated as uncertainties during the simulation. For each of the 1000 receptors, represented by each set of time-independent factors, 250 simulations of various combinations exposure frequency and meal size were performed for each epoch in the exposure duration.

### Computational Methods

All of the simulations were performed with *Crystal Ball Pro* v. 4.0e (Decisioneering, Inc.) and *Excel 97* (Microsoft). All simulations were repeated 20 times with different random number seeds. The precision of all 20 estimates of the 95th percentile of risk (50th percentile uncertainty) were within 3% of each other. A representative run was chosen for inclusion here. For each probabilistic method, the 50th and 95th percentiles of risk are shown (Figure 4). These percentiles represent the CTE and RME risk estimates, respectively (Simon, 1998; USEPA, 1999). Spreadsheet programming with Microsoft *Visual Basic for Applications* (VBA) was used as needed. All spreadsheets and data are available from the author. Sensitivity analysis was performed using the Spearman Rank Correlation Coefficient performed with *Crystal Ball* or *Statistica* software (StatSoft, Inc.)

## RESULTS

### Deterministic RME Risk Assessment for Fish Consumption

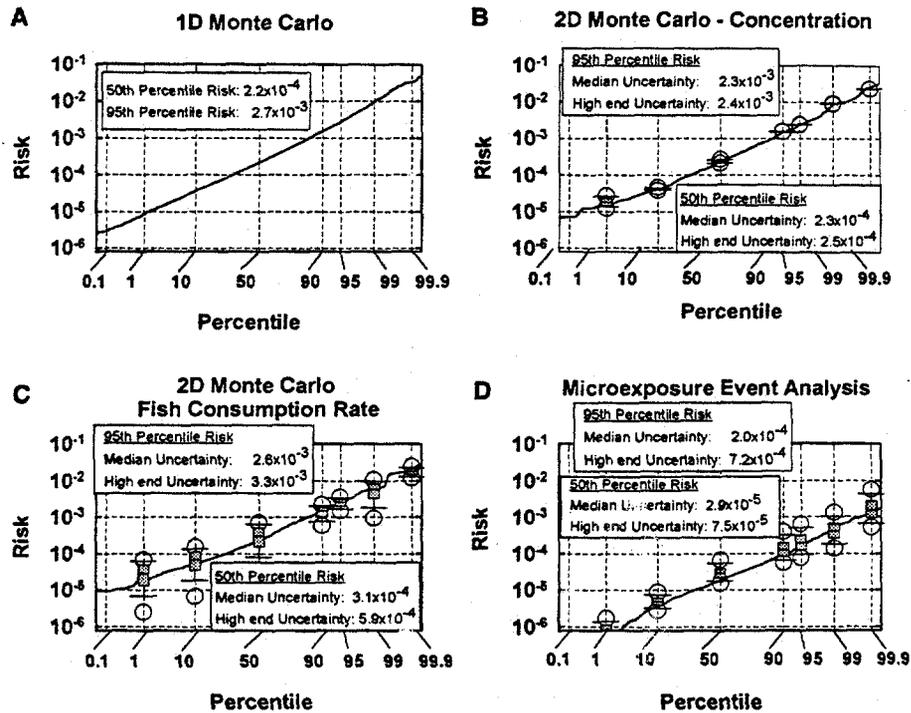
The values used in the standard risk equation (USEPA, 1989) are given in Table 1. The RME excess lifetime cancer risk thus calculated was  $3.9 \times 10^{-3}$ . Exposure Duration (ED) is the only factor that would change when using CTE assumptions because in the RME scenario, concentration, exposure frequency, and meal size are central values (USEPA, 1989; USEPA, 1992; Table 1). The ED would change to 9 years and the excess lifetime cancer risk estimated using CTE values was  $1.2 \times 10^{-3}$ .

### One-Dimensional Monte Carlo Simulation

The 95th percentile of the distribution of risks from the 1D Monte Carlo simulation was  $2.7 \times 10^{-3}$  and the 50th percentile was  $2.2 \times 10^{-4}$  (Figure 2A). Sensitivity analysis indicated the three most influential exposure factors were exposure duration, exposure frequency, and ingestion rate (Table 4).

### Two-Dimensional Monte Carlo Simulation to Assess Uncertainty in Concentration

The uncertainty at 95th percentile of variability in risk ranged from  $2.3 \times 10^{-3}$  at the 5th percentile to  $2.4 \times 10^{-3}$  at the 95th percentile. The



**Figure 4.** Results of the four risk assessment methods. The line plots of risk vs. probability show variability in risk. The box plots show uncertainty at selected percentiles. (A) 1D Monte Carlo Simulation. (B) 2D Monte Carlo Simulation considering uncertainty in concentration. (C) 2D Monte Carlo Simulation considering uncertainty in fish consumption rate. (D) Microexposure event analysis.

uncertainty at the 50th percentile of variability in risk ranged from  $2.1 \times 10^{-4}$  at the 5th percentile to  $2.5 \times 10^{-4}$  at the 95th percentile (Figure 2B). Sensitivity analysis indicated the three most influential exposure factors were exposure duration, exposure frequency, and meal size (Table 4).

#### Two-Dimensional Monte Carlo Simulation to Assess Uncertainty in Ingestion Rate

The uncertainty at the 95th percentile of variability in risk ranged from  $1.8 \times 10^{-3}$  at the 5th percentile to  $3.3 \times 10^{-3}$  at the 95th percentile. The uncertainty at the 50th percentile of variability in risk ranged from  $1.1 \times 10^{-4}$  at the 5th percentile to  $5.9 \times 10^{-4}$  at the 95th percentile. Sensitivity analysis indicated the three most influential exposure factors were exposure duration, exposure frequency, and meal size (Table 4). The latter two factors were expressed implicitly the fish consumption rate (Eq. 3).

**Table 5. Age-specific parameters for the Microexposure Event Analysis.**

Ages	Percent of local population	Body weight (kg) (mean $\pm$ SD)	Upper limit of ingestion rate (g/meal)
0-6	5	14.4 $\pm$ 2.35	150
7-18	16	50.2 $\pm$ 11.6	500
18-25	30	73.7 $\pm$ 12.7	1200
25-35	26	78.7 $\pm$ 13.7	1200
35-45	12	80.8 $\pm$ 13.4	1200
45-55	10	81.0 $\pm$ 13.6	1200
55-65	8	78.8 $\pm$ 12.8	1000
65-75	7	74.8 $\pm$ 12.8	800

#### Microexposure Event Analysis

The uncertainty at the 95<sup>th</sup> percentile of variability in risk ranged from  $6.1 \times 10^{-5}$  at the 5<sup>th</sup> percentile to  $7.2 \times 10^{-4}$  at the 95<sup>th</sup> percentile. The uncertainty at the 50<sup>th</sup> percentile of variability in risk ranged from  $1.2 \times 10^{-5}$  at the 5<sup>th</sup> percentile to  $7.5 \times 10^{-5}$  at the 95<sup>th</sup> percentile. Sensitivity analysis at both the 50<sup>th</sup> and 95<sup>th</sup> percentiles of variability indicated that exposure frequency, meal size, and concentration were the three most influential exposure factors.

#### Sensitivity Analysis

The results of sensitivity analysis on all four risk assessment methods are compared in Table 4. The 1D simulation and both 2D simulations had similar results, indicating that exposure duration was the most influential parameter. In the MEE, exposure frequency was the most influential parameter. Concentration was relatively unimportant in the first three methods but more influential in MEE.

## DISCUSSION

#### Comparison of Risk Estimates from the Various Methods

The deterministic risk estimates and those from the 1D and 2D methods essentially were similar. The risk estimates from MEE were approximately an order of magnitude lower.

MEE is the only risk assessment methodology that incorporated changes in the concentration term. Concentration decreased almost throughout the

exposure duration (Figure 3A). In addition, exposure duration was calculated differently and its distribution was different in MEE than the other methods. The distribution used for exposure duration was LN(4.4, 2.90) for the 1D and both 2D simulations. However, for MEE the distribution of ED was LN(8.7, 2.27) obtained from a probability plot of the results. Hence, the decrease in concentration had a greater influence on the risk estimate from MEE than the increase in exposure duration.

Generally, one would expect the Spearman rank correlation coefficient for body weight to be negative because body weight appears in the denominator of the risk equation (Table 4; Eq. 1 and 2). However, in the 2D Monte Carlo considering uncertainty in fish consumption rate, the rank correlation coefficient for body weight was positive. Meal size values that were incorporated into the fish consumption rate were generated at the same time as body weight. In all simulations, the correlation between body weight and meal size was assumed to be 0.65. The effect of incorporating meal size into a daily fish consumption rate changes the influence of body weight on the risk estimate.

#### **Definition of Reasonable Maximum Exposure for Probabilistic Risk Assessment**

The 1992 Office of Research and Development Guidelines for Exposure Assessment (USEPA, 1992) states that the "high end" of exposure for a population occurs between the 90th and 99.9th percentiles, with the 99.9th percentile considered a bounding estimate. Superfund guidance on probabilistic risk assessment is being developed by EPA and suggests that the 50th percentile of risk should be considered a CTE estimate, and the 95th percentile of risk may be considered an RME estimate (Simon, 1998; USEPA, 1999). Hence, the same percentiles were chosen in this study.

#### **Degree of Uncertainty in Concentration and Ingestion Rate**

Greater uncertainty is present in the ingestion rate than concentration. Because of the bootstrap procedure used to obtain distributions for uncertainty in concentration, the concentration term for high fish consumers involved averaging a large number of fish meals. Hence, a large value for concentration at any given meal would tend to be "averaged" in with a large number of meals at lower concentrations. Hence, high values for concentration had a greater influence for low fish consumers (Table 3).

The distribution for the fish consumption rate for anglers at Lake Hartwell was LN(23.7, 2.79) g/day. This distribution is probably too high to be representative. The recreational angler survey interviewed predominantly adult males between 20 and 65 years, and, hence, may not be representative of adult females or children. Fifty-two survey results were available lake-wide and were used to represent the ingestion rate of anglers harvesting fish from the Seneca River arm. The study claimed that one participant ate fish meals of 1200 g —

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almost 3 lbs! Possibly the length-weight regression equations used were incorrect or the dress-out percentage of 40% was too high (Bales, 1993).

EPA's Exposure Factors Handbook suggests a fish consumption rate of 25 g/day to be used as the RME point estimate and 8 g/day to be used as the CTE point estimate (USEPA, 1997). A recent study of two low-income fish populations in the South recommended LN (20.4, 2.25) as a distribution of fish consumption rates for high fish consumers (Simon, 1999). Both the EPA recommended values and the distribution for high fish consumers indicate lower FCRs than observed at Lake Hartwell.

### Is the Degree of Complexity Appropriate?

The methodology of the various simulations included in this study is, of course, critical to their results. Probabilistic risk assessment is often viewed by regulators with scorn and suspicion. Regulators reviewing these risk assessments should insist on a clear presentation of both the methods and results. Those submitting probabilistic risk assessments to regulatory agencies must realize that providing the input distributions, details of the simulations and appropriate software is critical for acceptance by regulators. Advanced techniques in probabilistic risk assessment are necessarily complex but provide a potentially truer view of risks. This view is limited only by the representativeness of the data supporting the input distributions and the creativity and meticulousness of the risk analyst. If the details are presented clearly, the reasons for obtaining different results from different methods should be apparent.

### CONCLUSIONS

The 1D Monte Carlo method, the 2D Monte Carlo method considering concentration, and the 2D Monte Carlo method considering fish consumption rate yields results similar to the deterministic risk assessment. Microexposure event analysis gave a risk estimate approximately an order of magnitude less. This decrease is due to the incorporation of a concentration term that decreases with time.

Many of the procedures described in this paper are complex and combining them in a risk assessment leads to even greater complexity. Nonetheless, the key idea of this paper echoes the mandate of the 1995 Risk Characterization memorandum (USEPA, 1995). This key idea is the need for clarity and transparency.

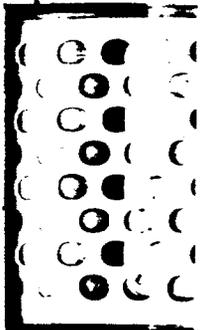
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