A STUDY TO ASSESS THE IMPACTS OF FRACTURED MEDIA IN MONTE-CARLO SIMULATIONS

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Acknowledgments

A number of individuals have been involved with this development. Dr. Zubair A. Saleem of the U.S.EPA, Office of Solid Waste, provided overall technical coordination and review throughout this work. The information on degrees of fracturing, and corresponding factors for modifying the hydraulic conductivity of the background non-fractured aquifers was provided by Dr. Steve Schmelling of the National Risk Management Research Laboratory, and Drs. Sang B. Lee and Jin-Song Chen of Dynamac Corporation. This report was prepared by Mr. Theodore Lillys of HydroGeoLogic, Inc..

1.0 INTRODUCTION

This report summarizes the completion of enhancements of the EPA's Composite Model for leachate migration with Transformation Products (EPACMTP) code (US EPA, 1996) to incorporate the presence of fractures at some sites in the Subtitle-D landfill database. A similar methodology has been incorporated into the HWIR99 Aquifer Module (U.S.EPA, 1999).

Results of preliminary analyses are presented to assist in assessing the impact of fractures on HWIR Monte-Carlo simulations.

2.0 BACKGROUND

2.1 EPACMTP

The EPA's Composite Model for leachate migration with Transformation Products (EPACMTP) code, is used by EPA Office of Solid Waste (OSW) to simulate the fate and transport of contaminants leaching from a land-based waste management unit through the underlying unsaturated and saturated zones. EPACMTP replaces EPACML as the best available tool to predict potential exposure at a downstream receptor well. EPACMTP offers improvements to EPACML by considering: 1) the formation and transport of transformation products; 2) the impact of groundwater mounding on groundwater velocity; 3) finite source as well as continuous source scenarios; and 4) metals transport.

Fate and transport processes simulated by the model include: advection, hydrodynamic dispersion, linear or nonlinear sorption, and chain-decay reactions. In cases where degradation of a waste constituent yields daughter products that are of concern, EPACMTP accounts for the formation and transport of up to six different daughter products. The composite model consists of a one-dimensional module that simulates infiltration and dissolved constituent transport through the unsaturated zone, which is coupled with a three-dimensional saturated zone module. The saturated zone module consists of a three-dimensional groundwater flow and a three-dimensional transport sub-module. The saturated zone groundwater flow sub-module accounts for the effects of leakage from the land disposal unit and regional recharge on the magnitude and direction of groundwater flow. The saturated zone transport sub-module accounts for three-dimensional advection and dispersion, chain decay reactions with up to seven different chemical species (i.e., parent with up to six daughter products), and linear or nonlinear equilibrium sorption.

2.2 HWIR99 AQUIFER MODULE

The aquifer simulation portion of the EPACMTP code has been extracted and modified to function as a stand-alone module. Included in this module is a new pseudo-three-dimensional submodule developed for HWIR99. The methodology described in Section 3 to include the effects due to fractures has been incorporated into the module. Details of the module are presented in US EPA, 1999).

3.0 ENHANCEMENT OF THE EPACMTP TO INCLUDE FRACTURE IMPACT ANALYSIS

In conjunction with a review by the Dynamac Corp. (U.S.EPA, 1998) for US EPAOSW, modifications to the OSW landfill database to account for the presence of fractured rock at sites listed in the database are to be incorporated into the EPACMTP to assess impacts of HWIR on ground-water pathways.

Using information from the Aquifer Vulnerability Report (US EPA, 1991) and the OSW data for landfills

(US EPA, 1986), Dynamac Corp. (US EPA, 1998) identified 126 out of 784 sites in the database that are situated in or bordering regions having "shallow permeable units which are highly vulnerable to contamination" (US EPA, 1998). Specifically, these units are classified as follows:

Soluble and Fractured Bedrock Aquifers – Class Ib;
Variably Covered Soluble and Fractured Bedrock Aquifers – Class Ibv; and
Units Bordering Soluble and Fractured Bedrock Aquifers – Class Ib*.

Each of the 126 sites was designated as belonging to one of the three classes. For the purpose of implementation, a multiplicative factor corresponding to one of the above classes is applied to the value of site's hydraulic conductivity to reflect the impact of fractures on contaminant transport at that site.

3.1 ENHANCEMENT IMPLEMENTATION

Implementation of a fracture multiplier within a Monte Carlo framework required the following modifications of the EPACMTP code and associated database files:

1) modification of OSW Subtitle-D landfill database to reflect membership in a particular fracture class;

2) modification of the input data file to control the application of the fracture multiplier;

3) modification of the EPACMTP code to read and interpret the above changes; and,

4) modification of the EPACMTP code to generate and apply a probabilistic hydraulic conductivity fracture multiplier.

3.1.1 Database Modifications

A fracture classification identifier is appended to each site record in the "LFSITE.DAT" input file for each of the 784 landfill sites. The parameter is read in I5 format from columns 60-65. Corresponding fracture identifiers and fracture classes are presented in Table 3.1.

Table 3.1 Fracture Identifiers used in Landfill Database

Fracture Identifier	Fracture Class
0	Not Fractured
1	Ib
2	Ib*
3	Ibv

3.1.2 Input File Modifications

Fracture Impact Analysis is allowed only if a landfill site is selected as the waste source (i.e., ISRC_TYP = 0 in General Parameter Record No. GP01 of the main input file). The following changes have been made to the input file to implement fracture analysis.

A new logical variable, FRACTURE, is read from General Parameter Record No. GP02 (columns 60-65) of the main input file. If FRACTURE is set equal to F(alse), then fracture multipliers are not applied. If FRACTURE is set equal to T(rue), only those sites with fracture identifiers greater than zero will have their hydraulic conductivity values scaled by a fracture multiplier selected from a distribution. Note that the default value of FRACTURE is F(alse). Also, FRACTURE is automatically set to F(alse) if ISRC_TYP ≠ 0.

3.1.3 Multiplier Determination

In accordance with the Monte Carlo analysis framework used in EPACMTP, uncertainty shall be incorporated into the selection of an arithmetic fracture multiplier via a logarithmic triangular probability density function (pdf) defined by data provided by Dynamac Corp. (US EPA, 1998). Two data sets were provide for testing, an initial version, referred to as Category I, and an updated version, Category II. The fracture classes Ib* and Ibv are combined into one class to reflect their similarity of impact on the ambient conductivity field. The distribution parameters are presented in the table below.

Table 3.2 Proposed Hydraulic Conductivity Multipliers

	Class Ib			Class Ib* or Ibv		
	Min	**Med**	**Max**	**Min**	**Med**	**Max**
Initial Proposed Multipliers Category I	1	10	100	1	5	50
Updated Proposed Multipliers Category II	14.8	125.9	1071.5	7.4	63	535.8

As mentioned above, the probability distribution is assumed to be triangular in log space. Given A ≤ x ≤ B, the value of the cumulative distribution function (cdf), *F(x)*, of a triangular pdf is defined as

$$F(x|A \le x \le M) = \frac{(x-A)^2}{(M-A)(B-A)} \quad \textbf{(3.1)}$$

$$F(x|B \ge x \ge M) = 1 - \frac{\left[1-\frac{x-A}{B-A}\right]^2}{1-\frac{M-A}{B-A}} \quad \textbf{(3.2)}$$

where: M is the median value of the distribution,

A is the minimum value of the distribution, and

B is the maximum value of the distribution.

Within the Monte-Carlo framework, a multiplier is determined by first generating a random value from the cdf, *F(x)*, assuming that

$$F(x) \in U[0,1]. \qquad \textbf{(3.3)}$$

Rewriting Equations 3.1 and 3.2 such that *F(x)* is the independent variable, a log space multiplier, *x*, can be determined given *F(x)*, A, M, and B, provided that A ≤ M ≤ B

$$x = A + \sqrt{F(x)(M-A)(B-A)}, \quad \forall\ x \le M \qquad \textbf{(3.4)}$$

$$x = A + (B-A)\left[1 - \sqrt{(1-F(x))\left(1 - \frac{M-A}{B-A}\right)}\right], \quad \forall\ x \ge M \qquad \textbf{(3.5)}$$

In this application,

$$\begin{aligned} A &= \log_{10}(Min) \\ M &= \log_{10}(Med) \\ B &= \log_{10}(Max) \end{aligned} \qquad \textbf{(3.6)}$$

where Min, Med, and Max represent values from columns in Table 3.1 for a multiplier category. A value of *x* is first generated using Equation 3.4. If *x* ≤ M, *x* is valid, other wise, *x* is generated using Equation 3.5. Once *x* is determined, the hydraulic conductivity, *K*, is updated to give *K'*

$$K' = K * 10^{x}. \qquad \textbf{(3.7)}$$

4.0 PRELIMINARY ASSESSMENT

4.1 ASSESSMENT RESULTS: QUASI-3D EPACMTP RUNS

A preliminary assessment of the impact of sites with fractured media on peak receptor well concentration predictions was performed using a version of the EPACMTP (US EPA, 1996) modified to incorporate amendments to the OSW Subtitle-D landfill database (US EPA, 1986) as per findings of Dynamac Corporation (US EPA, 1998). A combination of the vertically averaged areal solution and hybrid analytical-numerical (quasi 3D) solution was used for shallow and deep aquifers, respectively.

The bulk of the analysis consisted of three Monte-Carlo simulations based on the HWIR default landfill scenario: one simulation without fractures, and two simulations with fractures utilizing Category I and Category II multiplier distributions. Two additional Monte-Carlo simulations were performed constraining the receptor well location to be 100 meters down gradient of the source boundary along the plume centerline . One simulation incorporated Category II proposed hydraulic conductivity multipliers to model the impact of fractures, while the second simulation did not model fractured media. Each Monte-Carlo simulation consisted of 10,000 flow and transport realizations. Simulation results included peak receptor well concentrations and hydraulic conductivity values used to produce the peak well concentrations.

Results of the simulations are presented in Appendix A, Figures A.1 through A.8. Figures A.1 and A.2 compare hydraulic conductivity distributions for the case where fractures were not modeled, and the case where fractures were modeled using Category I and Category II hydraulic conductivity multipliers, respectively. These figures illustrate a shift to the right in the hydraulic conductivity distributions, the magnitude of shift increasing from Category I multipliers to Category II.

Figures A.3 and A.4 present the cumulative distributions of normalized peak receptor well concentrations for the case with and without fractures for Category I and Category II multipliers, respectively. Figures A.5 and A.6 present the cumulative distributions of the log of normalized peak receptor well concentrations for the case with and without fractures for Category I and Category II multipliers, respectively. All figures show negligible impact of increased hydraulic conductivity on peak receptor well concentration. Table 4.1 summarizes the data in these figures.

Figures A.7 and A.8 present the cumulative distributions of normalized peak receptor well concentrations and the log of normalized peak concentrations for the constrained well scenario with and without fractures for Category II. Again, the impact of the multipliers appears to be negligible.

Table 4.1 Selected Percentile Values from Quasi 3D Analysis

Percentile	Normalized Concentration Without Fractures	Normalized Concentration With Fractures-I	Percent Difference	Normalized Concentration With Fractures-II	Percent Difference
60	3.17E-21	8.06E-23	-97.46 *	4.72E-23	-98.51 *
75	1.47E-09	5.23E-10	-64.42 *	5.37E-10	-63.47 *
85	7.80E-05	7.59E-05	-2.69	7.34E-05	-5.90
90	1.07E-03	1.19E-03	11.22	1.20E-03	12.15
91	1.55E-03	1.72E-03	10.97	1.72E-03	10.97
92	2.12E-03	2.44E-03	15.09	2.47E-03	16.51
93	2.93E-03	3.50E-03	19.45	3.56E-03	21.50
94	4.07E-03	4.97E-03	22.11	4.91E-03	20.64
95	5.43E-03	6.75E-03	24.31	6.73E-03	23.94
96	7.93E-03	9.41E-03	18.66	8.99E-03	13.37
97	1.18E-02	1.34E-02	13.56	1.27E-02	7.63
98	1.78E-02	2.11E-02	18.54	2.01E-02	12.92
99	3.42E-02	3.90E-02	14.04	3.55E-02	3.80

* Normalized concentrations below 1.0E-06

$$Note: Percent Difference = \frac{Conc.\ with\ Fractures - Conc.\ without\ Fractures}{Conc.\ without\ Fractures} \times 100\%$$

4.2 ASSESSMENT RESULTS: AQUIFER MODULE (HWIR99) RUNS

The Aquifer module analysis consisted of two Monte-Carlo simulations based on the HWIR default landfill scenario: one simulation without fractures, and one simulation with fractures utilizing Category II multiplier distributions. Each Monte-Carlo simulation used the results of 10,000 fully three-dimensional EPACMTP flow and transport realizations. Parameter sets used in each of the 10,000 EPACMTP realizations were presented to the Vadose Zone and Aquifer modules for two additional simulations with and without fractures. Simulation results from both models included peak receptor well concentrations and hydraulic conductivity values used to produce the peak well concentrations.

4.2.1 EPACMTP Three-Dimensional Solution

Results of the simulations are presented in Appendix B, Figures B.1 through B.3. Figure B.1 compares hydraulic conductivity distributions for the case where fractures were not modeled, and the case where fractures were modeled using Category II hydraulic conductivity multipliers. This figure illustrate a shift to the right in the hydraulic conductivity distribution.

Figure B.2 presents the cumulative distributions of normalized peak receptor well concentrations for the case with and without fractures for Category II multipliers. Figure B.3 presents the cumulative distributions of the log of normalized peak receptor well concentrations for the case with and without fractures for Category II multipliers. All figures show negligible impact of increased hydraulic conductivity on peak receptor well concentration . Table 4.2 summarizes the data in these figures.

4.2.2 HWIR99 Pseudo Three-Dimensional Aquifer Module Solution

Results of the simulations are presented in Appendix C, Figures C.1 through C.3. The hydraulic conductivity distributions for the case where fractures were not modeled, and the case where fractures were modeled using Category II hydraulic conductivity multipliers are identical to the distributions in Section 4.2.1.

Figure C.1 presents the cumulative distributions of normalized peak receptor well concentrations for the case with and without fractures for Category II multipliers. Figures C.2 presents the cumulative distributions of the logarithm of normalized peak receptor well concentrations for the case with and without fractures for Category II multipliers. Both figures show negligible impact of increased hydraulic conductivity on peak receptor well concentration, however, the impacts are the opposite with respect to either of the preceding EPACMTP results. Table 4.3 summarizes the data in these figures.

Figures C.3 and C.4 present the cumulative distributions of the log of normalized peak concentrations for the both the three-dimensional and quasi three-dimensional solutions from EPACMTP, and the pseudo three-dimensional solution from the HWIR99 Aquifer module, with and without fractures for Category II, respectively.

Table 4.2 Selected Percentile Values from Fully 3D Analysis

Percentile	Normalized Concentration Without Fractures	Normalized Concentration With Fractures-II	Percent Difference
60	2.05E-15	5.49E-15	62.66
75	3.12E-10	5.05E-10	38.22
85	8.11E-07	1.07E-06	24.21
90	3.13E-05	4.38E-05	28.54
91	6.11E-05	8.18E-05	25.31
92	1.16E-04	1.54E-04	24.68
93	2.25E-04	3.00E-04	25.00
94	4.48E-04	6.11E-04	26.68
95	1.14E-03	1.58E-03	27.85
96	2.74E-03	3.31E-03	17.22
97	6.35E-03	7.11E-03	10.69
98	1.56E-02	1.59E-02	1.89
99	4.54E-02	4.44E-02	-2.25

$$Note: Percent Difference = \frac{Conc.\ with\ Fractures - Conc.\ without\ Fractures}{Conc.\ without\ Fractures} \times 100\%$$

Table 4.3 **Selected Percentile Values from Pseudo 3D Analysis**

Percentile	Normalized Concentration Without Fractures	Normalized Concentration With Fractures-II	Percent Difference
75	2.18E-11	1.34E-11	-38.53%
85	2.05E-06	1.42E-06	-30.73%
90	7.89E-05	6.85E-05	-13.18%
91	1.63E-04	1.43E-04	-12.27%
92	3.70E-04	3.43E-04	-7.30%
93	7.10E-04	6.56E-04	-7.61%
94	1.50E-03	1.37E-03	-8.67%
95	3.18E-03	2.72E-03	-14.47%
96	6.91E-03	5.78E-03	-16.35%
97	1.36E-02	1.22E-02	-10.29%
98	3.16E-02	2.71E-02	-14.24%
99	7.86E-02	6.66E-02	-15.27%

$$Note: Percent Difference = \frac{Conc.\ with\ Fractures - Conc.\ without\ Fractures}{Conc.\ without\ Fractures} \times 100\%$$

5.0 REFERENCES

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APPENDIX A

RESULTS: EPACMTP RUNS
QUASI-3D SOLUTION

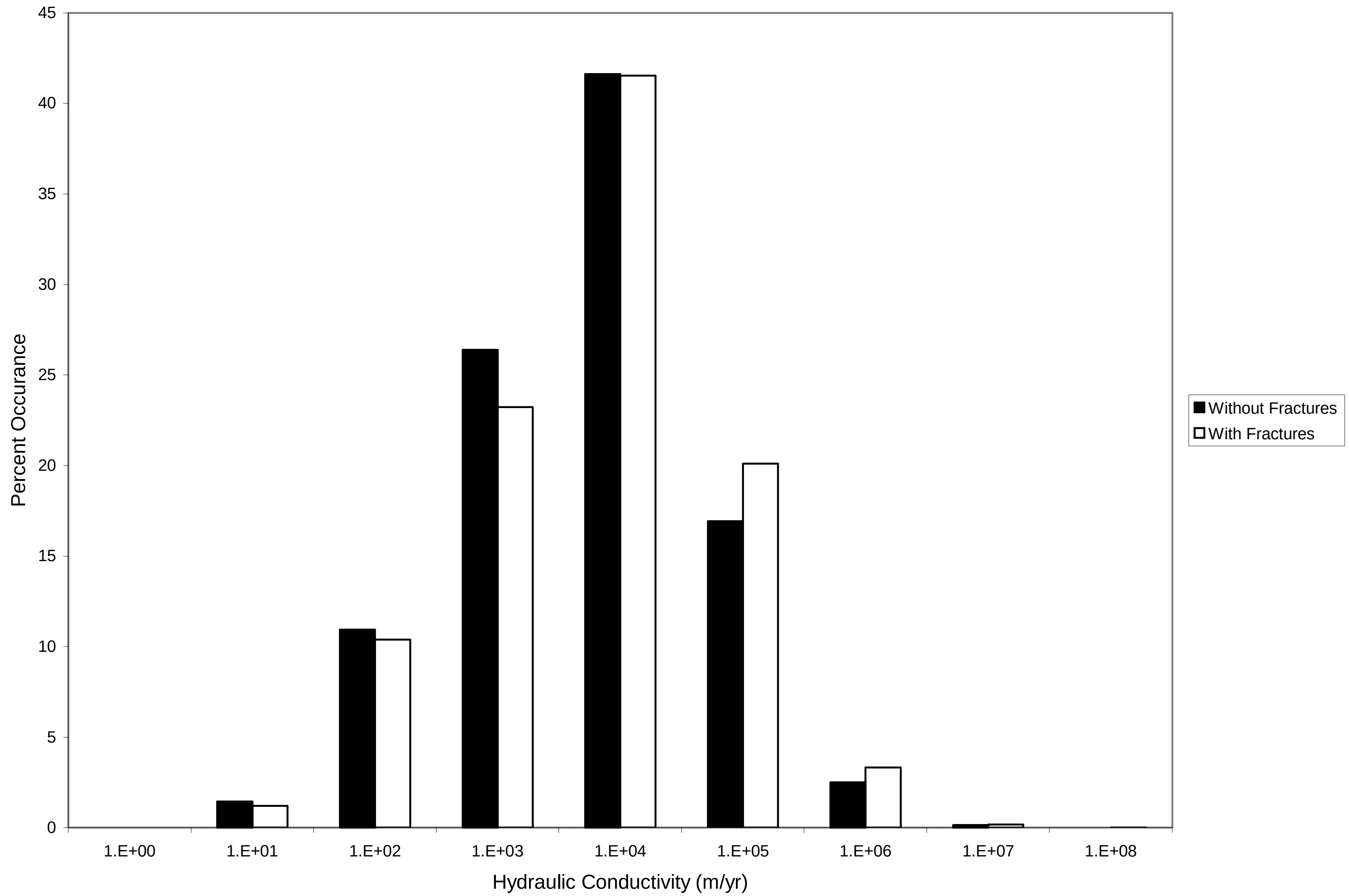

Figure A.1 Histogram of hydraulic conductivity distributions with and without fractures utilizing Category I hydraulic conductivity multiplier distribution parameters

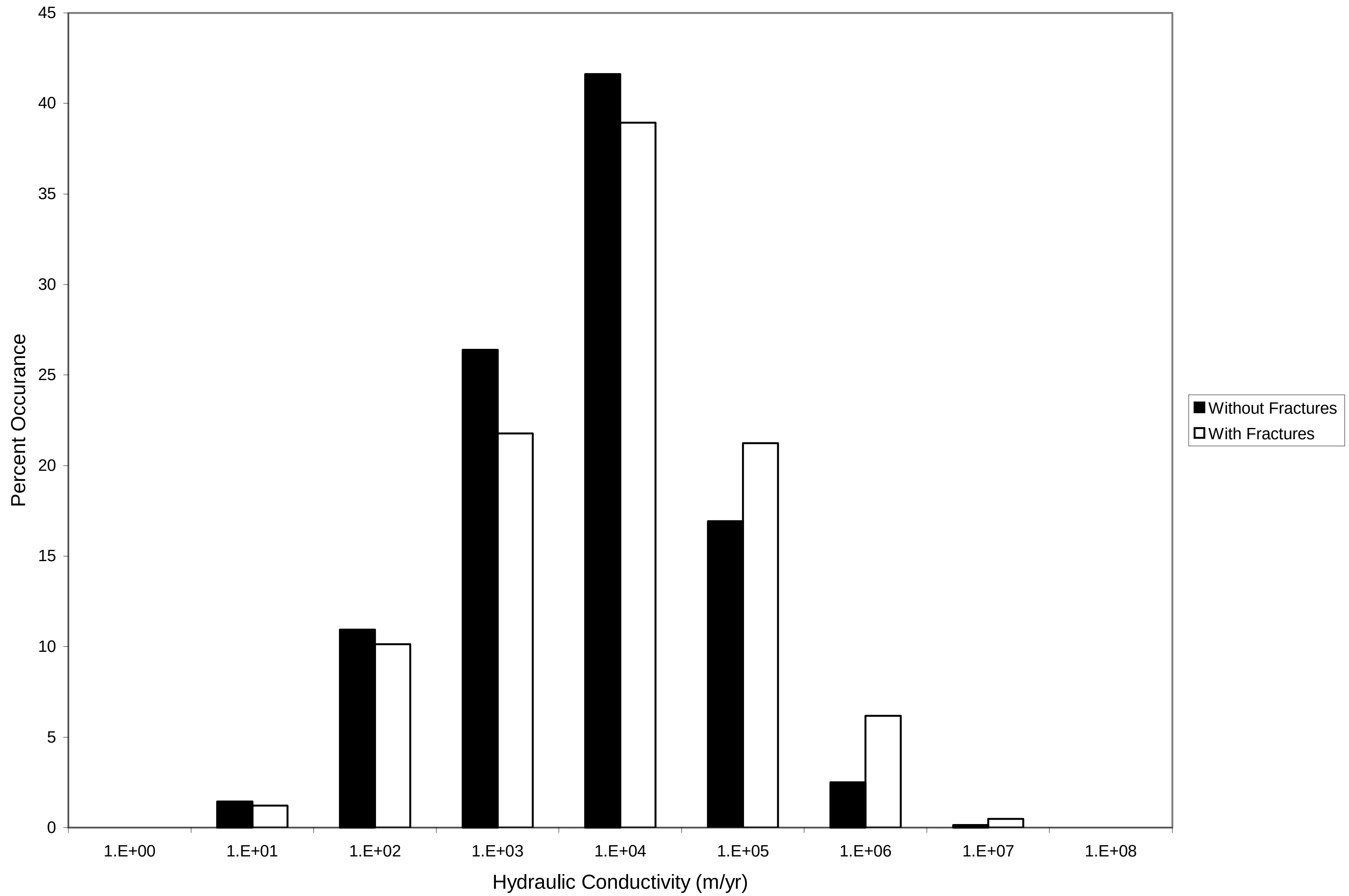

Figure A.2 Histogram of hydraulic conductivity distributions with and without fracture utilizing Category II hydraulic conductivity multiplier distribution parameters

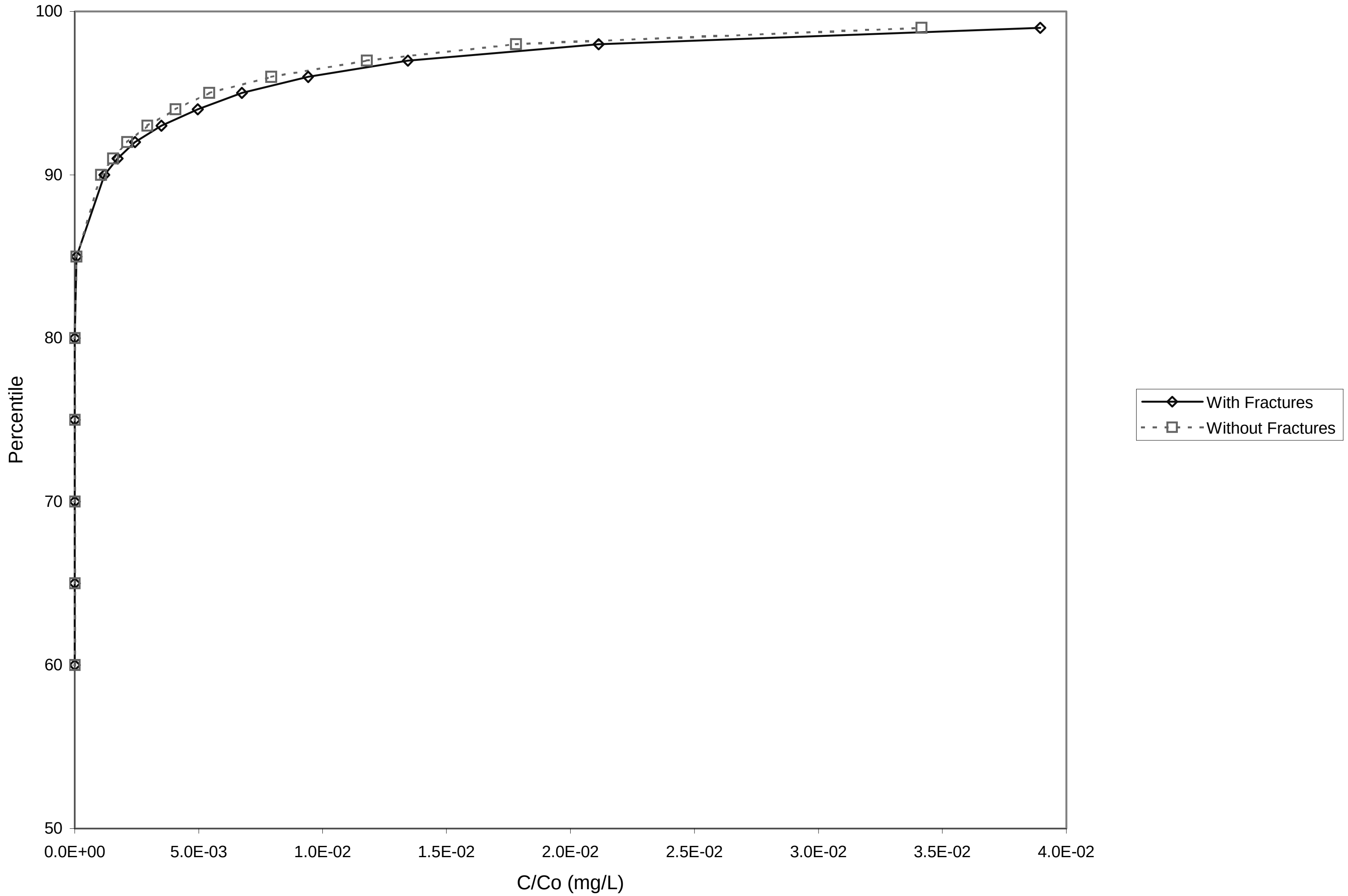

Figure A.3 **Percentiles of normalized concentration with and without fractures utilizing Category I hydraulic conductivity multiplier distribution parameters**

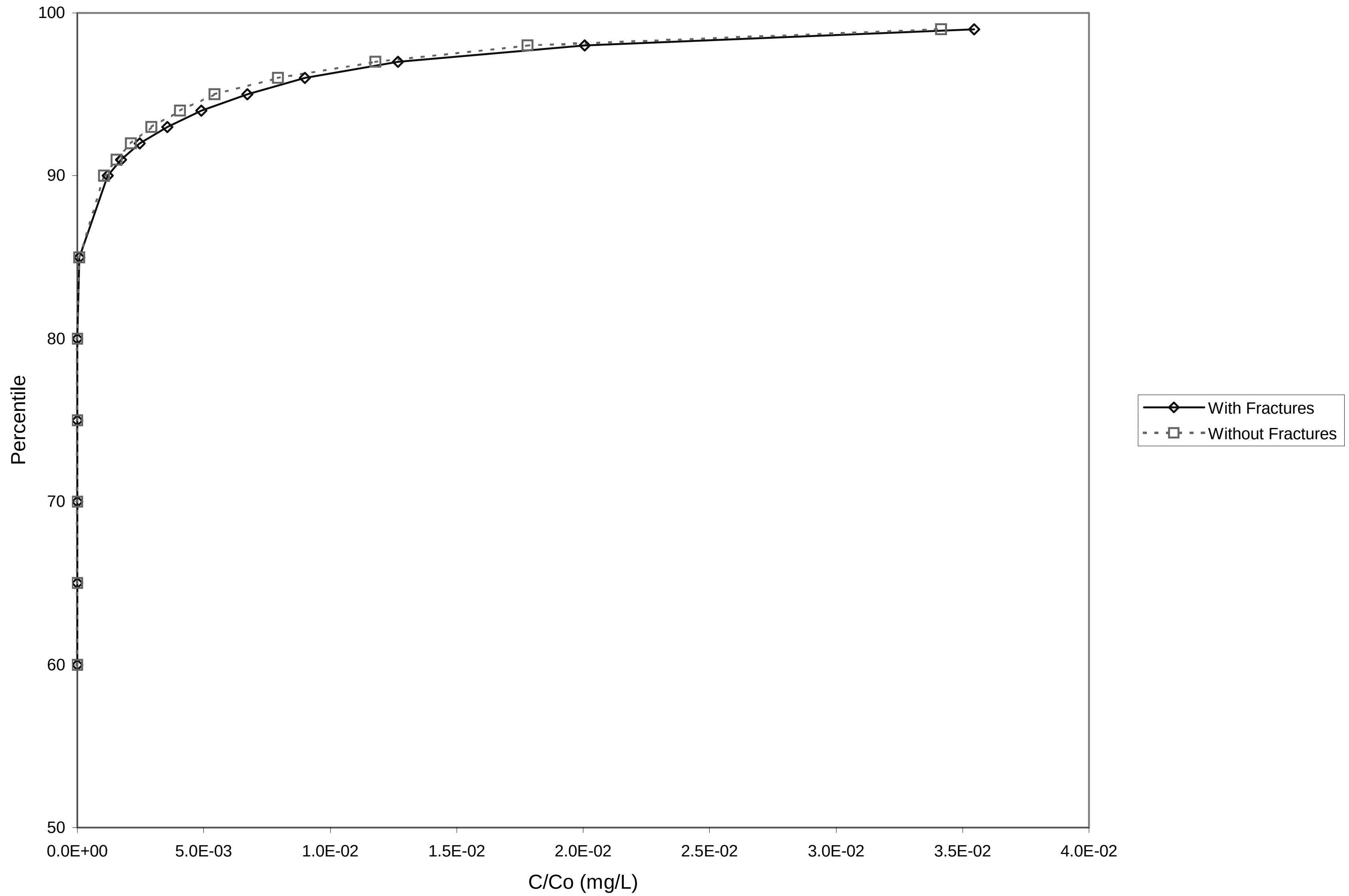

Figure A.4 **Percentiles of normalized concentration with and without fractures utilizing Category II hydraulic conductivity multiplier distribution parameters.**

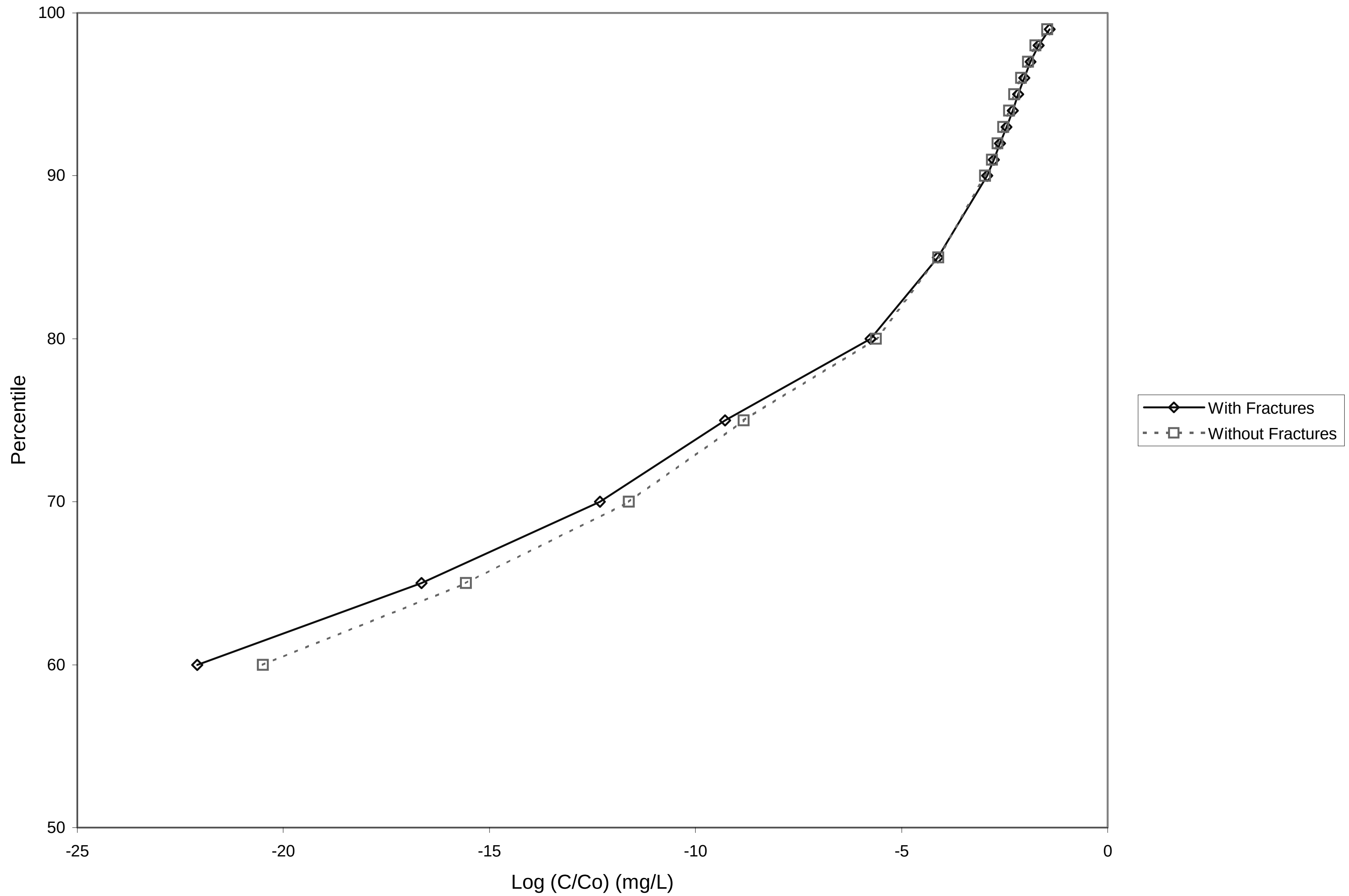

Figure A.5 Percentiles of the log of normalized concentration with and without fractures utilizing Category I hydraulic conductivity multiplier distribution parameters

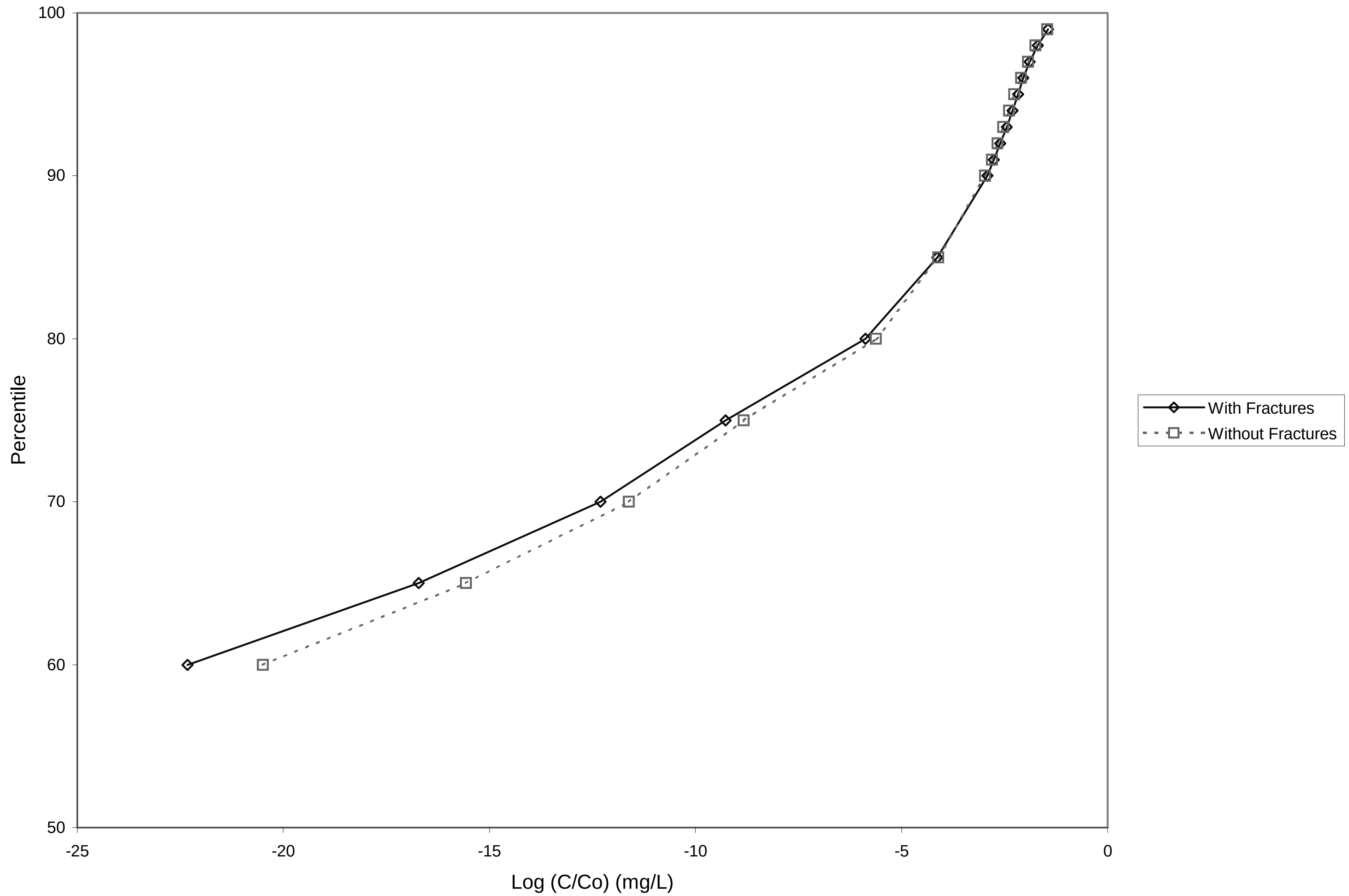

Figure A.6 **Percentiles of the log of normalized concentration with and without fractures utilizing Category II hydraulic conductivity multiplier distribution parameters**

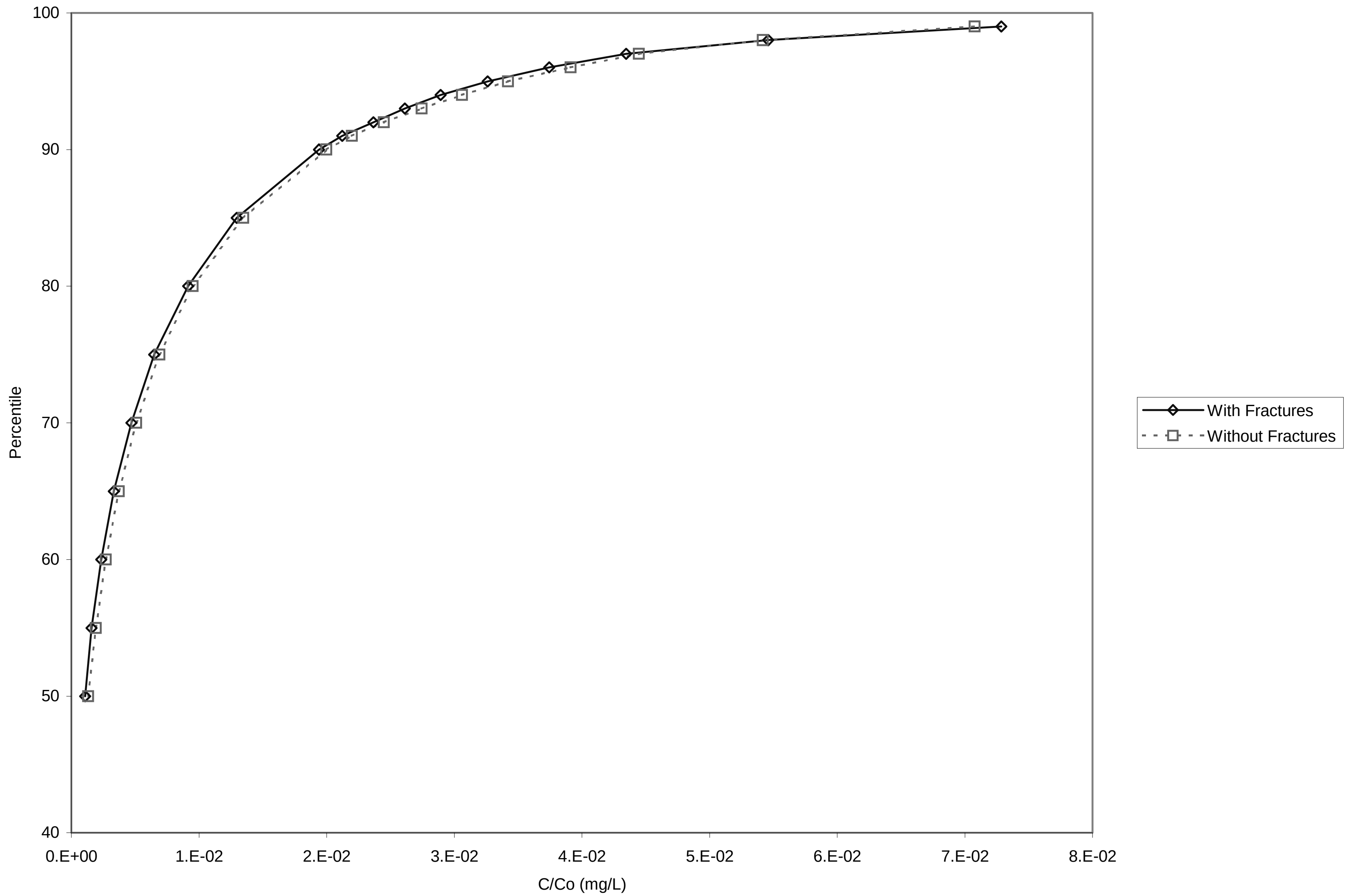

Figure A.7 Percentiles of normalized concentration with and without fractures utilizing Category II hydraulic conductivity multiplier distribution parameters where receptor well is located 100m along plume centerline

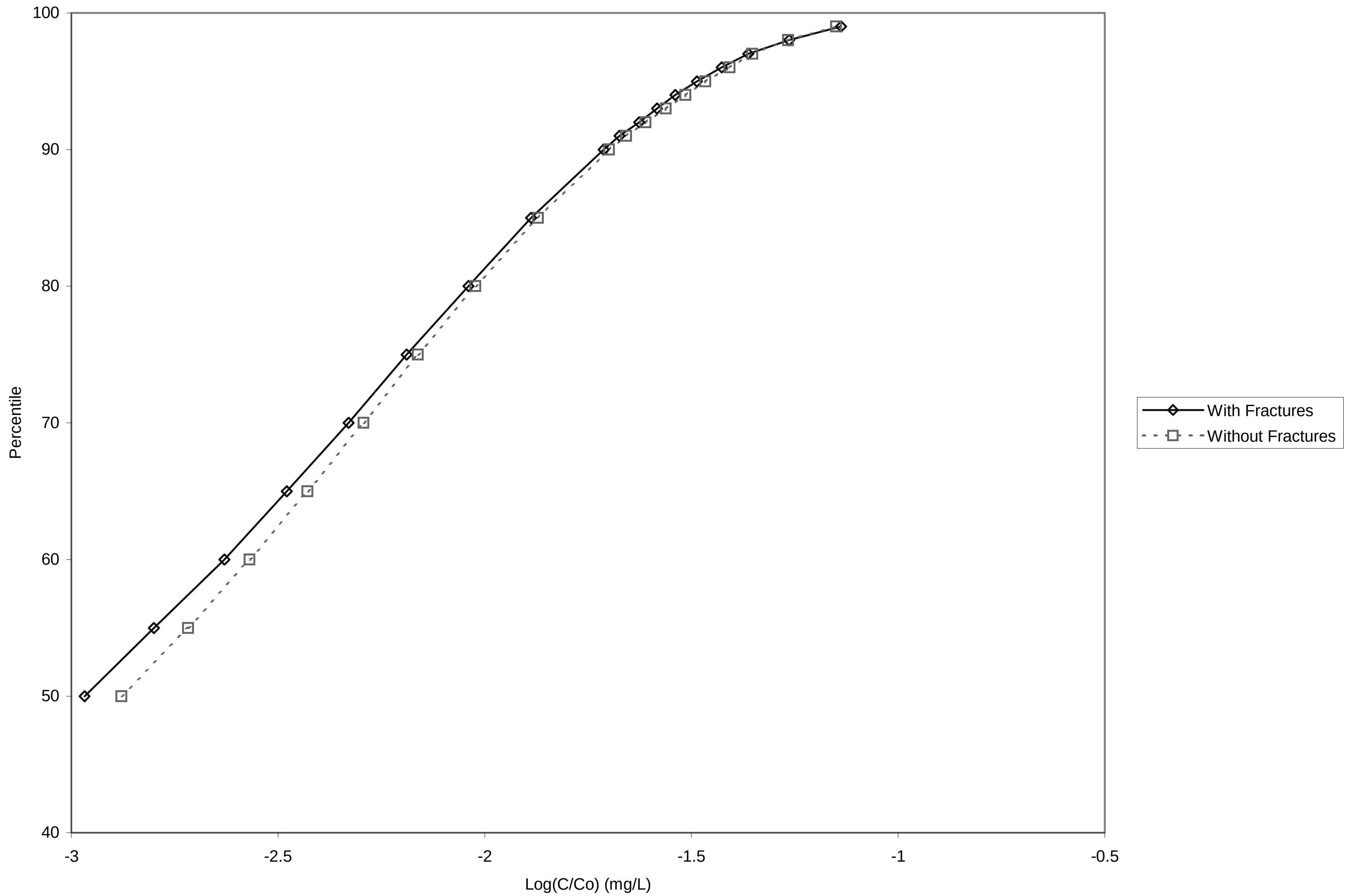

Figure A.8 Percentiles of the log of normalized concentration with and without fractures utilizing Category II hydraulic conductivity multiplier distribution parameters where receptor well is located 100m along plume centerline

APPENDIX B

RESULTS: EPACMTP RUNS FULLY-3D SOLUTION

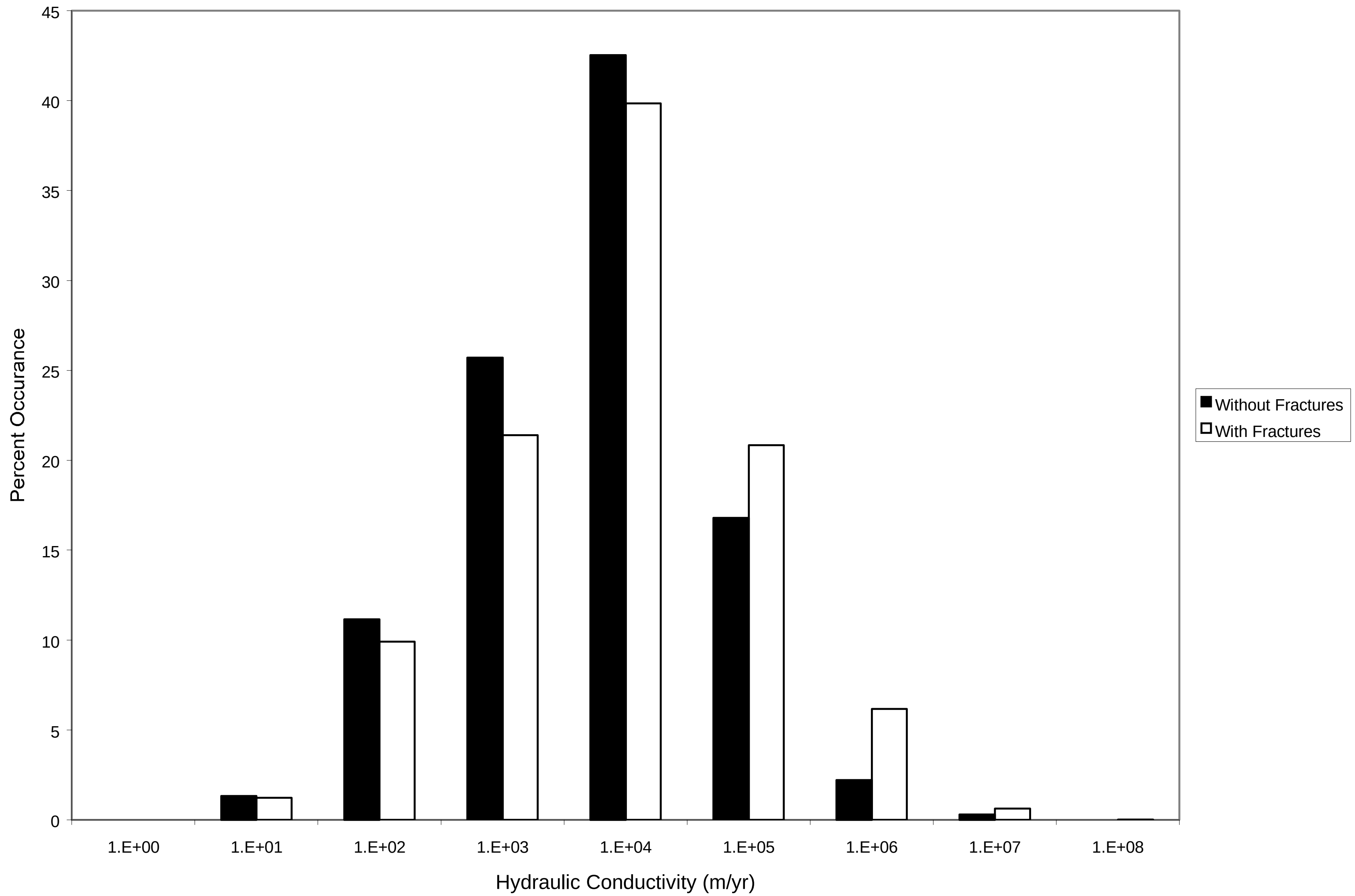

Figure B.1 **Histogram of hydraulic conductivity distributions with and without fractures utilizing Category II hydraulic conductivity multiplier distribution parameters from EPACMTP Full- 3D Monte-Carlo simulations**

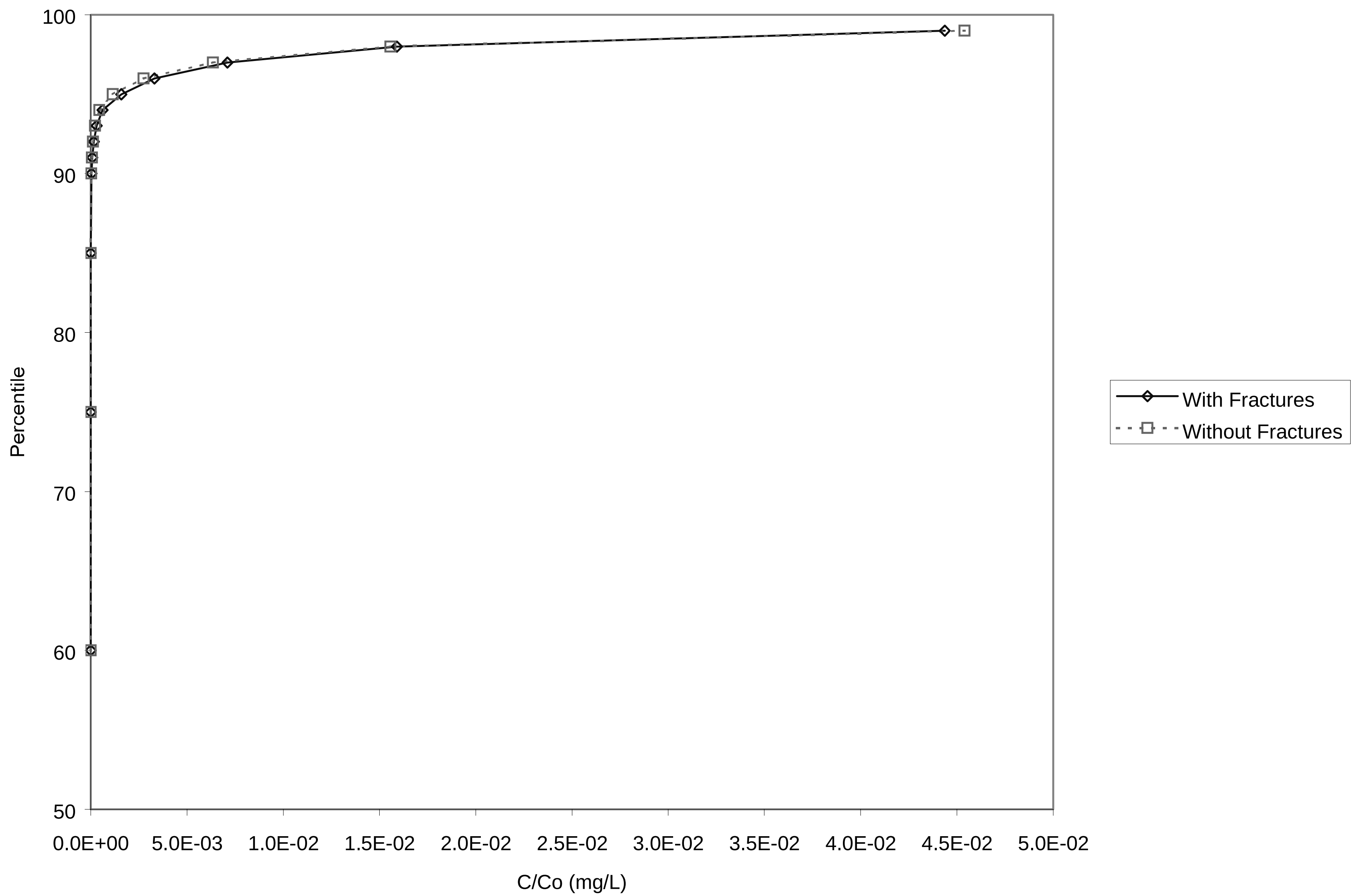

Figure B.2 Percentiles of normalized concentration with and without fractures utilizing Category II hydraulic conductivity multiplier distribution parameters from EPACMTP Fully- 3D Monte-Carlo simulations

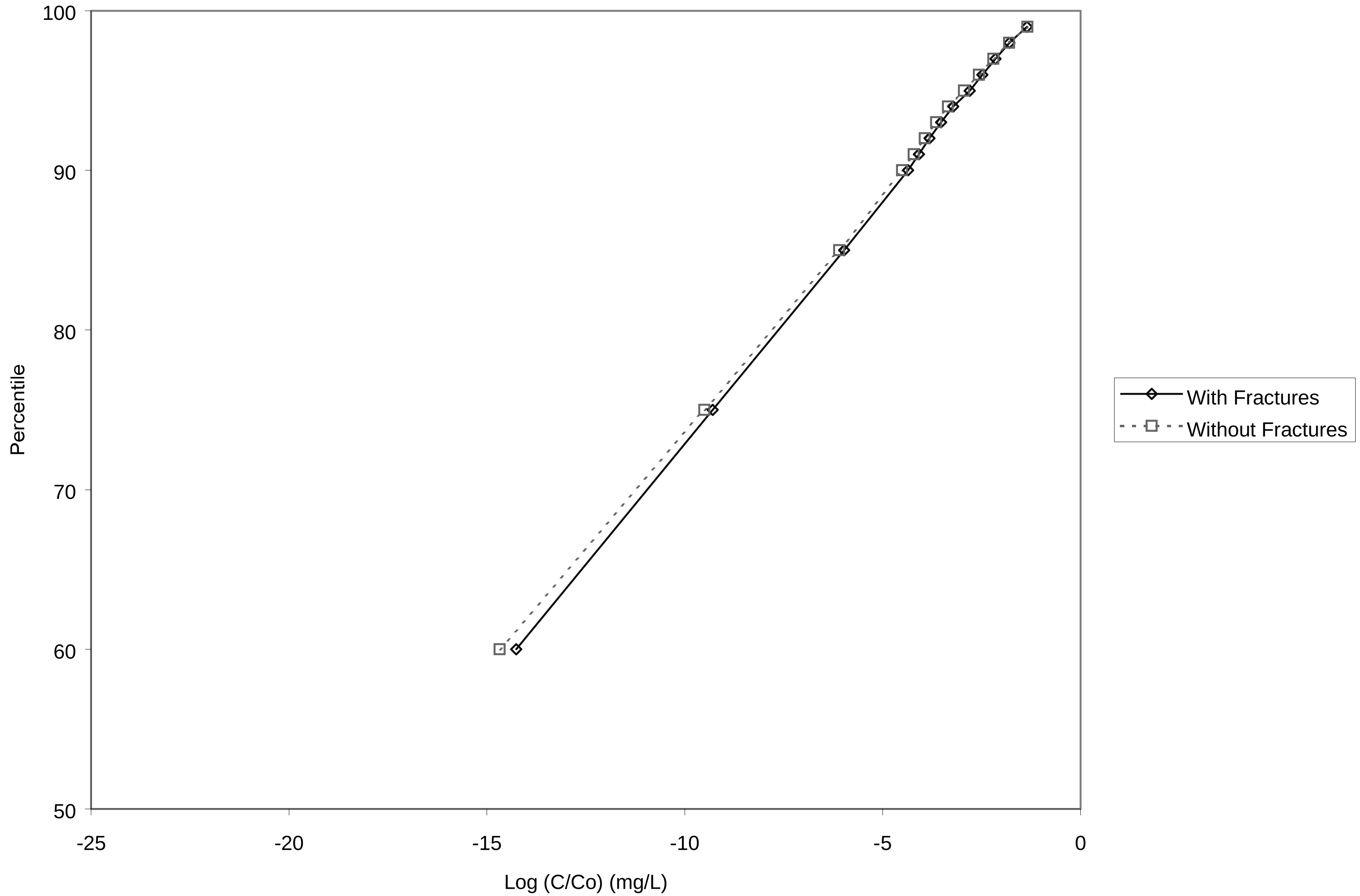

Figure B.3 Percentiles of the log of normalized concentration with and without fractures utilizing Category II hydraulic conductivity multiplier distribution parameters from EPACMTP Fully-3D Monte-Carlo simulations

APPENDIX C

RESULTS: MODULE RUNS
PSEUDO-3D SOLUTION

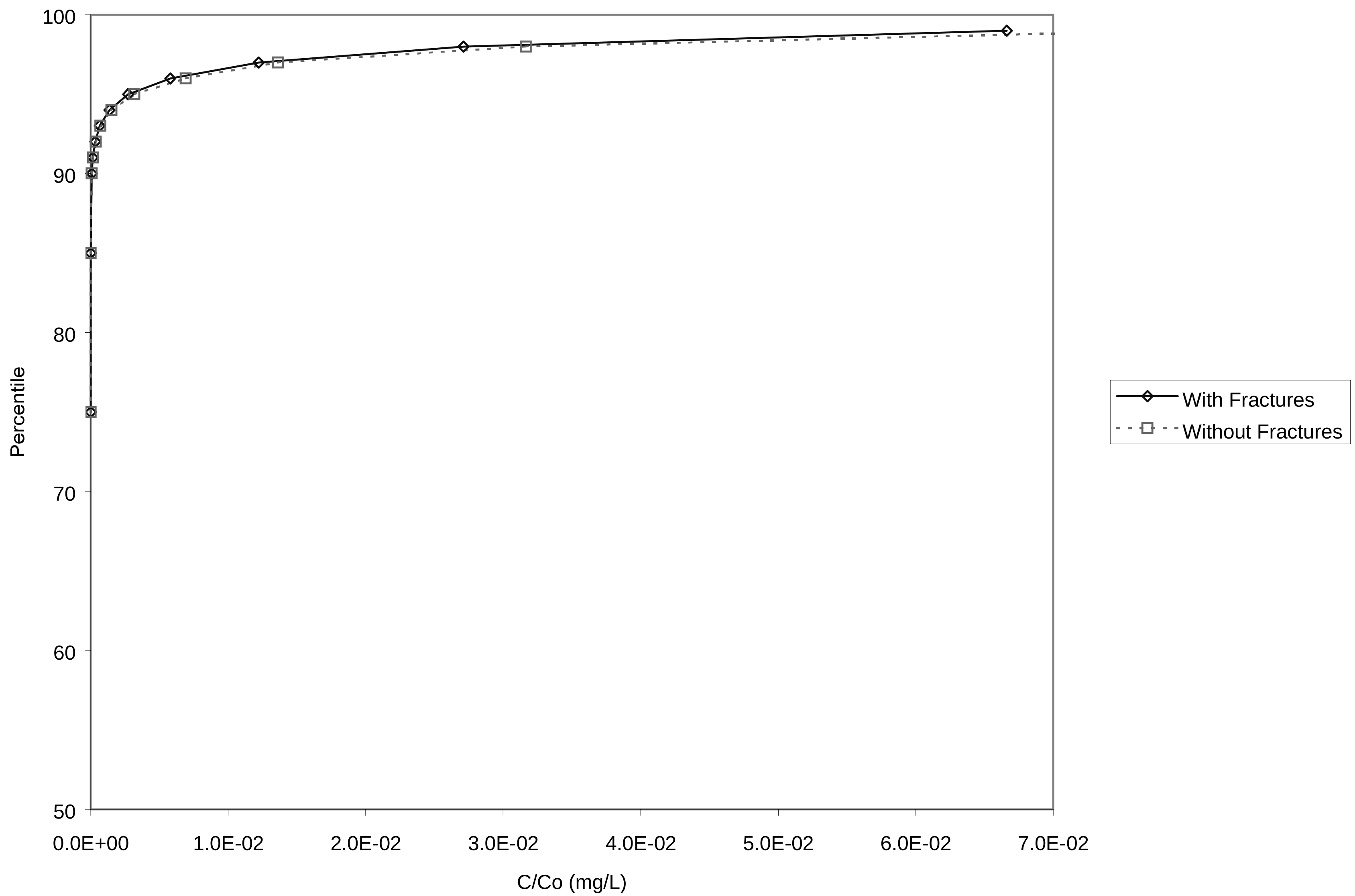

Figure C.1 Percentiles of normalized concentration with and without fractures utilizing Category II hydraulic conductivity multiplier distribution parameters from HWIR99 Aquifer module Monte-Carlo simulations

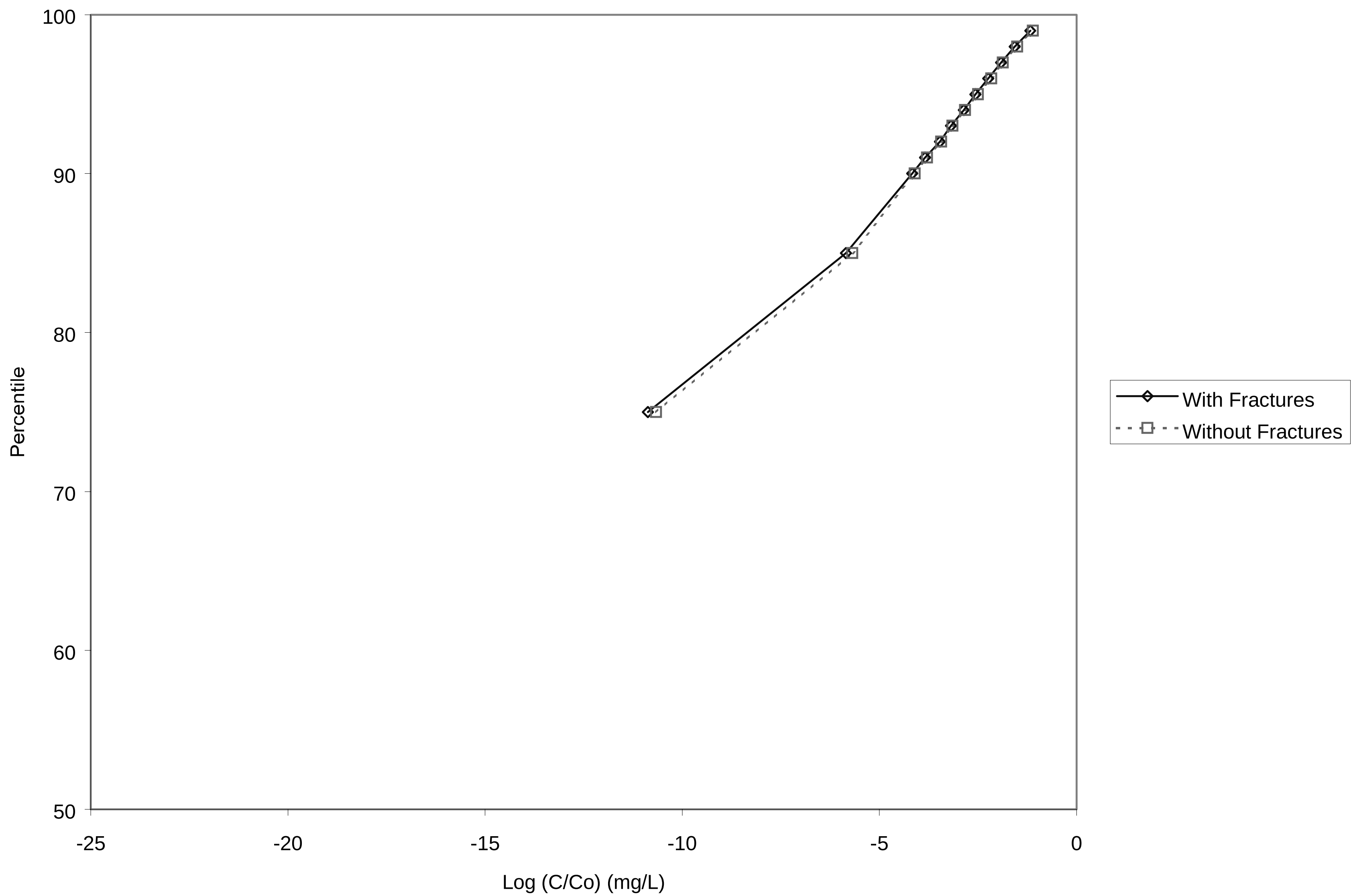

Figure C.2 Percentiles of the log of normalized concentration with and without fractures utilizing Category II hydraulic conductivity multiplier distribution parameters from the HWIR99 Aquifer modules Monte-Carlo simulations

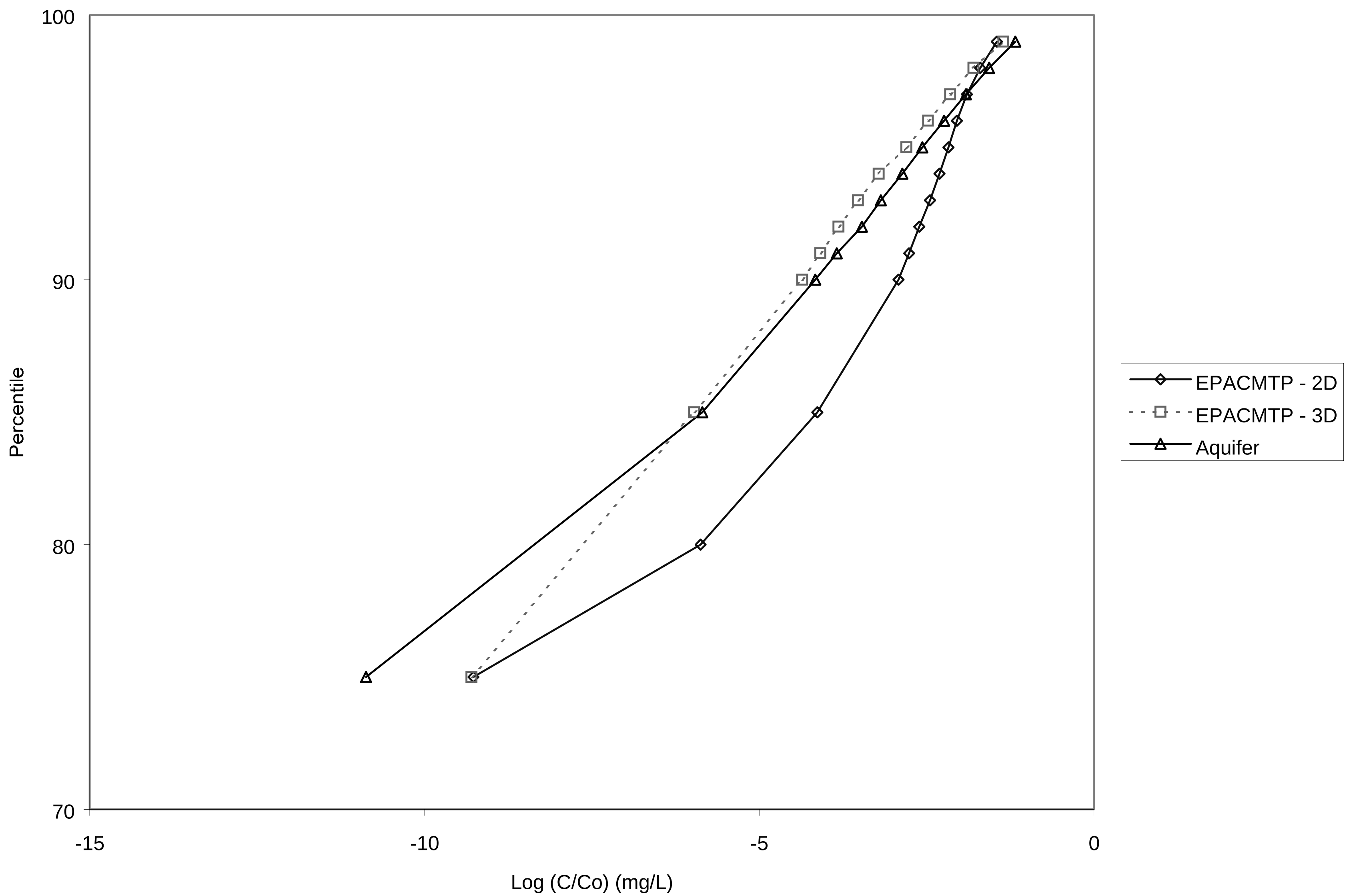

Figure C.3 Percentiles of the log of normalized concentration with fractures utilizing Category II hydraulic conductivity multiplier distribution parameters for EPACMTP -3D, Quasi-3D, and HWIR99 Aquifer module

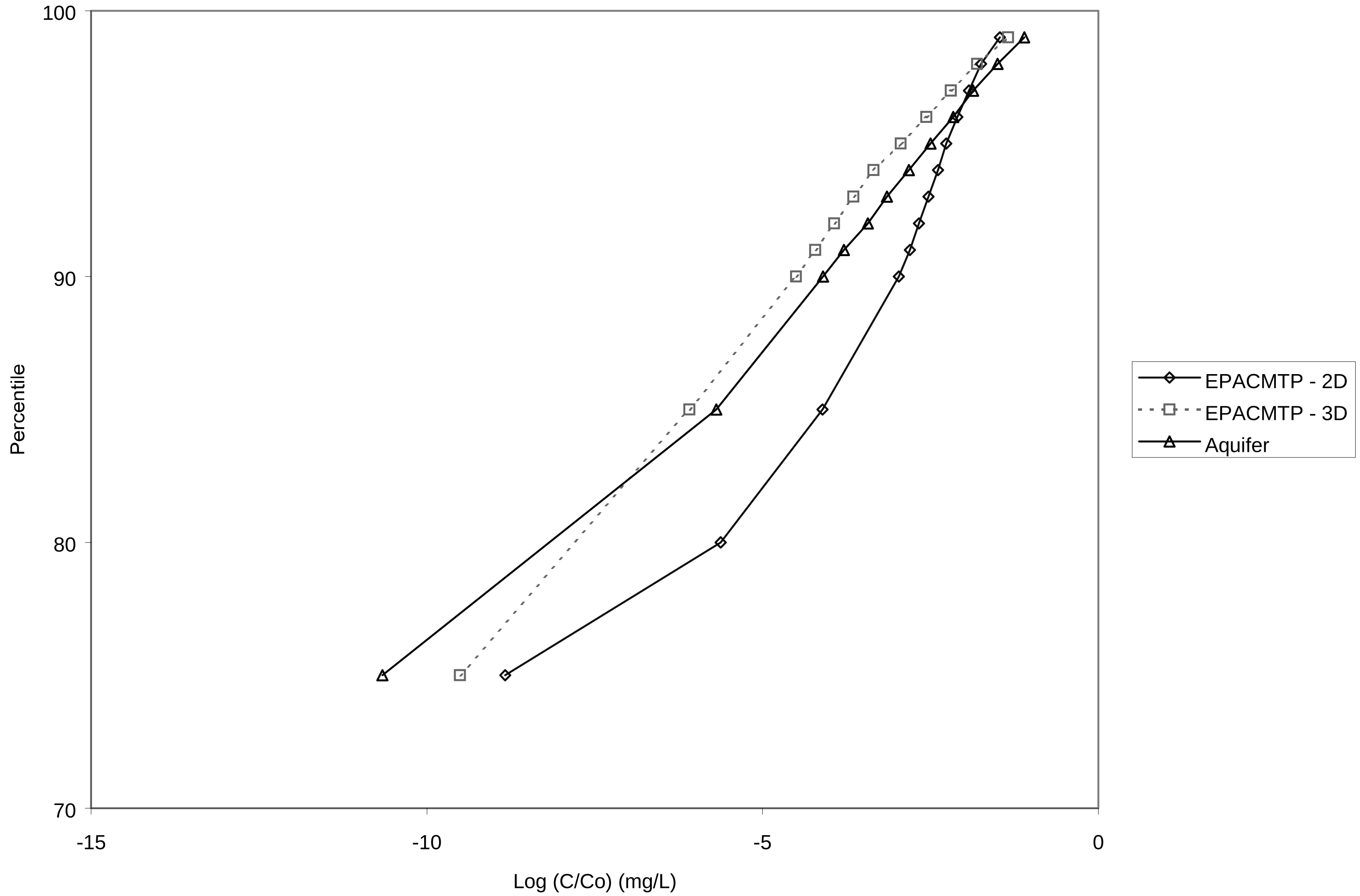

Figure C.4 **Percentiles of the log of normalized concentration without fractures for EPACMTP -3D, Quasi-3D, and HWIR99 Aquifer module**