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PARTITION COEFFICIENTS FOR METALS IN SURFACE WATER, SOIL, AND WASTE

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1.0 INTRODUCTION AND BACKGROUND

The purpose of this study was to develop contaminant partition coefficients for the surface water pathway and for the source model used in the multimedia approach for the Hazardous Waste Identification Rule (HWIR). Partition coefficients for certain metal contaminants in environmental media are needed to perform multimedia exposure and risk assessment modeling for HWIR. The multimedia model includes a surface water pathway model that requires partition coefficients to account for removal of contaminant from the solution phase and retardation of contaminant movement. The contaminants of interest are the metals: antimony (Sb), arsenic (As), barium (Ba), beryllium (Be), cadmium (Cd), chromium (Cr), cobalt (Co), copper (Cu), lead (Pb), molybdenum (Mo), mercury (Hg), nickel (Ni), selenium (Se), silver (Ag), thallium (Tl), tin (Sn), vanadium (V), and zinc (Zn). Methylated mercury (CH_3Hg^+) and cyanide (CN) are also of interest. In the surface water pathway, the HWIR modeling scenario includes several transport processes that require metal partition coefficients: (1) The overland transport of metal contaminants in runoff water in the watershed and the consequent partitioning between soil and water; (2) partitioning between the suspended load and the water in streams, rivers, and lakes; (3) partitioning between riverine or lacustrine sediment and its porewater; and (4) partitioning between dissolved organic carbon (DOC) and the inorganic solution species in the water of streams, rivers, and lakes.

The HWIR modeling scenario includes a source model for various types of waste management units that also requires partition coefficients. For the source model, the partition coefficients are used to represent the ratio of contaminant mass in the solid phase to that in the leachate (water) phase. There are five types of waste management units for which the source model requires partition coefficients: land application units, waste piles, landfills, treatment lagoons (surface impoundments), and aerated tanks.

This report describes the two-phase approach used in developing the needed partition coefficients. In the preferred method of obtaining the coefficients, a literature survey was performed to determine the range and statistical distribution of values that have been observed in field scenarios. This includes the collection of published partition coefficients for any of the metals in any of the environmental media of interest, or the estimation of partition coefficients from reported metal concentration data when feasible. The data retrieved in the literature search were recorded in a spreadsheet along with associated geochemical parameters (such as pH, sorbent content, etc.) when these were reported. It was anticipated that the literature search would not supply partition coefficients for all of the metals in all of the environmental media of interest. In the second-phase effort, statistical methods, geochemical speciation modeling, and expert judgement were used to provide reasonable estimates of partition coefficients not available from the literature.

2.0 LITERATURE SURVEY FOR METAL PARTITION COEFFICIENTS

A literature survey was conducted to obtain partition coefficients to describe the partitioning of metals between soil and soil-water, between suspended particulate matter (SPM) and surface water, between sediment and sediment-porewater, and between DOC and the dissolved inorganic phase in natural waters. In addition, partition coefficients were sought for equilibrium partitioning of metals between waste matrix material and the associated aqueous phase in land application units, waste piles, landfills, treatment lagoons, and aerated tanks. The literature survey encompassed periodical scientific and engineering materials and some non-periodicals including books and technical reports published by the U.S. EPA and other government agencies. Electronic searches of the following databases were included as part of the literature survey:

- Academic Press Journals (1995 - present)
- AGRICOLA (1970 - present)
- Analytical Abstracts (1980 - present)
- Applied Science and Technology Abstracts
- Aquatic Sciences and Fisheries Abstract Set (1981 - present)
- CAB Abstracts (1987 - present)
- Current Contents (1992 - present)
- Dissertation Abstracts (1981 - present)
- Ecology Abstracts (1982 - present)
- EIS Digest of Environmental Impact Statements (1985 - present)
- EI Tech Index (1987 - present)
- Environmental Engineering Abstracts (1990 - present)
- General Science Abstracts (1984 - present)
- GEOBASE (1980 - present)
- GEOREF (1785 - present)
- National Technical Information Service
- PapersFirst (1993 - present)
- Periodical Abstracts (1986 - present)
- Toxicology Abstracts (1982 - present)
- Water Resources Abstracts (1987 - present)

Two search strings were used in the electronic searches: "distribution coefficient" and "partition coefficient". Use of such general strings has the advantage of generating many citations, decreasing the probability that relevant articles will be missed, but also carrying a high labor burden because each citation returned must be examined for useful data. For metals that are not as well represented in the published literature, even more general search strings were used, sometimes with boolean operators (e.g., "barium" and "soil", "selenium" and "partitioning"). The work of identifying articles containing useful data from among all those retrieved was made easier by first reviewing the titles to eliminate those of obvious irrelevance, then reviewing the abstracts, which were usually available on-line. Abstracts of citations that showed promise for providing partition coefficients were printed and given a

code consisting of the first two letters of the lead author's last name and the last two digits of the year of publication. The code, along with the first few words of the article title, was entered in a log book for tracking. Logged articles were quickly reviewed at local university research libraries, and those containing relevant data were copied for a more thorough review at the office. Most of the articles were obtained from the University of Georgia Science Library or the Georgia Institute of Technology Library. As each copied article or report was reviewed, a summary page containing the assigned code was stapled to the front with notes indicating the type of data found in the paper and the location (page number, table number, etc.) of useful data. Partition coefficients and other data from the articles were then entered into an EXCEL 97 spreadsheet for compilation and analysis.

The geochemical parameters most likely to influence the partition coefficient were entered in the spreadsheet along with reported or calculated coefficients if such were specified in the source article or report. Examples of these are pH, total concentrations of metal and important metal complexing agents including DOC, and weight fraction of particulate organic matter and other sorbing materials. Physical parameters necessary to convert concentration ratios to partition coefficients in L/kg, including porosity, water content, and bulk density were also recorded when reported in the articles.

Approximately 245 articles and reports were copied and reviewed. A total of 1170 individual K_d values were obtained from these sources directly or calculated from reported media concentrations. This total does not include mean estimated K_d values reported in previously published compilations of K_d values (Baes and Sharp, 1983; Baes et al., 1984; Coughtrey et al., 1985; Thibault et al., 1990). (The data from previous compilations were recorded in the spreadsheet and used in guiding the final estimates of appropriate central tendency values as described in Section 3.1.3.) Approximately 80% of the 1170 values obtained from the literature pertained to the metals Cd, Co, Cr, Cu, Hg, Ni, Pb, and Zn. More K_d 's were recovered for Cd than any other metal, followed closely by Zn, Pb, and Cu. The most frequently reported type of K_d was that for suspended matter in streams, rivers and lakes. (Data pertaining to marine environments were generally avoided, but some data from estuaries were included if reported as corresponding to low salinity.) The second most frequently reported values pertained to partitioning in soil. Suspended matter and soil K_d 's together totaled 68% of the reported data. Table 1 below shows the median and range of literature K_d values for natural media for each metal and K_d type. (Shown as log K_d values.)

No directly reported partition coefficients for the waste systems of interest were discovered in the literature survey, and none are included in Table 1. There are many reasons for wishing to understand the behavior of metals in natural systems. The rich literature of soil science, plant nutrition, aquatic chemistry, geology, and toxicology are all examples of investigative areas of longstanding where metals partition coefficients are frequently encountered. The impetus for research with regard to waste systems is significantly different from that of natural systems. Moreover, the behavior of metals in waste materials are typically studied and reported prior to their disposal and consequent mixing with a host of other substances—few studies have focused on the behavior of metals within disposal units containing a (usually unknown) mixture of materials. Most studies involving metal concentrations in waste are

concerned with predicting the metal concentration in leachate by means of a physical test (a leach test). Section 3.2 presents further findings with regard to leach tests and appropriate metal partition coefficients for waste systems.

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Table 1

Median, range, and number of samples (N) for partition coefficients (log K_d in L/kg) from the literature search. Range or median specified without N are from a previous compilation. Open spaces represent combinations of media-type and metal for which either no data was found, or too little data was found to provide meaningful statistics.

Metal	Soil/Water	Suspended Matter /Water	Sediment/ Water	DOC/Water
Ag	median	2.6	4.9	3.6
	range	1.0 - 4.5	4.4 - 6.3	2.1 - 5.8
	N	21	15	2
As	median	3.4	4.0	2.5
	range	0.3 - 4.3	2.0 - 6.0	1.6 - 4.3
	N	22	25	18
Ba	median		4.0	
	range	0.7 - 3.4	2.9 - 4.5	
	N		14	
Be	median	3.1	4.1	4.5
	range	1.7 - 4.1	2.8 - 6.9	3.0 - 5.3
	N	2	17	
Cd	median	2.9	4.7	3.6
	range	0.1 - 5.0	2.8 - 6.3	0.5 - 7.3
	N	41	67	21
Co	median	2.1	4.7	3.3
	range	(-1.2) - 4.2	3.2 - 6.3	2.9 - 6.3
	N	11	29	3
Cr(III)	median	3.9	5.1	4.5
	range	1.0 - 4.8	3.9 - 6.0	
	N	43	25	
Cr(VI)	median	1.1		
	range	(-0.7) - 3.3		
	N	24	1	
Cu	median	2.7	4.7	4.2
				5.5

Table 1 (continued)

Median, range, and number of samples (N) for partition coefficients (log K_d in L/kg) from the literature search. Range or median specified without N are from a previous compilation. Open spaces represent combinations of media-type and metal for which either no data was found, or too little data was found to provide meaningful statistics.

Metal	Soil/Water	Suspended Matter /Water	Sediment/ Water	DOC/Water
range	0.2 - 3.6	3.1 - 6.1	0.7 - 6.2	2.5 - 7.0
N	20	70	12	17
Hg				
median	3.8	5.3	4.9	5.4
range	2.2 - 5.8	4.2 - 6.9	3.8 - 6.0	5.3 - 5.6
N	17	35	2	3
CH ₃ Hg				
median	2.8	5.4	3.9	
range	1.3 - 4.8	4.2 - 6.2	2.8 - 5.0	
N	11	2	4	
Mo				
median	1.1		2.5	
range	(-0.2) - 2.7			
N	8			
Ni				
median	3.1	4.6	4.0	5.1
range	1.0 - 3.8	3.5 - 5.7	0.4 -	4.7 - 5.4
N	18	30	5	4
Pb				
median	4.2	5.6	5.1	5.1
range	0.7 - 5.0	3.4 - 6.5	2.0 - 7.0	3.8 - 5.6
N	33	48	24	9
Sb				
median	2.4		4.0	
range	0.1 - 2.7		2.5 - 4.8	2.7 - 4.3
N	6		3	
Se				
median	2.1	4.2	3.6	
range	-0.3 - 2.4	3.2 - 4.7		
N	23	2		
Sn				
median	2.8	5.6	4.7	
range	2.1 - 4.0	4.9 - 6.3		
N		3		

Table 1 (continued)

Median, range, and number of samples (N) for partition coefficients (log K_d in L/kg) from the literature search. Range or median specified without N are from a previous compilation. Open spaces represent combinations of media-type and metal for which either no data was found, or too little data was found to provide meaningful statistics.

Metal	Soil/Water	Suspended Matter /Water	Sediment/ Water	DOC/Water
Tl median			3.2	
range			3.0 - 3.5	
N			6	

Table 1 (continued)

Median, range, and number of samples (N) for partition coefficients (log K_d in L/kg) from the literature search. Range or median specified without N are from a previous compilation. Open spaces represent combinations of media-type and metal for which either no data was found, or too little data was found to provide meaningful statistics.

Metal	Soil/Water	Suspended Matter /Water	Sediment/ Water	DOC/Water
V				
median				
range	0.6 - 2.7			
N	1			
Zn				
median	3.1	5.1	3.7	4.9
range	(-1.0) - 5.0	3.5 - 6.9	1.5 - 6.2	4.6 - 6.4
N	21	75	18	9
CN				
median	3.0			
range	0.7 - 3.6			
N	3			

Partition coefficients used in several recent U.S. EPA risk assessments are presented in Appendix A. Because the origin of these data is generally unknown, they were not included in the collection of K_d values appearing elsewhere in the spreadsheet, nor were they included in the statistical summary of K_d values obtained from the literature.

3.0 ANALYSIS OF RETRIEVED DATA AND DEVELOPMENT OF PARTITION COEFFICIENT VALUES

The data gathered from published sources were insufficient to establish a reasonable range for the partition coefficient for all metals in all media-types. The second part of the effort was directed at augmenting the values obtained from the literature so as to provide a reasonable range and central tendency for each metal in each media-type. Statistical analysis of retrieved data, geochemical modeling, and expert judgement were all used in developing the partition coefficients. The nature of the available data for natural media systems and waste systems was different to the extent that it seemed best to consider these separately.

3.1 DEVELOPMENT OF PARTITIONING COEFFICIENTS IN NATURAL MEDIA

In analyzing the partitioning data collected from the literature for soil and surface water systems, we attempted to identify the shape of the probability distribution for each metal in each medium. For a particular metal in a particular medium, the degree to which the literature sample is truly representative of the population of metal partition coefficients is dependent on the number of sample points, the actual variability of important medium properties that influence partitioning (pH, concentration of sorbing phases, etc.), and how well this variability is represented in the sample. In some cases, it was necessary to eliminate data points from the literature sample to avoid obvious bias. For example, the sample of literature K_d values for Cr(III) in soil included values obtained in a pH titration of three soils such that each of the three was represented by 8 different K_d values. Although they provide interesting data on the dependence of K_d on pH in these soils, multiple measurements from the same soil and values determined at other than the ambient soil pH introduce bias in the natural probability distribution of K_d . Therefore, for each of these soils, one of the eight K_d values was picked randomly and the other seven were discarded in deriving the probability distribution. In similar fashion, the sample of literature data for each metal and media-type was edited before attempting to identify the underlying distribution.

Statistical tests were performed to determine the shape of the frequency distribution of K_d for each metal and media-type. The tests employed widely recognized techniques available in the statistical package Analyze-It (version 1.32), an module add-on for Microsoft EXCEL 97. In only a few cases were the data sufficient to identify the underlying distribution with any degree of certainty. Many of the samples, including the most complete samples (largest sample size), gave a positive test for normality after transforming the available data to log space, suggesting that the frequency distribution of the underlying population of K_d values for a particular metal in a particular medium is most likely log-normal. The Shapiro-Wilk test and the Kolmogorov-Smirnov test were used to test the log transformed samples for normality. A positive test in Shapiro-Wilk does not ensure a normal distribution. Rather, it provides a measure of confidence that the sample data are not inconsistent with a normal distribution. The Shapiro-Wilk test is a general test for normality; it is not necessary to know the population mean or standard deviation. The Kolmogorov-Smirnov test was used when results from the Shapiro-Wilk test were negative

In some cases, there were too few representative data points in the sample to have confidence in the descriptive statistics of the data. In these cases, three methods were used to augment the available data in estimating the mean, standard deviation, and minimum and maximum K_d values. The three methods were: estimation from linear regression equations developed from the literature samples, estimation from the results of geochemical speciation modeling, and estimation by expert judgement. Each of these is discussed below.

3.1.1 Estimation from Regression Equations Based on Literature Data

Of the 13 metals for which literature data were retrieved characterizing K_d in soil, sediment, and suspended matter, 12 of them exhibited the progression $K_{d, SPM} > K_{d, sediment} > K_{d, soil}$ (determined by comparison of mean values). In the two other cases where at least two of the K_d types could be characterized from the literature data, both conformed to this pattern. In addition, consistency was noted in the magnitude of K_d for metals within a specific media. For the best represented metals, the following K_d (affinity) patterns were observed (based on mean K_d):

Soils:	Pb > Cr ^{III} > Hg > As > Zn = Ni > Cd > Cu > Ag > Co
Sediment:	Pb > Hg > Cr ^{III} > Cu > Ni > Zn > Cd > Ag > Co > As
SPM:	Pb > Hg > Cr ^{III} = Zn > Ag > Cu = Cd = Co > Ni > As

There is some shuffling about of the affinity order among these media-types, as might be expected for a data set that is doubtlessly incomplete. It may be that the As affinity for soils in our literature sample is too high. Nevertheless, the similarities are worthy of note. Some aspects of the overall trend are in agreement with the hard-soft acid-base (HSAB) concepts of Pearson (1963). Pb and Hg have higher affinity than HSAB predicts. Certainly, there are multiple adsorbing surfaces present in all of these materials. The consistency of affinity relationships among these metals suggests that the distribution of K_d is partly due to characteristics unique to the metals themselves and partly due to characteristics associated with the sorbing surfaces. Regardless of the cause, it appears feasible to exploit these relationships to provide an estimate of K_d for a metal in one media if its value in another could be ascertained. For example, the literature data provided a reasonable number of samples of K_d in soils and suspended matter for the nine metals Ag, Cd, Co, Cr(III), Cu, Hg, Ni, Pb, and Zn. For each of these metals, the mean values of K_d in soil was in the neighborhood of two orders of magnitude less than the mean value in suspended matter. This trend was characterized more exactly by developing a linear regression equation that was exploited to estimate mean K_d values for metals for which the literature provided an estimate of mean K_d in soil, but not in suspended matter (or the opposite). In a similar manner, linear regression equations were developed to estimate the mean K_d in sediment from the literature estimate of mean K_d in soil or suspended matter, or the mean soil K_d from that in sediment or suspended matter. The regression equations were developed from cases where the literature survey data provided reasonable estimates of the mean K_d for at least two of the three media. The metals used in developing the regression equations included cadmium, copper, zinc, and other metals that were better represented in the literature. The distribution was assumed to be log-normal so that the regression equations were actually based on mean log K_d and were

used to predict mean log K_d . The standard deviation was estimated from the mean and minimum values assuming the minimum value represents two standard deviations from the mean. It was also estimated in like manner using the mean and maximum values. The larger of the two estimates of standard deviation was retained as the final estimate. The regression equations used are shown in Table 2 along with the number of observations on which each equation is based, the correlation coefficient (r^2), and the 95% confidence interval for the slope and intercept.

Table 2
Linear Regression Equations used to Estimate Mean log K_d Values (L/kg) in Natural media.

Used to Estimate	Dependent Variable	slope (+/- 95% CI)	intercept (+/- 95% CI)	r^2	N
mean log K_d sediment	mean log K_d soil	1.080 (1.035)	0.796 (3.190)	0.79	5
mean log K_d sediment	mean log K_d suspended matter	1.418 (1.923)	-3.179 (9.868)	0.65	5
mean log K_d suspended matter	mean log K_d soil	0.380 (0.444)	3.889 (1.338)	0.37	9
mean log K_d suspended matter	mean log K_d sediment	0.457 (0.619)	3.257 (2.555)	0.65	5
mean log K_d soil	mean log K_d sediment	0.728 (0.697)	0.071 (2.878)	0.79	5
mean log K_d soil	mean log K_d suspended matter	0.969 (1.136)	-1.903 (5.703)	0.37	9

The regressions equations were also used to estimate mean K_d values for suspended matter and sediments from an estimate of the mean K_d in soil obtained from geochemical speciation modeling.

3.1.2 Estimation From Geochemical Speciation Modeling

Geochemical speciation modeling was used to estimate soil/water partitioning if regression equations could not be used. The partitioning of metal cations between DOC and the inorganic portion of the solution phase was also estimated by speciation modeling. In both cases, the U.S. EPA geochemical speciation model MINTEQA2 version 4.0 (Allison et al., 1990) was used to estimate the K_d values. The input data for MINTEQA2 was developed from various sources.

Modeling details for soil partition coefficients

The concentrations of major ions were the average concentrations in river water as reported by Stumm and Morgan (1996). The soil water phosphate concentration was obtained from Bohn et al. (1979). The ionic strength was held constant at 0.005 M after a sensitivity test in the range 0.01 to 0.001 M revealed that the impact was significantly less than other important variables. Model values for several of the most significant variables affecting K_d were varied over reasonable ranges in order to capture the expected range in K_d . These master variables include pH, concentration of dissolved organic carbon (DOC), concentration of particulate organic carbon (POC), and concentration of metal oxide binding sites. The range for each of these was characterized by low, medium, and high values, and the model was executed at all possible combinations of these settings. The pH range corresponded to that reported from the STORET database (U.S. EPA, 1996a) with a slight downward adjustment (6.5 for the medium value instead of 6.8, and 4.5 for the low value instead of 4.9) to account for the more acidic environment of surface watershed soils. The concentrations used for DOC were 0.5, 5.0, and 50.0 mg/L, taken as a reasonable range in soil water. The POC concentrations were obtained from analysis of shallow silt-loam soils from a soils database (Carsel et al., 1988 and R. Parrish, personal communication). The low, medium, and high values were as corresponds to the 10th, 50th, and 90th percentiles, respectively, for particulate organic matter (0.41, 1.07, and 2.12 wt%).

The dominant metal oxide sorbing surface was assumed to be hydrous ferric oxide (HFO). Because we had little reliable information as to the appropriate concentration range, and also in consideration of the importance of this variable in determining K_d , the HFO concentration was used as a calibrating variable. The low, medium, and high values were first set to correspond to the values used in U.S. EPA (1996a). Those values were based on a specialized extraction of reactive Fe from a set of 12 samples from aquifers and soils. The mean K_d for Cd, Cu, Ni, Pb, and Zn were computed using these values in MINTEQA2. These were compared with mean K_d values for these metals in soil from the literature survey. The low, medium, and high HFO concentrations were scaled in subsequent modeling such that the mean K_d value from MINTEQA2 was within the 95% confidence interval of the mean literature K_d value for each of these metals. (Each MINTEQA2 execution resulted in 81 different K_d values due to utilizing all different combinations of low, medium, and high for the four different master variables. The mean value from MINTEQA2 was taken as the average of the three K_d values corresponding to the medium setting of pH, DOC, and HFO and the low POC; the medium settings of pH, DOC, and HFO, and the medium POC; and the medium settings of pH, DOC, and HFO, and the high setting of POC.) Appendix B shows a typical MINTEQA2 input file used in estimating K_d for soil/water.

The minimum and maximum K_d values were established from the available literature data and the MINTEQA2 results. The distribution was assumed to be log-normal. Once the mean log K_d value for a metal was established for soil from the modeling exercise, the regression equations were used to estimate mean values for sediment and suspended matter if these were lacking in the literature data. The standard deviation was estimated as described above for linear regression estimates.

Modeling details for DOC partition coefficients

The partitioning of metals between DOC and other inorganic forms in water is not usually reported in terms of a partitioning coefficient. In fact, specialized algorithms within speciation models are frequently employed to estimate the fraction of metal bound with DOC based on the pH, major ion composition of the solution, and ionic strength. The development of such specialized methods for estimating metal binding with DOC is an ongoing research area. MINTEQA2 includes a specialized sub-model for estimating DOC interactions—the Gaussian distribution model (Dobbs et al., 1989; Allison and Perdue, 1994). This model represents DOC as a mixture of many types of metal binding sites. The probability of occurrence of a binding site with a particular log K is given by a normal probability function defined by a mean log K and standard deviation in log K. A limitation of the DOC binding calculations in MINTEQA2 and similar models is that the metal-DOC reactions necessary to obtain results are available only for a limited number of metal cations and for none of the anionic metals. MINTEQA2 includes mean log K values for the metal cations Cd, Cu, Ba, Be, Cr(III), Ni, Pb, and Zn. For other metal cations of interest (Ag, Co, Hg(II), Sn(II), and Tl(I)) it was necessary to estimate the mean log K for DOC binding for use with the Gaussian model. For Hg(II), the estimate of the mean log K was determined from a regression of “known” mean log K values with the binding constants for humic- and fulvic acid (HA and FA, respectively) as given by Tipping (1994). The metals Cd, Cu, Ni, Pb, and Zn were represented in the database of HA and FA binding constants, so these were used to develop the regression relationship:

$$\text{mean log } K_{\text{DOC,Hg}} = -0.610 \text{ log } K_{\text{HA,Hg}} + 4.206 \text{ log } K_{\text{FA,Hg}} - 3.645 \quad (1)$$

This relationship was derived with a correlation coefficient (r^2) of 0.95. It was used to estimate a mean log $K_{\text{DOC,Hg}}$ of 9.0 for Hg+ 2 binding with DOC.

The mean log K for the other cations (Ag^+ , Co^{2+} , Sn^{2+} , and Tl^+) were derived from a linear free energy relationship using the first hydrolysis constants ($\text{log } K_{\text{OH}}$) and the binding constant for acetate ($\text{log } K_{\text{Acet}}$). The $\text{log } K_{\text{OH}}$ and $\text{log } K_{\text{Acet}}$ for the metals Cd, Cu, Fe, Ni, Pb, and Zn were used to derive the following relationship:

$$\text{mean log } K_{\text{DOC}} = 0.3595 \text{ log } K_{\text{OH}} + 0.6932 \text{ log } K_{\text{acet}} + 0.7974 \quad (2)$$

The correlation coefficient (r^2) for this relationship is 0.98. It was used to estimate the mean $\text{log } K_{\text{DOC}}$ for Ag^+ , Co^{2+} , Sn^{2+} , and Tl^+ for use in MINTEQA2 modeling. The mean $\text{log } K_{\text{DOC}}$ values estimated for these metals were 2.0, 3.3, 6.6, and 1.0, respectively.

The estimation procedures outlined above cannot reliably be extended to anions. However, anions are typically not as strongly bound to organic matter. We therefore have used

MINTEQA2 to estimate K_d values with DOC for cationic metals only and have included conservative estimates for the anions based on judgement alone.

The concentrations of major ions used in estimating metal-DOC binding using MINTEQA2 were the average concentrations in river water as reported by Stumm and Morgan (1996). The concentration of DOC and the pH were treated as master variables with each assigned three levels corresponding to low, medium, and high. The medium value was the mean of the reported river and stream samples from the literature survey, and the low and high values were selected to encompass the range observed in the literature survey data. Specifically, the low, medium, and high DOC were 0.89, 8.9, and 89 mg/L, respectively, and the low, medium, and high pH were 4.9, 7.3, and 8.1, respectively. The binding of each of the metal cations was computed in nine simulations that represented all possible combinations of pH and DOC concentration level. The mean value K_d value for the cations was represented by the value computed by MINTEQA2 when the pH and DOC concentration were set to their mean values in surface water. A typical MINTEQA2 input file used to estimate metal partitioning with DOC is shown in Appendix C.

The results computed using MINTEQA2 for both soils and DOC were used to augment the partitioning data collected in the literature survey. Although it was considered reasonable to use MINTEQA2 to estimate mean partition coefficients, it is not possible to establish the shape of the distribution from the MINTEQA2 results. However, there is no compelling reason to suppose other than the log-normal distribution suggested by the literature survey data.

3.1.3 Estimation from Expert Judgement

When neither the regression equations nor MINTEQA2 could reasonably be used to estimate the mean log K_d , the mean value was estimated subjectively using expert judgement. Factors considered included any values obtained from the literature survey, reported mean values or ranges from previous compilations, similarities of behavior among metals, and qualitative statements from articles and reports. The minimum and maximum K_d values from the literature were used if reasonable values were available. Otherwise, these were also estimated by expert judgement. In either case, the standard deviation was estimated as described above for linear regression.

Finally, a relative confidence level (*CL*) was subjectively assigned to each of the final values presented. The *CL* values range from 1 to 4 with the highest confidence corresponding to a value of 1, and the lowest to a value of 4. In general, estimates based on the literature survey for a well-studied metal with a large literature sample was deemed to merit a *CL* of 1. Data for a metal not represented in the literature for which the final values were purely estimates from MINTEQA2 or other means with a notable degree of expert judgement were assigned a *CL* of 4. Many data were determined in circumstances that warrant a *CL* between these extremes (e.g., a range was given in the literature, a value was available from a previous compilation, estimates from combinations of these circumstances could be combined

with estimates from modeling, etc.). In these cases, a *CL* of 2 or 3 was assigned as seemed best.

The metal partition coefficients in soil, sediment, suspended matter, and DOC are presented in Tables 3, 4, 5, and 6, respectively. The method used to arrive at each estimate is indicated for each metal and media-type, as is the subjectively assigned confidence level.

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Table 3

Metal partition coefficients ($\log K_d$) in kg/L for soil/soil water. Values in italics were estimated by regression or from MINTEQA2 results. An entry of “log-normal” in bold indicates that the sample data gave a positive result in the Shapiro-Wilk test for normality of the log-transformed data. An entry of “log-normal” in parentheses means that data were not sufficient to establish the distribution, but log-normal has been assumed. Relative confidence in the data is indicated by the CL value of 1 to 4 (1= highest, 4= lowest).

Metal	Distribution (assumed)	Median	Mean	Std. Dev.	Min	Max	Comments
Ag (I)	Log Normal	2.6	2.6	0.8	1.0	4.5	From literature data (raw, n= 21); CL= 1
As ^a	(log-normal)	3.4	3.2	0.7	0.3	4.3	From literature data (raw, n= 21); oxidation state usually not specified in literature; CL= 2
Ba(II)	(log-normal)	---	<i>2.0</i>	<i>0.7</i>	0.7	3.4	Suspended matter K_d regression equation for mean; CL= 2
Be(II)	(log-normal)	---	<i>2.2</i>	<i>1.0</i>	1.7	4.1	Suspended matter K_d regression equation for mean; CL= 3
Cd(II)	Log Normal	2.9	2.7	0.8	0.1	5.0	From literature data (edited, n= 37); CL= 1
Co(II)	Log Normal	2.1	2.1	1.2	-1.2	4.1	From literature data (raw, n= 11); CL= 1
Cr(III)	Log Normal	3.9	3.8	0.4	1.0	4.7	From literature data (raw, n= 22); CL= 2
Cr(VI)	(log-normal)	1.1	0.8	0.8	-0.7	3.3	From literature data (raw, n= 24); CL= 2
Cu(II)	Log Normal	2.7	2.5	0.6	0.1	3.6	From literature data (raw, n= 20); CL= 1
Hg(II)	Log Normal	3.8	3.6	0.7	2.2	5.8	From literature data (raw, n= 17); CL= 1
MeHg	Log Normal	2.8	2.7	0.6	1.3	4.8	From literature data (raw, n= 11); CL= 2
Mo(VI)	(log-normal)	1.1	1.3	0.6	-0.4	2.7	From literature data (raw, n= 5); oxidation state not always specified in literature data; CL= 3
Ni(II)	Log Normal	3.1	2.9	0.5	1.0	3.8	From literature data (raw, n= 19); CL= 1

Table 3 (continued)

Metal partition coefficients ($\log K_d$) in kg/L for soil/soil water. Values in italics were estimated by regression or from MINTEQA2 results. An entry of “log-normal” in bold indicates that the sample data gave a positive result in the Shapiro-Wilk test for normality of the log-transformed data. An entry of “log-normal” in parentheses means that data were not sufficient to establish the distribution, but log-normal has been assumed. Relative confidence in the data is indicated by the CL value of 1 to 4 (1= highest, 4= lowest).

Metal	Distribution (assumed)	Median	Mean	Std. Dev.	Min	Max	Comments
Pb(II)	(log-normal)	4.1	3.7	1.2	0.7	5.0	From literature data (edited, n= 31); CL= 2
Sb ^b	(log-normal)	---	2.3	1.1	0.1	2.7	From literature data (mean is the average of several reported mean values, n= 5); CL= 4
Se(IV) ^c	(log-normal)	1.4	1.3	0.4	-0.3	2.4	From literature data (edited, n= 11); CL= 2
Se(VI)	(log-normal)	---	<i>-0.2</i>	<i>1.1</i>	<i>-2.0</i>	<i>2.0</i>	Mean estimated from MINTEQA2 result; min, max are guesses; CL= 4
Sn(II)	(log-normal)	---	2.7	0.7	2.1	4.0	From literature data, CL= 3
Tl(I)	(log-normal)	---	<i>0.5</i>	<i>0.9</i>	<i>-1.2</i>	<i>1.5</i>	Estimated from MINTEQA2 result. CL= 4
V(V)	(log-normal)	---	<i>1.7</i>	<i>1.5</i>	<i>0.5</i>	<i>2.5</i>	Mean, min, max from suspended matter K_d regression equation; CL= 4
Zn(II)	(log-normal)	3.1	2.7	1.0	-1.0	5.0	From literature data (raw, n= 21); CL= 1
CN-	(log-normal)	---	<i>0.7</i>	<i>1.6</i>	<i>-2.4</i>	<i>1.3</i>	Estimated from MINTEQA2 result. CL= 4

^a Published partitioning data for As does not allow differentiation of As(III) and As(V). It is probable that published values represent results involving both oxidation states.

^b Published partitioning data for Sb is rare and does not allow differentiation of Sb(III) and Sb(V).

^c Positive result in Shapiro-Wilk test for normality of data not log-transformed. But sample size is small and data may not be very representative.

Table 4

Metal partition coefficients ($\log K_d$) in kg/L for sediment/porewater. Values in italics were estimated by regression or from MINTEQA2 results. An entry of “log-normal” in bold indicates that the sample data gave a positive result in the Shapiro-Wilk test for normality of the log-transformed data. An entry of “log-normal” in parentheses means that data were not sufficient to establish the distribution, but log-normal has been assumed. Relative confidence in the data is indicated by the *CL* value of 1 to 4 (1= highest, 4= lowest).

Metal	Distribution (assumed)	Median	Mean	Std. Dev.	Min	Max	Comments
Ag(I)	(log-normal)	---	3.6	1.1	2.1	5.8	Mean from soil K_d regression equation; min, max from literature data; <i>CL</i> = 3
As ^a	Log-normal	2.2	2.4	0.7	1.6	4.3	From literature data; Oxidation state not specified in literature data; <i>CL</i> = 2
Ba(II)	(log-normal)	---	2.5	0.8	0.9	3.2	Mean, min, max from suspended matter K_d regression equation; <i>CL</i> = 3
Be(II)	(log-normal)	---	2.8	1.9	0.8	6.5	Mean, min, max from suspended matter K_d regression equation; <i>CL</i> = 3
Cd(II)	Log-normal	3.7	3.3	1.8	0.5	7.3	From literature data (n= 14, edited); <i>CL</i> = 1
Co(II)	(log-normal)	---	3.1	1.0	2.9	3.6	Mean from soil K_d regression equation; min, max from literature data; <i>CL</i> = 3
Cr(III)	(log-normal)	---	4.9	1.5	1.9	5.9	Mean, min, max from soil K_d regression equation; <i>CL</i> = 4
Cr(VI)	(log-normal)	---	1.7	1.4	0.0	4.4	Mean, min, max from soil K_d regression equation; <i>CL</i> = 4
Cu(II)	Log-normal	4.1	3.5	1.7	0.7	6.2	From literature data (raw, n = 12); <i>CL</i> = 1
Hg(II)	(log-normal)	---	4.9	0.6	3.8	6.0	From literature data (raw, n= 2); <i>CL</i> = 2
MeHg	(log-normal)	---	3.9	0.5	2.8	5.0	From literature data (edited, n= 2), <i>CL</i> = 2
Mo(VI)	(log-normal)	---	2.5	0.8	0.4	3.7	Mean from literature data (reported mean value with oxidation state not specified); min, max from soil K_d regression equation; <i>CL</i> = 4

Table 4 (continued)

Metal partition coefficients ($\log K_d$) in kg/L for sediment/porewater. Values in italics were estimated by regression or from MINTEQA2 results. An entry of “log-normal” in bold indicates that the sample data gave a positive result in the Shapiro-Wilk test for normality of the log-transformed data. An entry of “log-normal” in parentheses means that data were not sufficient to establish the distribution, but log-normal has been assumed. Relative confidence in the data is indicated by the CL value of 1 to 4 (1= highest, 4= lowest).

Metal	Distribution (assumed)	Median	Mean	Std. Dev.	Min	Max	Comments
Ni(II)	(log-normal)	---	3.9	1.8	0.3	4.0	Mean from soil K_d regression equation; min, max from literature data; CL= 3
Pb(II)	Log-normal	5.1	4.6	1.9	2.0	7.0	From literature data (edited, n= 14); CL= 1
Sb ^b	(log-normal)	---	3.6	1.8	0.6	4.8	From literature data (reported mean value); CL= 4
Se(IV)	(log-normal)	---	3.6	1.2	1.0	4.0	Mean from literature data (reported mean value); min, max are guesses; CL= 4
Se(VI)	(log-normal)	---	0.6	1.2	-1.4	3.0	Mean, min, max from soil K_d regression equation; CL= 4
Sn(II)	(log-normal)	---	3.7	0.7	3.1	5.1	Mean, min, max from soil K_d regression equation; CL= 3
Tl(I)	(log-normal)	---	1.3	1.1	-0.5	3.5	Mean, min from soil K_d regression equation; max from literature data; CL= 4
V(V)	(log-normal)	---	2.1	0.9	0.4	3.2	Mean, min, max from suspended matter K_d regression equation; CL= 4
Zn(II)	(log-normal)	4.8	4.1	1.6	1.5	6.2	From literature data (edited, n= 13); CL= 1
CN-	(log-normal)	---	1.6	1.7	-1.8	2.2	Mean, min, max from soil K_d regression equation; CL= 4

^a Published metal partitioning data does not allow differentiation of As(III) and As(V). It is probable that the data presented include results for both oxidation states.

^b Published partitioning data for Sb is rare and does not allow differentiation of Sb(III) and Sb(V).

Table 5

Metal partition coefficients ($\log K_d$) in kg/L for suspended matter/water. Values in italics were estimated by regression or from MINTEQA2 results. An entry of “log-normal” in bold indicates that the sample data gave a positive result in the Shapiro-Wilk test for normality of the log-transformed data. An entry of “log-normal” in parentheses means that data were not sufficient to establish the distribution, but log-normal has been assumed. Relative confidence in the data is indicated by the *CL* value of 1 to 4 (1= highest, 4= lowest).

Metal	Distribution (assumed)	Median	Mean	Std. Dev.	Min	Max	Comments
Ag(I)	Log-normal	5.2	5.2	0.6	4.4	6.3	From literature data (edited, n= 9); <i>CL</i> = 2
As ^a	(log-normal)	4.0	3.9	0.5	2.0	6.0	From literature data (raw, n= 25); oxidation state not specified in the literature data; <i>CL</i> = 2
Ba(II)	Log-normal	4.0	4.0	0.4	2.9	4.5	From literature data (raw, n= 14); <i>CL</i> = 2
Be(II)	Log-normal	4.1	4.2	0.7	2.8	6.8	From literature data (raw, n= 17); <i>CL</i> = 2
Cd(II)	Log-normal	5.0	4.9	0.6	2.8	6.3	From literature data (edited, n= 38); <i>CL</i> = 1
Co(II)	Log-normal	4.7	4.8	0.8	3.2	6.3	From literature data (edited, n= 20); <i>CL</i> = 1
Cr(III)	Log-normal	5.1	5.1	0.4	3.9	6.0	From literature data (raw, n= 25); assumes unspecified oxidation state is (III); <i>CL</i> = 2
Cr(VI)	(log-normal)	---	4.2	0.5	3.6	5.1	Mean, min, max from soil K_d regression equation; <i>CL</i> = 4
Cu(II)	Log-normal	4.7	4.7	0.4	3.1	6.1	From literature data (edited, n= 42); <i>CL</i> = 1
Hg(II)	Log-normal ^b	5.3	5.3	0.4	4.2	6.9	From literature data (edited, n= 26); <i>CL</i> = 1
MeHg	(log-normal)	---	4.9	0.7	4.2	6.2	Mean from soil K_d regression equation; min, max from literature data; <i>CL</i> = 3
Ni(II)	Log-normal ^b	4.3	4.4	0.4	3.5	5.7	From literature data (edited, n= 25); <i>CL</i> = 1
Mo(VI)	(log-normal)	---	4.4	1.0	3.7	4.9	Mean, min, max from soil K_d regression equation; <i>CL</i> = 4
Pb(II)	(log-normal) ^c	5.7	5.7	0.4	3.4	6.5	From literature data (edited, n= 38); <i>CL</i> = 1

Table 5 (continued)

Metal partition coefficients (log K_d) in kg/L for suspended matter/water. Values in italics were estimated by regression or from MINTEQA2 results. An entry of “log-normal” in bold indicates that the sample data gave a positive result in the Shapiro-Wilk test for normality of the log-transformed data. An entry of “log-normal” in parentheses means that data were not sufficient to establish the distribution, but log-normal has been assumed. Relative confidence in the data is indicated by the *CL* value of 1 to 4 (1= highest, 4= lowest).

Metal	Distribution (assumed)	Median	Mean	Std. Dev.	Min	Max	Comments
Sb ^d	(log-normal)	---	<i>4.8</i>	<i>0.5</i>	<i>3.9</i>	<i>4.9</i>	Mean, min, max from soil K_d regression equation; <i>CL</i> = 4
Se(IV)	(log-normal)	---	<i>4.4</i>	<i>0.4</i>	<i>3.8</i>	<i>4.8</i>	Mean, min, max from soil K_d regression equation; <i>CL</i> = 4
Se(VI)	(log-normal)	---	<i>3.8</i>	<i>1.0</i>	<i>3.1</i>	<i>4.6</i>	Mean, min, max from soil K_d regression equation; <i>CL</i> = 4
Sn(II)	(log-normal)	---	<i>4.9</i>	<i>0.8</i>	<i>4.7</i>	6.3	Mean, min from soil K_d regression equation; max from literature data; <i>CL</i> = 4
Tl(I)	(log-normal)	---	<i>4.1</i>	<i>1.0</i>	<i>3.0</i>	<i>4.5</i>	Mean from soil K_d regression equation; other parameters are guesses; <i>CL</i> = 4
V(V)	(log-normal)	---	<i>3.7</i>	<i>0.6</i>	<i>2.5</i>	<i>4.5</i>	Mean from literature data (raw, n= 5); min, max are guesses; oxidation state not always specified in literature; <i>CL</i> = 3
Zn(II)	Log-normal	5.1	5.0	0.5	3.5	6.9	From literature data (edited, n= 47); <i>CL</i> = 1
CN-	(log-normal)	---	<i>4.2</i>	<i>0.6</i>	<i>3.0</i>	<i>4.4</i>	Mean, min, max from soil K_d regression equation; <i>CL</i> = 4

- ^a Positive result for Shapiro-Wilk test for normality of data not log-transformed. But published metal partitioning data does not allow differentiation of As(III) and As(V). It is probable that the data represented include results for both oxidation states.
- ^b Failed Shapiro-Wilk test for normality of log-transformed data, but passed the Kolmogorov-Smirnov test and histogram exhibits log-normal character
- ^c Failed Shapiro-Wilk and the Kolmogorov-Smirnov test for normality of log-transformed data, but histogram exhibits log-normal character
- ^d Published partitioning data for Sb is rare and does not allow differentiation of Sb(III) and Sb(V).

Table 6

Metal partition coefficients ($\log K_d$) in kg/L for partitioning between DOC and inorganic solution species. Values in italics were estimated by regression or from MINTEQA2 results. Log-normal distributions are assumed. Relative confidence in the data is indicated by the *CL* value of 1 to 4 (1= highest, 4= lowest).

Metal	Distribution (assumed)	Mean	Std. Dev.	Min	Max	Comment
Ag(I)	(log-normal)	<i>2.5</i>	<i>1.0</i>	<i>1.5</i>	<i>4.5</i>	Mean estimated from MINTEQA2 results; other parameters are guesses; <i>CL</i> = 3
As	(log-normal)	<i>2.0</i>	<i>1.0</i>	<i>0.0</i>	<i>3.0</i>	No data, values are conservative guesses; <i>CL</i> = 4
Ba(II)	(log-normal)	<i>3.6</i>	<i>1.0</i>	<i>2.5</i>	<i>4.0</i>	Mean estimated from MINTEQA2 results, values for other parameters are guesses; <i>CL</i> = 3
Be(II)	(log-normal)	<i>2.1</i>	<i>1.0</i>	<i>1.1</i>	<i>3.8</i>	All parameters estimated from MINTEQA2 results; <i>CL</i> = 3
Cd(II)	(log-normal)	<i>3.8</i>	<i>0.9</i>	<i>2.0</i>	<i>5.5</i>	Mean estimated from MINTEQA2 results; min, max are guesses; <i>CL</i> = 3
Co(II)	(log-normal)	<i>3.8</i>	<i>0.9</i>	<i>2.0</i>	<i>5.5</i>	Mean estimated from MINTEQA2 results; min, max are guesses; <i>CL</i> = 3
Cr(III)	(log-normal)	<i>1.1</i>	<i>1.6</i>	<i>-0.6</i>	<i>4.3</i>	Mean estimated from MINTEQA2 results; min, max are guesses; <i>CL</i> = 4
Cr(VI)	(log-normal)	<i>2.0</i>	<i>1.0</i>	<i>0.0</i>	<i>3.0</i>	No data, values are conservative guesses; <i>CL</i> = 4
Cu(II)	(log-normal)	<i>5.4</i>	<i>1.1</i>	<i>2.5</i>	<i>7.0</i>	From literature data (raw, n= 17); <i>CL</i> = 2
Hg(II)	(log-normal)	<i>5.4</i>	<i>1.2</i>	<i>3.0</i>	<i>6.0</i>	Mean from literature data (raw, n= 3); min, max are guesses; <i>CL</i> = 4
MeHg	(log-normal)	<i>5.0</i>	<i>1.1</i>	<i>2.8</i>	<i>5.5</i>	Mean, min, max estimated based on relative K_d 's of Hg(II) and MeHg for suspended matter and Hg(II) K_d with DOC.
Ni(II)	(log-normal)	<i>3.7</i>	<i>0.9</i>	<i>1.9</i>	<i>5.4</i>	Mean estimated from MINTEQA2 results; min, max are guesses; <i>CL</i> = 3
Mo(VI)	(log-normal)	<i>2.0</i>	<i>1.0</i>	<i>0.0</i>	<i>3.0</i>	No data, values are conservative guesses; <i>CL</i> = 4
Pb(II)	(log-normal)	<i>4.9</i>	<i>0.5</i>	<i>3.8</i>	<i>5.6</i>	From literature data (raw, n= 9); <i>CL</i> = 2

Table 6 (continued)

Metal partition coefficients ($\log K_d$) in kg/L for partitioning between DOC and inorganic solution species. Values in italics were estimated by regression or from MINTEQA2 results. Log-normal distributions are assumed. Relative confidence in the data is indicated by the *CL* value of 1 to 4 (1= highest, 4= lowest).

Metal	Distribution (assumed)	Mean	Std. Dev.	Min	Max	Comment
Sb	(log-normal)	<i>2.0</i>	<i>1.0</i>	<i>0.0</i>	<i>3.0</i>	No data, values are conservative guesses; <i>CL</i> = 4
Se(IV)	(log-normal)	<i>2.0</i>	<i>1.0</i>	<i>0.0</i>	<i>3.0</i>	No data, values are conservative guesses; <i>CL</i> = 4
Se(VI)	(log-normal)	<i>2.0</i>	<i>1.0</i>	<i>0.0</i>	<i>3.0</i>	No data, values are conservative guesses; <i>CL</i> = 4
Sn(II)	(log-normal)	<i>2.0</i>	<i>1.0</i>	<i>0.0</i>	<i>3.0</i>	No data, values are conservative guesses; <i>CL</i> = 4
Tl(I)	(log-normal)	<i>1.6</i>	<i>1.0</i>	<i>0.0</i>	<i>3.0</i>	Mean estimated from MINTEQA2, values for other parameters are guesses; <i>CL</i> = 4
V(V)	(log-normal)	<i>2.0</i>	<i>1.0</i>	<i>0.0</i>	<i>3.0</i>	No data, values are conservative guesses; <i>CL</i> = 4
Zn(II)	(log-normal)	<i>5.1</i>	<i>0.7</i>	<i>4.6</i>	<i>6.4</i>	From literature data (raw, n= 9); <i>CL</i> = 3
CN-	(log-normal)	<i>2.0</i>	<i>1.0</i>	<i>0.0</i>	<i>3.0</i>	No data, values are conservative guesses; <i>CL</i> = 4

3.2 DEVELOPMENT OF PARTITIONING COEFFICIENTS FOR WASTE SYSTEMS

The multimedia, multi-pathway risk assessment for HWIR utilizes a source model that assumes equilibrium partitioning in land application units (LAUs), waste piles, landfills, treatment lagoons (surface impoundments), and aerated tanks. The available data for characterizing the partitioning of metals in waste consists almost exclusively of leach test results for specific wastes. The literature search did not produce any study that specifically provides measured partitioning coefficients for metals in the mixed materials present in waste management units.

Several studies have addressed the issue of the applicability of leach test data in predicting the leachate concentration from landfills (U.S. EPA, 1991). The U.S. EPA Toxicity Characteristic Leaching Procedure (TCLP) was specifically designed to predict leachate concentrations for wastes co-disposed with municipal solid waste. Recent papers present the idea that the concentration observed in any leach test depends a great deal on leaching time and the cumulative solid-liquid ratio (van der Sloot et al., 1996). Three “regimes” are recognized in the leaching process (de Groot and van der Sloot, 1992): 1) leaching concentration controlled by initial wash-off of loosely adhered contaminant, 2) leaching concentration controlled by dissolution of primary materials and perhaps re-precipitation of more stable phases, and 3) leaching concentration controlled by the diffusion of waste constituent from the interior of waste particles to the particle surface. The time of onset and duration of these regimes is highly variable and is interrelated with the life-cycle of the waste system (acetogenesis, methanogenesis, etc.). The chemical composition (major ion concentration and concentration of metal-complexing organic ligands) is also important in determining the leaching concentration that will be observed in any particular case. In general, it would seem that the highest concentrations are expected during the initial wash-off period, with concentrations declining thereafter. An immediately obvious question is: What period is of concern in the modeling for the HWIR rulemaking? Since, the model does not allow a time-variable partition coefficient, it would seem that an aggregate partition coefficient that represents an average over time would be desired. Unfortunately, there is currently no way to know whether the “partitioning” observed in a TCLP test corresponds to such an average value. Most authors seem to regard the TCLP as an aggressive test that may overestimate metal concentrations. However, there is no consensus on this point.

In view of the lack of data describing partitioning of metals in different types of waste units, the following simplifications are proposed:

- 1) For land application units, the partition coefficients for soils presented in Table 3 should be used. This simplification assumes that the partitioning behavior of metals in an LAU is likely to be dominated by the sorptive characteristics of the soil underlying the unit.
- 2) For surface impoundments and aerated tanks, the partition coefficients for suspended matter presented in Table 5 should be used. This seems a reasonable step in that partitioning in such systems must involve sorption to suspended particles and sediments. The composition and quantity of suspended and sedimented sorbing particles must be quite variable, but there is no source of data on which to base modeling or other estimating techniques.

3) Waste piles and landfills should be treated the same as regards metal partitioning.

Adopting these simplifications, it is necessary to derive estimates of metal partition coefficients for waste piles and landfills only. The sections below detail how these have been estimated from available TCLP and similar leach tests that present both solid phase and corresponding leachate concentrations. We have used statistical methods and geochemical speciation modeling to extend results to metals not represented in reported TCLP or other leach test results and to examine the similarity between expected waste partitioning and partitioning in natural media.

3.2.1 Estimation from Analysis of Data Presented in the Literature

There are numerous papers and journal articles describing results from a TCLP or similar leach test for a particular waste. These published studies often focus on waste constituent leachability before and after a waste stabilization or treatment process. There are many published studies of leachability of metals from incinerator ash with the aim of investigating the suitability of the ash materials for disposal or for use in construction. Frequently, leach test results (leachate concentrations) are reported without the corresponding concentration in the solid phase. This omission makes those data useless in estimating expected partitioning. The literature survey produced 203 leach test results for which both leachate and solid phase data are presented. Table 7 shows the range and mean values of effective partition coefficients for each metal for which sufficient data was found. We refer to these as effective partition coefficients because they are simply the ratio of metal in the solid and solution phases as represented in the leach test results. They may or may not represent equilibrium partitioning.

Several authors discussed the similarities in metal leachability over a range of different materials. A study by van der Sloot et al. (1996) examined the leaching behavior of Cd and Zn from various ash materials, shredded municipal solid waste, sewage sludge-amended soil, and soil. Similar characteristics were noted in pH dependent leaching of both Cd and Zn from the nine different materials studied. Differences among the different materials were attributed to waste-specific chemical parameters that caused a different chemical speciation. The authors gave an example of Cd complexation with chloride which they investigated using MINTEQA2. The increased leachability of Cd in some of the ash materials was correlated with chloride concentration in the waste.

Flyhammar (1997) concluded that there are similarities in the metal binding properties of municipal solid waste (MSW) and sediments. He found that the fractionation of metals among various available and reactive forms (as determined by sequential chemical extractions) was similar between fresh MSW and an oxic sediment. Similarities were also found in the fractionation patterns of aged MSW and anoxic sediments.

Table 7

Effective partition coefficients based on reported solid phase and solution phase metals concentrations from leach tests reported in the literature. N is number of samples; mean and range are expressed in log units (L/kg).

Metal	N	Mean	Range
As	11	2.8	1.0 - 5.1
Ba	7	3.0	1.8 - 3.7
Be	2	2.8	2.7 - 6.8
Cd	31	1.3	0 - 3.9
Co	6	2.8	1.6 - 3.8
Cr(III)	27	3.0	0.6 - 6.2
Cr(VI)	6	4.1	2.2 - 6.2
Cu	16	3.3	2.0 - 5.1
Hg	8	3.1	1.7 - 4.4
Ni	12	2.3	1.3 - 4.7
Pb	31	2.7	0.0 - 4.9
Sb	4	2.7	1.7 - 3.2
V	4	2.9	2.7 - 3.1
Zn	23	2.6	1.2 - 4.7

The consistency in the affinity relationships of metals noted in Section 3.1.1 and the similarities noted by these authors in the fractionation and behavior of metals in waste versus that in soils and sediments leads to the supposition that the partitioning behavior of metals in mixed waste systems might not be altogether different from that of a natural medium. It would perhaps be surprising if the relative affinities for different metals in waste were markedly different from their relative affinities in natural materials. There may certainly be some deviations due to the presence of one or more complexing agents in waste systems that have a preference for complexing certain of the metals. However, in the absence of data to quantify this effect, and also in consideration of the paucity of actual partitioning data for waste systems, we have developed a regression equation that predicts waste K_d from soil K_d . We chose to use soil K_d as the predictor because a comparison of K_d values for soils, sediments and suspended matter suggests that the solid to liquid concentration ratio is important in determining the magnitude of K_d . This ratio for waste is probably more similar to that of soils than any other medium. Also, we note that landfilled waste is typically covered with soil to form soil/waste layers within a landfill cell. In developing this relationship, we used the effective partition coefficients for the metals for which we had the

most complete (largest) sample. The regression equation thus determined is $\log K_{d,waste} = 0.7 \log K_{d,soil} + 0.3$. The relationship has a correlation coefficient of (r^2) of 0.4 implying that 40% of the variation in $\log K_{d,waste}$ from the leach test data is predicted.

3.2.2 Estimation from Geochemical Speciation Modeling

The MINTEQA2 geochemical speciation model was used to investigate the range of metal partitioning coefficients for landfills. The input requirements of the model for estimating metal partitioning include the concentrations of major ions, the pH, the concentrations of sorbing phases, and the DOC concentration. Four landfill modeling scenarios were developed, distinguished primarily by the concentrations of major ions, the DOC concentration, the POC concentration, and the pH. The scenarios included landfills containing municipal solid waste in the acetogenic stage and in the methanogenic stage, a monofill containing ash from incineration of municipal solid waste (MSWI ash), and a monofill containing cement kiln dust (CKD).

For each of the MINTEQA2 modeling scenarios, a hydrous ferric oxide sorbing phase was assumed. A particulate organic carbon sorbent was also assumed for the acetogenic and methanogenic MSW landfills. Particulate organic carbon was assumed to have been consumed in the incineration process for the MSWI and CKD scenarios. The concentration of the sorbent is crucial in determining the number of sites available for metal sorption. Unfortunately, the concentration of sorbent appropriate in waste systems is subject to a very high degree of uncertainty. The uncertainty arises from the variable composition of wastes that are disposed in landfills and the possible changes in composition over time as leachate percolates through the materials. It is not unlikely that surfaces exposed to landfill gas and leachate undergo changes with respect to their sorptive character over time. Possible changes include dissolution or precipitation of oxide or organic surface coatings. These processes have not been studied in actual landfill samples in sufficient detail to allow quantitative representation. Kersten et al. (1997) cited evidence of sorption control of Pb leaching in MSWI leach tests. They attempted to model the observed Pb concentrations by utilizing a speciation model with surface complexation sorption reactions parameterized for the constant capacitance model assuming hydrous ferric oxide as the sorbent. They obtained reasonable results assuming 0.7 g/L for the HFO concentration and using a site density of 1.35×10^{-4} mol sites/g HFO. The MINTEQA2 modeling presented here utilized a similar surface complexation model (the diffuse-layer model). Kersten et al. (1997) had noted that their sorbent concentration was perhaps too low, so the modeling was conducted both with their value of 0.7 g/L, and using 7 g/L as a reasonable upper-range value. In both cases, a site density 1.35×10^{-4} mol sites/g HFO was used.

The values of other parameters and constituent concentrations used in the modeling for the four scenarios are shown in Table 8. After concentration of sorbing sites, the most critical model parameter is pH, so the modeling was conducted at three different pH values for each scenario. The three pH values used for the acetogenic and methanogenic scenarios (4.5, 6.1, 7.5 and 7.5, 8.0, 9.0, respectively) were in keeping with the minimum, maximum and mean pH cited for these landfill stages in a study of 15 landfills by Ehrig (1992). The major ion

concentrations for the acetogenic and methanogenic scenarios were also as specified in Ehrig (1992). The three pH values for the MSWI scenario (8.0, 9.0, 10.0) were selected to define a reasonable range and central tendency value for this scenario. These values were based on data collected in the literature review portion of this study, as were the major ion concentrations for the MSWI scenario. The pH values associated with the CKD scenario were selected with due consideration to the highly alkaline conditions associated with this material, but they lack statistical significance. An example MINTEQA2 input file for each of the scenarios is presented in Appendix D.

It should be noted that the confidence level associated with all of the modeling parameters for waste systems is low. There is not an extensive database of observations from which to extract reasonable model values for most of these parameters, especially the concentration of sorbents and sorbing sites. Without reliable information for characterizing the sorbents, it is not possible to accurately establish the total system concentrations of competing ions (Ca, Mg, etc.) that should be used in the model. The results must be interpreted in light of this shortcoming.

Table 8
Important parameters and constituent concentrations used in MINTEQA2 modeling of landfills in the acetogenic and methanogenic stages and MSWI and CKD monofills.

Model Parameter	Scenario			
	MSW Acetogenic	MSW Methanogenic	MSWI Ash Monofill	CKD Monofill
pH	4.5, 6.1, 7.5 ^a	7.5, 8.0, 9.0 ^a	8.0, 9.0, 10.0 ^b	9.0, 10.0, 11.0 ^c
Ca	6000 ^d	975 ^d	1,700 ^b	2850 ^f
Mg	625 ^d	500 ^d	10 ^b	10 ^f
Na	1350 ^e	1350 ^e	300 ^b	300 ^f
K	1100 ^e	1100 ^e	380 ^b	400 ^f
CO ₃	500 ^c	250 ^c	50 ^c	50 ^f
Cl	2100 ^e	2100 ^e	1,200 ^b	380 ^f
Fe	780 ^e	---	---	---
SO ₄	500 ^d	80 ^d	1,400 ^b	630 ^f
Ionic Strength (M)	0.1 ^c	0.1 ^c	0.1 ^c	0.1 ^c
DOC	100 ^c	50 ^c	15 ^c	15 ^c
POC	100,000 ^c	50,000 ^c	---	---

^a Minimum, average, and maximum values reported in Ehrig (1992)

^b Obtained from analysis of data MSWI obtained in literature survey

^c Reasonable guesses

^d Computed from typical dissolved values reported in Ehrig (1992) and assuming equilibrium with the model sorbents at the median pH for acetogenic and methanogenic cases.

^e Reported as typical values in Ehrig (1992)

^f Generated from simulation of TCLP on CKD using MINTEQA2 (U.S. EPA, 1998b)

The partitioning coefficients estimated from the MINTEQA2 modeling exercise for several metals are shown in Table 9. The values presented were converted to units of L/kg by assuming that one liter of leachate solution is associated with 5 kg of waste material. The range in estimated partition coefficients is shown for each scenario. In interpreting these results, it must be remembered that no statistical significance can be assigned because none can be associated with most of the model input parameters. At best, these results should be

regarded as indicating a possible range of central tendency values, and even this must be qualified because the results are so sensitive to several poorly characterized parameters, most notably, the concentration of sorbents. The results also reflect only a single concentration value for each of the major ions— variability in these concentrations will influence metal partitioning. Some ions exert greater influence on the partitioning of particular metals. For example, the low partition coefficients associated with Cd appear to be related to complexation with chloride, which is entered at high concentrations in all scenarios. This effect is in keeping with observations by others (van der Sloot et al., 1996). Another major ion whose concentration level may influence metal partitioning is calcium. At the high concentrations of these ions in waste systems, especially MSWI ash and CKD, the competition for binding sites can become very important with regard to trace metal binding. For those metals whose partitioning is significantly influenced by the concentration level of a major ion, it is expected that this fact would contribute to a broader range of observed partition coefficients in real systems than that calculated in this modeling exercise.

Table 9
Estimated range in log partition coefficients (L/kg) for selected metals determined from MINTEQA2 modeling.

Metal	Estimated log K_d (L/kg)			
	MSW Acetogenesis	MSW Methanogenesis	MSWI Ash Monofill	CKD Monofill
Be	0.8 - 3.9	3.3 - 4.4	(-0.4) - 4.0	---
Cd	(-0.3) - 0.0	0.6 - 1.7	(-1.0) - 1.1	(-0.4) - 1.2
Co	0.2 - 0.3	0.9 - 1.8	(-0.9) - 0.4	(-2.0) - 0.2
Cr(III)	1.1 - 3.5	3.8 - 4.8	(-0.2) - 3.2	---
Cu	1.1 - 1.9	2.0 - 2.5	0.0 - 2.9	(-2.0) - 2.1
Ni	0.2 - 0.4	1.1 - 1.9	(-0.04) - 1.1	(- 1.5) - 0.9
Pb	1.7 - 2.7	3.3 - 4.2	2.4 - 3.6	0.7 - 3.4
Zn	0.4 - 0.7	1.5 - 2.1	(-0.6) - 1.3	---

In comparing the partition coefficients estimated using MINTEQA2 with those for soils, there is greater agreement with values predicted by the derived regression equation ($\log K_{d,waste} = 0.7 \log K_{d,soil} + 0.3$; see Section 3.2.1) for some metals than for others. (The measure of “agreement” for a metal is whether the value predicted by the equation using the mean soil K_d value of Table 3 falls within the range of MINTEQA2 estimates for that metal. Using this rather lax requirement for agreement, the modeled K_d values for Be, Cr(III), Cu, and Pb agree, those of Cd and Ni do not agree, and those of Co and Zn are marginal.) Like the literature-reported K_d values for natural media, Pb and Cr(III) tend to have high K_d

estimates from MINTEQA2 . In general, the results for the acetogenic and methanogenic landfill scenarios agree more closely with the regression relationship with soil K_d values than do the more alkaline cases for ash and CKD. It is probable that the lower K_d values in the latter are due to the combination of high major ion concentrations that compete for sorbing sites and solubilize the metals by complexation, and the absence of particulate organic carbon in the model systems.

In view of the uncertainties inherent in the model results, a possible alternative for representing metal partitioning in waste piles and landfills is to use the regression equation presented in Section 3.2.1. This has the advantage of preserving the relative affinities among metals that has been noted as common to the natural media. However, the model results do suggest that the K_d values in alkaline systems may be significantly lower than in municipal landfills. This might be accounted for by treating the slope and intercept coefficients in the regression as variables subject to uncertainty that can be represented in the monte carlo iterations. In the overall modeling strategy of HWIR, if the frequency of occurrence of a highly alkaline waste system can be established and used in the monte carlo realizations, the coefficients could be adjusted to give lower K_d values for the appropriate fraction of realizations to reflect alkaline systems. This topic needs further study, as does the entire issue of equilibrium partitioning in waste. It should be noted that of the several studies reviewed whose authors suggested mechanisms controlling the leachate concentrations of metals, most advocated a mineral solubility control rather than equilibrium partitioning (Bäverman et al., 1997; Kersten et al., 1997; Johnson et al., 1996; Eighmy et al., 1995; Yan and Neretnieks, 1995; Fruchter et al., 1990; Moretti et al., 1988; Gould et al., 1988). However, the difficulty in distinguishing solubility controls from effects of sorption is also noted. It is possible that metals are initially mobilized by dissolution of solid phases, especially in ash and CKD, but that surface coatings that form upon aging eventually control solution phase metal concentrations via sorption (van der Sloot et al., 1996). More research is need to quantify these processes in waste systems.

4.0 REFERENCES

The reference list includes the complete bibliography of papers, articles, and reports that were copied and reviewed in the literature search. Those articles which provided data for spreadsheet entry are identified by a code in square brackets at the end of the citation. The code can be cross-referenced to spreadsheet entries. Further explanation of spreadsheet entries is provided in the spreadsheet itself.

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APPENDIX A

**METAL PARTITION COEFFICIENTS USED IN
SOME PREVIOUS U.S. EPA RISK ASSESSMENTS**

Metal	Risk Assessment	Type of Kd	Kd(L/kg)	
			Single Value	Range
Ag	US EPA Region 6 Combustion [USEPA96b]	soil/water	---	0.1 - 110
	US EPA Region 6 Combustion [USEPA96b]	suspended matter /water	---	0.1 - 110
	US EPA Region 6 Combustion [USEPA96b]	sediment/water	---	0.1 - 110
	Soil-Screening Guidance [USEPA96c]	soil/water	---	0.1 - 110
	Sewage Sludge Rule, Round 2 [USEPA96d]	soil/water	290	---
As	US EPA Region 6 Combustion [USEPA96b]	soil/water	---	25 - 31
	US EPA Region 6 Combustion [USEPA96b]	suspended matter /water	---	25 - 31
	US EPA Region 6 Combustion [USEPA96b]	sediment/water	---	25 - 31
	Sewage Sludge Rule [USEPA92]	waste/leachate	20	---
	Sewage Sludge Rule [USEPA92]	suspended matter /water	63,700	---
	Soil-Screening Guidance [USEPA96c]	soil/water	---	25 - 31
	Chlorinated Aliphatics Listing [USEPA?]	soil/water	29	---
Ba	US EPA Region 6 Combustion [USEPA96b]	soil/water	---	11 - 52
	US EPA Region 6 Combustion [USEPA96b]	suspended matter /water	---	11 - 52
	US EPA Region 6 Combustion [USEPA96b]	sediment/water	---	11 - 52
	Soil-Screening Guidance [USEPA96c]	soil/water	---	11 - 52
	Sewage Sludge Rule, Round 2 [USEPA96d]	soil/water	6	---
	Chlorinated Aliphatics Listing [USEPA?]	soil/water	530	---
Be	US EPA Region 6 Combustion [USEPA96b]	soil/water	---	23 - 100,000
	US EPA Region 6 Combustion [USEPA96b]	suspended matter /water	---	23 - 100,000
	US EPA Region 6 Combustion [USEPA96b]	sediment/water	---	23 - 100,000
	Soil-Screening Guidance [USEPA96c]	soil/water	---	23 - 100,000
	Sewage Sludge Rule, Round 2 [USEPA96d]	soil/water	43	---

Metal	Risk Assessment	Type of Kd	Kd(L/kg)	
			Single Value	Range
Cd	US EPA Region 6 Combustion [USEPA96b]	soil/water	---	15 - 4300
	US EPA Region 6 Combustion [USEPA96b]	suspended matter /water	---	15 - 4300
	US EPA Region 6 Combustion [USEPA96b]	sediment /water	---	15 - 4300
	Sewage Sludge Rule [USEPA92]	waste/leachate	431	---
	Sewage Sludge Rule [USEPA92]	suspended matter /water	174,000	---
	Soil-Screening Guidance [USEPA96c]	soil/water	---	15 - 4300
	Chlorinated Aliphatics Listing [USEPA?]	soil/water	162	---
Co	Chlorinated Aliphatics Listing [USEPA?]	soil/water	45	---
Cr	US EPA Region 6 Combustion [USEPA96b]	soil/water	---	1200 - 4.3E06
	US EPA Region 6 Combustion [USEPA96b]	suspended matter /water	---	1200 - 4.3E06
	US EPA Region 6 Combustion [USEPA96b]	sediment /water	---	1200 - 4.3E06
	Sewage Sludge Rule [USEPA92]	waste/leachate	59	---
	Sewage Sludge Rule [USEPA92]	suspended matter /water	255,000	---
	Soil-Screening Guidance [USEPA96c]	soil/water	---	1200 - 4.3E06
Cr(VI)	US EPA Region 6 Combustion [USEPA96b]	soil/water	---	14 - 31
	US EPA Region 6 Combustion [USEPA96b]	suspended matter /water	---	14 - 31
	US EPA Region 6 Combustion [USEPA96b]	sediment /water	---	14 - 31
	Soil-Screening Guidance [USEPA96c]	soil/water	---	14 - 31
	Chlorinated Aliphatics Listing [USEPA?]	soil/water	18	---
Cu	Sewage Sludge Rule [USEPA92]	waste/leachate	98	---
	Sewage Sludge Rule [USEPA92]	suspended matter /water	132,000	---
	Chlorinated Aliphatics Listing [USEPA?]	soil/water	22	---
Hg	US EPA Region 6 Combustion [USEPA96b]	soil/water	1000	---
	US EPA Region 6 Combustion [USEPA96b]	suspended matter /water	1000	---

Metal	Risk Assessment	Type of Kd	Kd(L/kg)	
			Single Value	Range
	US EPA Region 6 Combustion [USEPA96b]	sediment /water	3000	---
	Sewage Sludge Rule [USEPA92]	waste/leachate	330	---
	Sewage Sludge Rule [USEPA92]	suspended matter /water	125,000	---
	Soil-Screening Guidance [USEPA96c]	soil/water	---	0.04 - 200
Mo	Chlorinated Aliphatics Listing [USEPA?]	soil/water	20	---
Ni	US EPA Region 6 Combustion [USEPA96b]	soil/water	---	16 - 1900
	US EPA Region 6 Combustion [USEPA96b]	suspended matter /water	---	16 - 1900
	US EPA Region 6 Combustion [USEPA96b]	sediment /water	---	16 - 1900
	Sewage Sludge Rule [USEPA92]	waste/leachate	63	---
	Sewage Sludge Rule [USEPA92]	suspended matter /water	100,000	---
	Soil-Screening Guidance [USEPA96c]	soil/water	---	16 - 1900
	Chlorinated Aliphatics Listing [USEPA?]	soil/water	82	---
Pb	US EPA Region 6 Combustion [USEPA96b]	soil/water	900	---
	US EPA Region 6 Combustion [USEPA96b]	suspended matter /water	900	---
	US EPA Region 6 Combustion [USEPA96b]	sediment /water	900	---
	Sewage Sludge Rule [USEPA92]	waste/leachate	621	---
	Sewage Sludge Rule [USEPA92]	suspended matter /water	185,000	---
	Chlorinated Aliphatics Listing [USEPA?]	soil/water	280,000	---
Sb	US EPA Region 6 Combustion [USEPA96b]	soil/water	45	---
	US EPA Region 6 Combustion [USEPA96b]	suspended matter /water	45	---
	US EPA Region 6 Combustion [USEPA96b]	sediment /water	45	---
	Soil-Screening Guidance [USEPA96c]	soil/water	45	---
	Sewage Sludge Rule, Round 2 [USEPA96d]	soil/water	6	---
Se	US EPA Region 6 Combustion [USEPA96b]	soil/water	---	2.2 - 18

Metal	Risk Assessment	Type of Kd	Kd(L/kg)	
			Single Value	Range
	US EPA Region 6 Combustion [USEPA96b]	suspended matter /water	---	2.2 - 18
	US EPA Region 6 Combustion [USEPA96b]	sediment /water	---	2.2 - 18
	Soil-Screening Guidance [USEPA96c]	soil/water	---	2.2 - 18
Tl	US EPA Region 6 Combustion [USEPA96b]	soil/water	---	44 - 96
	US EPA Region 6 Combustion [USEPA96b]	suspended matter /water	---	44 - 96
	US EPA Region 6 Combustion [USEPA96b]	sediment /water	---	44 - 96
	Soil-Screening Guidance [USEPA96c]	soil/water	---	44 - 96
V	Soil-Screening Guidance [USEPA96c]	soil/water	1000	---
	Sewage Sludge Rule, Round 2 [USEPA96d]	soil/water	39	---
	Chlorinated Aliphatics Listing [USEPA?]	soil/water	50	---
Zn	US EPA Region 6 Combustion [USEPA96b]	soil/water	62	---
	US EPA Region 6 Combustion [USEPA96b]	suspended matter /water	62	---
	US EPA Region 6 Combustion [USEPA96b]	sediment /water	62	---
	Soil-Screening Guidance [USEPA96c]	soil/water	---	16 - 530
	Chlorinated Aliphatics Listing [USEPA?]	soil/water	40	---
CN	Soil-Screening Guidance [USEPA96c]	soil/water	9.9	---
	Sewage Sludge Rule, Round 2 [USEPA96d]	soil/water	0.0014	---

APPENDIX B

**EXAMPLE INPUT FILE FOR THE MINTEQA2
MODEL USED TO ESTIMATE PARTITIONING IN SOIL**

Estimate Kd in soil/soil water

MMMM: Md Dissolved OM , Md FeO Sorbent, Md Particulate OM , Md pH

17.00 MG/L 0.010 3.56000E+00

0 1 1 0 2 3 1 0 1 0 0 1 2

Co_soil.prn 200

5.00 19100. 145.00 0.000 0.00

4 1 7

5.940E-01 600.00 0.000 0.000 81

330	0.000E+00	-4.90 y	/H+ 1
200	1.000E-03	-12.32 y	/Co+ 2
150	1.320E+01	-2.92 y	/Ca+ 2
460	3.600E+00	-3.24 y	/Mg+ 2
410	1.200E+00	-4.13 y	/K+ 1
500	5.300E+00	-3.02 y	/Na+ 1
140	5.200E+01	-2.51 y	/CO3-2
180	5.700E+00	-3.37 y	/Cl-1
580	5.000E-01	-6.02 y	/PO4-3
732	6.600E+00	-3.58 y	/SO4-2
90	6.200E-02	-4.00 y	/H3BO3
144	0.000E+00	-6.00 y	/DOM1
145	0.000E+00	-6.00 y	/DOM1
811	3.337E-05	-4.45 y	/ADS1TYP1
812	1.335E-03	-2.84 y	/ADS1TYP2
813	0.000E+00	0.00 y	/ADS1PSIo

3 1

330 6.5000 0.0000 /H+ 1

6 1

813 0.0000 0.0000 /ADS1PSIo

2 74

8113302 = FeOH2+	0.0000	7.2900	0.000	0.000	1.00	0.00	0.00	0.0000
0.00 3 1.000 811 1.000 330 1.000 813	0.000	0	0.000	0	0.000	0	0.000	0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0	0.000	0	0.000	0	0.000	0	0.000	0
0 0.000 0 0.000 0 0.000 0	0.000	0	0.000	0	0.000	0	0.000	0
8113301 = FeO-	0.0000	-8.9300	0.000	0.000	-1.00	0.00	0.00	0.0000
0.00 3 1.000 811 -1.000 330 -1.000 813	0.000	0	0.000	0	0.000	0	0.000	0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0	0.000	0	0.000	0	0.000	0	0.000	0
0 0.000 0 0.000 0 0.000 0	0.000	0	0.000	0	0.000	0	0.000	0
8123302 = FeOH2+	0.0000	7.2900	0.000	0.000	1.00	0.00	0.00	0.0000
0.00 3 1.000 812 1.000 330 1.000 813	0.000	0	0.000	0	0.000	0	0.000	0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0	0.000	0	0.000	0	0.000	0	0.000	0
0 0.000 0 0.000 0 0.000 0	0.000	0	0.000	0	0.000	0	0.000	0
8123301 = FeO-	0.0000	-8.9300	0.000	0.000	-1.00	0.00	0.00	0.0000
0.00 3 1.000 812 -1.000 330 -1.000 813	0.000	0	0.000	0	0.000	0	0.000	0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0	0.000	0	0.000	0	0.000	0	0.000	0
0 0.000 0 0.000 0 0.000 0	0.000	0	0.000	0	0.000	0	0.000	0
8111000 = FeOHBa+ 2	0.0000	5.4600	0.000	0.000	2.00	0.00	0.00	0.0000
0.00 3 1.000 811 1.000 100 2.000 813	0.000	0	0.000	0	0.000	0	0.000	0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0	0.000	0	0.000	0	0.000	0	0.000	0
0 0.000 0 0.000 0 0.000 0	0.000	0	0.000	0	0.000	0	0.000	0
8121000 = FeOBa+	0.0000	-7.2000	0.000	0.000	1.00	0.00	0.00	0.0000
0.00 4 1.000 812 1.000 100 -1.000 330 1.000 813	0.000	0	0.000	0	0.000	0	0.000	0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0	0.000	0	0.000	0	0.000	0	0.000	0
0 0.000 0 0.000 0 0.000 0	0.000	0	0.000	0	0.000	0	0.000	0

8111500 = FeOHCa+ 2 0.0000 4.9700 0.000 0.000 2.00 0.00 0.00 0.0000
 0.00 3 1.000 811 1.000 150 2.000 813 0.000 0 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0

8121500 = FeOCa+ 0.0000 -5.8500 0.000 0.000 1.00 0.00 0.00 0.0000
 0.00 4 1.000 812 1.000 150 -1.000 330 1.000 813 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0

8124600 = FeOMg+ 0.0000 -4.6000 0.000 0.000 1.00 0.00 0.00 0.0000
 0.00 4 1.000 812 1.000 460 -1.000 330 1.000 813 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0

8118700 = FeOTl 0.0000 -3.5000 0.000 0.000 0.00 0.00 0.00 0.0000
 0.00 3 1.000 811 1.000 870 -1.000 330 0.000 0 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0

8128700 = FeOTl 0.0000 -6.9000 0.000 0.000 0.00 0.00 0.00 0.0000
 0.00 3 1.000 812 1.000 870 -1.000 330 0.000 0 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0

8110200 = FeOAg 0.0000 -1.7200 0.000 0.000 0.00 0.00 0.00 0.0000
 0.00 3 1.000 811 1.000 20 -1.000 330 0.000 0 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0

8120200 = FeOAg 0.0000 -5.3000 0.000 0.000 0.00 0.00 0.00 0.0000
 0.00 3 1.000 812 1.000 20 -1.000 330 0.000 0 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0

8115400 = FeONi+ 0.0000 0.3700 0.000 0.000 1.00 0.00 0.00 0.0000
 0.00 4 1.000 811 1.000 540 -1.000 330 1.000 813 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0

8125400 = FeONi+ 0.0000 -2.5000 0.000 0.000 1.00 0.00 0.00 0.0000
 0.00 4 1.000 812 1.000 540 -1.000 330 1.000 813 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0

8112000 = FeOCo+ 0.0000 -0.4600 0.000 0.000 1.00 0.00 0.00 0.0000
 0.00 4 1.000 811 1.000 200 -1.000 330 1.000 813 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0

8122000 = FeOCo+ 0.0000 -3.0100 0.000 0.000 1.00 0.00 0.00 0.0000
 0.00 4 1.000 812 1.000 200 -1.000 330 1.000 813 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0

8111600 = FeOCd+ 0.0000 0.4700 0.000 0.000 1.00 0.00 0.00 0.0000
 0.00 4 1.000 811 1.000 160 -1.000 330 1.000 813 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0

8121600 = FeOCd+ 0.0000 -2.9000 0.000 0.000 1.00 0.00 0.00 0.0000
 0.00 4 1.000 812 1.000 160 -1.000 330 1.000 813 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0

8119500 = FeOZn+ 0.0000 0.9900 0.000 0.000 1.00 0.00 0.00 0.0000
 0.00 4 1.000 811 1.000 950 -1.000 330 1.000 813 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0

```

0 0.000 0 0.000 0 0.000 0
8129500 = FeOZn+      0.0000 -1.9900 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 4 1.000 812 1.000 950 -1.000 330 1.000 813 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8112310 = FeOCu+     0.0000 2.8900 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 4 1.000 811 1.000 231 -1.000 330 1.000 813 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8123100 = FeOCu+     0.0000 0.6000 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 4 1.000 812 1.000 231 -1.000 330 1.000 813 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8116000 = FeOPb+     0.0000 4.6500 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 4 1.000 811 1.000 600 -1.000 330 1.000 813 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8126000 = FeOPb+     0.0000 0.3000 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 4 1.000 812 1.000 600 -1.000 330 1.000 813 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8111100 = FeOBe+     0.0000 5.7000 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 4 1.000 811 1.000 110 -1.000 330 1.000 813 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8121100 = FeOBe+     0.0000 3.3000 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 4 1.000 812 1.000 110 -1.000 330 1.000 813 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8113610 = FeOHg+     0.0000 13.9500 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 5 1.000 811 1.000 361 -2.000 2 1.000 330 1.000 813 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8123610 = FeOHg+     0.0000 12.6400 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 5 1.000 812 1.000 361 -2.000 2 1.000 330 1.000 813 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8117900 = FeOSn+     0.0000 15.1000 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 5 1.000 811 1.000 790 -2.000 2 1.000 330 1.000 813 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8127900 = FeOSn+     0.0000 13.0000 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 5 1.000 812 1.000 790 -2.000 2 1.000 330 1.000 813 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8112110 = FeOCrOH+   0.0000 11.6300 0.000 0.000 1.00 0.00 0.00 0.0000
0.00 4 1.000 811 1.000 211 -1.000 2 1.000 813 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8110600 = FeH2AsO3   0.0000 5.4100 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 3 1.000 811 1.000 60 -1.000 2 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8120600 = FeH2AsO3   0.0000 5.4100 0.000 0.000 0.00 0.00 0.00 0.0000
0.00 3 1.000 812 1.000 60 -1.000 2 0.000 0 0.000 0 0.000 0

```



```

0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8110900 = FeH2BO3      0.0000  0.6200  0.000  0.000 0.00 0.00 0.00 0.0000
0.00 3 1.000 811 1.000 90 -1.000 2 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8120900 = FeH2BO3      0.0000  0.6200  0.000  0.000 0.00 0.00 0.00 0.0000
0.00 3 1.000 812 1.000 90 -1.000 2 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8115800 = FeH2PO4      0.0000  31.2900  0.000  0.000 0.00 0.00 0.00 0.0000
0.00 4 1.000 811 1.000 580 3.000 330 -1.000 2 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8125800 = FeH2PO4      0.0000  31.2900  0.000  0.000 0.00 0.00 0.00 0.0000
0.00 4 1.000 812 1.000 580 3.000 330 -1.000 2 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8115801 = FeHPO4-      0.0000  25.3900  0.000  0.000-1.00 0.00 0.00 0.0000
0.00 5 1.000 811 1.000 580 2.000 330 -1.000 2 -1.000 813 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8125801 = FeHPO4-      0.0000  25.3900  0.000  0.000-1.00 0.00 0.00 0.0000
0.00 5 1.000 812 1.000 580 2.000 330 -1.000 2 -1.000 813 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8115802 = FePO4-2      0.0000  17.7200  0.000  0.000-2.00 0.00 0.00 0.0000
0.00 5 1.000 811 1.000 580 1.000 330 -1.000 2 -2.000 813 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8125802 = FePO4-2      0.0000  17.7200  0.000  0.000-2.00 0.00 0.00 0.0000
0.00 5 1.000 812 1.000 580 1.000 330 -1.000 2 -2.000 813 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8110610 = FeH2AsO4     0.0000  8.6100  0.000  0.000 0.00 0.00 0.00 0.0000
0.00 3 1.000 811 1.000 61 -1.000 2 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8120610 = FeH2AsO4     0.0000  8.6100  0.000  0.000 0.00 0.00 0.00 0.0000
0.00 3 1.000 812 1.000 61 -1.000 2 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8110611 = FeHASO4-     0.0000  2.8100  0.000  0.000-1.00 0.00 0.00 0.0000
0.00 5 1.000 811 1.000 61 -1.000 2 -1.000 330 -1.000 813 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8120611 = FeHASO4-     0.0000  2.8100  0.000  0.000-1.00 0.00 0.00 0.0000
0.00 5 1.000 812 1.000 61 -1.000 2 -1.000 330 -1.000 813 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8119032 = FeHVO4-     0.0000  -3.7000  0.000  0.000-1.00 0.00 0.00 0.0000
0.00 5 1.000 811 1.000 903 -2.000 330 1.000 2 -1.000 813 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
0 0.000 0 0.000 0 0.000 0
8129032 = FeHVO4-     0.0000  -3.7000  0.000  0.000-1.00 0.00 0.00 0.0000

```

0.00 5 1.000 812 1.000 903 -2.000 330 1.000 2 -1.000 813 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8117320 = FeSO4- 0.0000 7.7800 0.000 0.000-1.00 0.00 0.00 0.0000
 0.00 5 1.000 811 1.000 732 1.000 330 -1.000 2 -1.000 813 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8127320 = FeSO4- 0.0000 7.7800 0.000 0.000-1.00 0.00 0.00 0.0000
 0.00 5 1.000 812 1.000 732 1.000 330 -1.000 2 -1.000 813 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8117321 = FeOHSeO4-2 0.0000 0.7900 0.000 0.000-2.00 0.00 0.00 0.0000
 0.00 3 1.000 811 1.000 732 -2.000 813 0.000 0 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8127321 = FeOHSeO4-2 0.0000 0.7900 0.000 0.000-2.00 0.00 0.00 0.0000
 0.00 3 1.000 812 1.000 732 -2.000 813 0.000 0 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8117610 = FeSeO3- 0.0000 4.2900 0.000 0.000-1.00 0.00 0.00 0.0000
 0.00 4 1.000 811 1.000 761 -1.000 2 -1.000 813 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8127610 = FeSeO3- 0.0000 4.2900 0.000 0.000-1.00 0.00 0.00 0.0000
 0.00 4 1.000 812 1.000 761 -1.000 2 -1.000 813 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8117611 = FeOHSeO3-2 0.0000 -3.2300 0.000 0.000-2.00 0.00 0.00 0.0000
 0.00 4 1.000 811 1.000 761 -1.000 330 -2.000 813 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8127611 = FeOHSeO3-2 0.0000 -3.2300 0.000 0.000-2.00 0.00 0.00 0.0000
 0.00 4 1.000 812 1.000 761 -1.000 330 -2.000 813 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8117620 = FeSeO4- 0.0000 7.7300 0.000 0.000-1.00 0.00 0.00 0.0000
 0.00 5 1.000 811 1.000 762 1.000 330 -1.000 2 -1.000 813 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8127620 = FeSeO4- 0.0000 7.7300 0.000 0.000-1.00 0.00 0.00 0.0000
 0.00 5 1.000 812 1.000 762 1.000 330 -1.000 2 -1.000 813 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8117621 = FeOHSeO4-2 0.0000 0.8000 0.000 0.000-2.00 0.00 0.00 0.0000
 0.00 3 1.000 811 1.000 762 -2.000 813 0.000 0 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8127621 = FeOHSeO4-2 0.0000 0.8000 0.000 0.000-2.00 0.00 0.00 0.0000
 0.00 3 1.000 812 1.000 762 -2.000 813 0.000 0 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8112120 = FeCrO4- 0.0000 10.8500 0.000 0.000-1.00 0.00 0.00 0.0000
 0.00 5 1.000 811 1.000 212 1.000 330 -1.000 2 -1.000 813 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0

8122120 = FeCrO4- 0.0000 10.8500 0.000 0.000-1.00 0.00 0.00 0.0000
 0.00 5 1.000 812 1.000 212 1.000 330 -1.000 2 -1.000 813 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8114800 = FeMoO4- 0.0000 9.5000 0.000 0.000-1.00 0.00 0.00 0.0000
 0.00 5 1.000 811 1.000 480 1.000 330 -1.000 2 -1.000 813 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8124800 = FeMoO4- 0.0000 9.5000 0.000 0.000-1.00 0.00 0.00 0.0000
 0.00 5 1.000 812 1.000 480 1.000 330 -1.000 2 -1.000 813 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8114801 = FeOHMoO4-2 0.0000 2.4000 0.000 0.000-2.00 0.00 0.00 0.0000
 0.00 3 1.000 811 1.000 480 -2.000 813 0.000 0 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8124801 = FeOHMoO4-2 0.0000 2.4000 0.000 0.000-2.00 0.00 0.00 0.0000
 0.00 3 1.000 812 1.000 480 -2.000 813 0.000 0 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8117410 = FeSbO(OH)4 0.0000 8.4000 0.000 0.000 0.00 0.00 0.00 0.0000
 0.00 4 1.000 811 1.000 741 1.000 330 -2.000 2 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8127410 = FeSbO(OH)4 0.0000 8.4000 0.000 0.000 0.00 0.00 0.00 0.0000
 0.00 4 1.000 812 1.000 741 1.000 330 -2.000 2 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8117411 = FeOHSbO(OH)4 0.0000 1.3000 0.000 0.000-1.00 0.00 0.00 0.0000
 0.00 4 1.000 811 1.000 741 -1.000 2 -1.000 813 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8127411 = FeOHSbO(OH)4 0.0000 1.3000 0.000 0.000-1.00 0.00 0.00 0.0000
 0.00 4 1.000 812 1.000 741 -1.000 2 -1.000 813 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8111430 = FeCN 0.0000 13.0000 0.000 0.000 0.00 0.00 0.00 0.0000
 0.00 4 1.000 811 1.000 143 1.000 330 -1.000 2 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8121430 = FeCN 0.0000 13.0000 0.000 0.000 0.00 0.00 0.00 0.0000
 0.00 4 1.000 812 1.000 143 1.000 330 -1.000 2 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8111431 = FeOHCN- 0.0000 5.7000 0.000 0.000-1.00 0.00 0.00 0.0000
 0.00 3 1.000 811 1.000 143 -1.000 813 0.000 0 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0
 8121431 = FeOHCN- 0.0000 5.7000 0.000 0.000-1.00 0.00 0.00 0.0000
 0.00 3 1.000 812 1.000 143 -1.000 813 0.000 0 0.000 0 0.000 0
 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0
 0 0.000 0 0.000 0 0.000 0

APPENDIX C

**EXAMPLE INPUT FILE FOR THE MINTEQA2
MODEL USED TO ESTIMATE PARTITIONING WITH DOC**

Compute Kd-DOC in riverwater

MXXM: Md Dissolved OM , No FeO Sorbent, No Particulate OM , Md pH

16.00 MG/L 0.000 8.90000E-06

0 1 1 0 2 3 0 0 1 0 0 1 2

Co_doc.prn 200

0.00 8.90 144.00 0.000 0.00

0 0 0

330	0.000E+00	-4.90 y	/H+ 1
200	1.000E-03	-12.32 y	/Co+ 2
150	1.320E+01	-2.92 y	/Ca+ 2
460	3.600E+00	-3.24 y	/Mg+ 2
410	1.200E+00	-4.13 y	/K+ 1
500	5.300E+00	-3.02 y	/Na+ 1
492	6.010E+00	-3.00 y	/NO3-
140	5.200E+01	-2.51 y	/CO3-2
180	5.700E+00	-3.37 y	/Cl-1
732	6.600E+00	-3.58 y	/SO4-2
144	0.000E+00	-6.00 y	/DOM1

3 1

330 7.3000 0.0000 /H+ 1

APPENDIX D

**EXAMPLE INPUT FILE FOR THE MINTEQA2
MODEL USED TO ESTIMATE PARTITIONING WITH WASTE
SYSTEMS**

Estimate partitioning in acetogenic landfill. Assumes 0.7gFeOOH/L
 DLM; uses 3x site densities used in Ke97; Mean major ions.

17.00 MG/L 0.100 5.00000E+00

0 1 1 0 2 3 1 0 1 0 2 1 2

3 H+ 1 ACTIVITY mol/L

1 330 1.000

4.50 6.10 7.50

Co_waste.prn 200

100.00 99999. 145.00 0.000 0.00

4 1 7

7.000E-01 600.00 0.000 0.000 81

330	0.000E+00	-4.90 y	/H+ 1
200	1.000E-03	-12.32 y	/Co+ 2
150	6.000E+03	-2.92 y	/Ca+ 2
460	6.250E+02	-3.24 y	/Mg+ 2
140	5.000E+02	-2.51 y	/CO3-2
500	1.350E+03	-3.37 y	/Na+
410	1.100E+03	-3.37 y	/K+
180	2.100E+03	-3.37 y	/Cl-1
280	7.800E+02	-9.00 y	/Fe+ 2
732	5.000E+02	-3.58 y	/SO4-2
144	0.000E+00	-6.00 y	/DOM1
145	0.000E+00	-6.00 y	/DOM1
811	2.363E-06	-4.45 y	/ADS1TYP1
812	9.212E-05	-2.84 y	/ADS1TYP2
813	0.000E+00	0.00 y	/ADS1PSIo

3 1
 330 4.0000 0.0000 /H+ 1

6 1
 813 0.0000 0.0000 /ADS1PSIo

2 74

(same HFO reactions as for soil/water partitioning; see Appendix B)

Estimate partitioning in methanogenic landfill. Assumes 0.7gFeOOH/L
 DLM; uses 3x site densities used in Ke97; Mean major ions.

17.00 MG/L 0.100 5.00000E+ 00

0 1 1 0 2 3 1 0 1 0 2 1 2

3 H+ 1 ACTIVITY mol/L

1 330 1.000

7.50 8.00 9.00

Co_waste.prn 200

50.00 50000. 145.00 0.000 0.00

4 1 7

7.000E-01 600.00 0.000 0.000 81

330	0.000E+ 00	-4.90 y	/H+ 1
200	1.000E-03	-12.32 y	/Co+ 2
150	9.750E+ 01	-2.92 y	/Ca+ 2
460	5.000E+ 02	-3.24 y	/Mg+ 2
140	2.500E+ 02	-2.51 y	/CO3-2
500	1.350E+ 03	-3.37 y	/Na+
410	1.100E+ 03	-3.37 y	/K+
180	2.100E+ 03	-3.37 y	/Cl-1
732	8.000E+ 01	-3.58 y	/SO4-2
144	0.000E+ 00	-6.00 y	/DOM1
145	0.000E+ 00	-6.00 y	/DOM1
811	2.363E-06	-4.45 y	/ADS1TYP1
812	9.212e-05	-2.84 y	/ADS1TYP2
813	0.000E+ 00	0.00 y	/ADS1PSIo

3 1

330 7.0000 0.0000 /H+ 1

6 1

813 0.0000 0.0000 /ADS1PSIo

2 74

(same HFO reactions as for soil/water partitioning; see Appendix B)

Estimate partitioning in MSWI ash monofill. Assumes 0.7gFeOOH/L
 DLM; uses 3x site densities used in Ke97; Mean major ions.

17.00 MG/L 0.100 5.00000E+00

0 1 1 0 2 3 1 0 1 0 2 1 2

3 H+ 1 ACTIVITY mol/L

1 330 1.000

8.00 9.00 10.00

Co_waste.prn 200

15.00 0. 0.00 0.000 0.00

4 1 7

7.000E-01 600.00 0.000 0.000 81

330	0.000E+00	-4.90 y	/H+ 1
200	1.000E-03	-12.32 y	/Co+ 2
150	1.700E+03	-2.92 y	/Ca+ 2
460	1.000E+01	-3.24 y	/Mg+ 2
140	5.000E+01	-2.51 y	/CO3-2
500	3.000E+02	-3.37 y	/Na+
410	3.800E+02	-3.37 y	/K+
180	1.200E+03	-3.37 y	/Cl-1
732	1.400E+03	-3.58 y	/SO4-2
144	0.000E+00	-6.00 y	/DOM1
811	2.363E-06	-4.45 y	/ADS1TYP1
812	9.212e-05	-2.84 y	/ADS1TYP2
813	0.000E+00	0.00 y	/ADS1PSIo

3 1

330 4.0000 0.0000 /H+ 1

6 1

813 0.0000 0.0000 /ADS1PSIo

2 74

(same HFO reactions as for soil/water partitioning; see Appendix B)

Estimate partitioning in CKD monofill. Assumes 7.0gFeOOH/L
 DLM; uses 3x site densities used in Ke97; Mean major ions.

17.00 MG/L 0.100 5.00000E+00

0 1 1 0 2 3 1 0 1 0 2 1 2

3 H+ 1 ACTIVITY mol/L

1 330 1.000

9.00 10.00 11.00

Co_waste.prn 200

15.00 0. 0.00 0.000 0.00

4 1 7

7.000E-00 600.00 0.000 0.000 81

330	0.000E+00	-4.90 y	/H+ 1
200	1.000E-03	-12.32 y	/Co+ 2
150	2.850E+03	-2.92 y	/Ca+ 2
460	1.000E+01	-3.24 y	/Mg+ 2
140	5.000E+01	-2.51 y	/CO3-2
500	3.000E+02	-3.37 y	/Na+
410	4.000E+02	-3.37 y	/K+
180	3.800E+02	-3.37 y	/Cl-1
732	6.300E+02	-3.58 y	/SO4-2
144	0.000E+00	-6.00 y	/DOM1
811	2.363E-05	-4.45 y	/ADS1TYP1
812	9.212E-04	-2.84 y	/ADS1TYP2
813	0.000E+00	0.00 y	/ADS1PSIo

3 1

330 4.0000 0.0000 /H+ 1

6 1

813 0.0000 0.0000 /ADS1PSIo

2 74

(same HFO reactions as for soil/water partitioning; see Appendix B)

Draft