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

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NOTICE

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FOREWORD

The National Exposure Research Laboratory Ecosystems Research Division (ERD) in Athens, Georgia, conducts process, modeling, and field research to assess the exposure risks of humans and ecosystems to both chemical and non-chemical stressors. This research provides data, modeling, tools, and technical support to EPA Program and Regional Offices, state and local governments, and other customers, enabling achievement of Agency and ORD strategic goals for the protection of human health and the environment.

ERD research includes studies of the behavior of contaminants, nutrients, and biota in environmental systems, and the development of mathematical models to assess the response of aquatic systems, watersheds, and landscapes to stresses from natural and anthropogenic sources. ERD field and laboratory studies support process research, model development, testing and validation, and the characterization of variability and prediction uncertainty.

Leading-edge computational technologies are developed to integrate core science research results into multi-media (air, surface water, ground water, soil, sediment, biota), multi-stressor, and multi-scale (organism, population, community, ecosystem; field site, watershed, regional, national, global) modeling systems that provide predictive capabilities for complex environmental exposure scenarios face by the Agency.

Exposure models are distributed and supported via the EPA Center for Exposure Assessment Modeling (CEAM) (www.epa.gov/athens/ceampubl), the Watershed and Water Quality Model Technical Support Center (www.epa.gov/athens/wwqtsc), and through access to Internet tools (www.epa.gov/athens/onsite).

This research project is a component of the ERD hazardous waste research program, which seeks to better understand the environmental cycling, exposure, and risk arising from the release of organic and inorganic pollutants from treatment facilities. In this project, metal partition coefficients were developed for the watershed, surface water, and source models used in the Multimedia, Multi-pathway, Multi-receptor Exposure and Risk Assessment (3MRA) technology. Knowledge and data gained in this evaluation will be used to improve exposure and risk analysis capabilities for heavy metals evaluated by the 3MRA and other models used by EPA in various regulatory programs.

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ABSTRACT

This report presents metal partition coefficients for the surface water pathway and for the source model used in the Multimedia, Multi-pathway, Multi-receptor Exposure and Risk Assessment (3MRA) technology under development by the U.S. Environmental Protection Agency. Partition coefficients values are presented for partitioning between soil and water; partitioning between the suspended sediment load and the water in streams, rivers, and lakes; partitioning between riverine or lacustrine sediment and its porewater; and partitioning between dissolved organic carbon (DOC) and the inorganic solution species in the water of streams, rivers, and lakes. Some partition coefficients are also presented to represent metal partitioning between the solid phase of waste and its associated leachate. Partition coefficients are presented for antimony (Sb), arsenic (As), barium (Ba), beryllium (Be), cadmium (Cd), chromium (Cr), cobalt (Co), copper (Cu), lead (Pb), molybdenum (Mo), mercury (Hg), methylated mercury (CH_3Hg), nickel (Ni), selenium (Se), silver (Ag), thallium (Tl), tin (Sn), vanadium (V), and zinc (Zn).

A two-phase approach was used in developing the needed partition coefficients. In the first-phase, a literature survey was performed to determine the range and statistical distribution of values that have been observed in field studies. This included the collection of published partition coefficients for any of the metals in any of the environmental media of interest, or our estimation of partition coefficients from reported metal concentration data when feasible. In the second-phase effort, statistical methods, geochemical speciation modeling, and expert judgement were used to provide reasonable estimates of those partition coefficients not obtained from our literature search and data processing. The report concludes with a discussion of the many sources of uncertainty in the reported metal partition coefficients.

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1.0 INTRODUCTION AND BACKGROUND

The purpose of this study was to develop metal partition coefficients for the surface water pathway and for the source model used in the Multimedia, Multi-pathway, Multi-receptor Exposure and Risk Assessment (3MRA) technology under development by the U.S. Environmental Protection Agency. The 3MRA technology provides for screening-level human and ecological risk assessments for chronic exposure to chemicals released from land-based waste management units (WMUs) managed under the Hazardous Waste Identification Rule (HWIR). The multimedia 3MRA model includes a surface water pathway model that requires the partition coefficient for each metal to be modeled.

In natural media, metal contaminants undergo reactions with ligands in water and with surface sites on the solid materials with which the water is in contact. Reactions in which the metal is bound to the solid matrix are referred to as sorption reactions and metal that is bound to the solid is said to be sorbed. The metal partition coefficient (K_d; also known as the sorption distribution coefficient) is the ratio of sorbed metal concentration (expressed in mg metal per kg sorbing material) to the dissolved metal concentration (expressed in mg metal per L of solution) at equilibrium.

$$K_d = \frac{\text{sorbed metal concentration } (mg\ /\ kg)}{\text{dissolved metal concentration } (mg\ /\ L)} \qquad \textbf{(1)}$$

During transport of metals in soils and surface water systems, metal sorption to the solid matrix results in a reduction in the dissolved concentration of metal and this affects the overall rate of metal transport. Thus, transport models such as those used in various pathways in the 3MRA incorporate the metal K_d into the overall retardation factor (the ratio of the average linear particle velocity to the velocity of that portion of the plume where the contaminant is at 50 percent dilution). The use of K_d in 3MRA transport modeling implies the assumption that local equilibrium between the metal solutes and the sorbents is attained. This implies that the rate of sorption reactions is fast relative to advective-dispersive transport of the metal.

For a particular metal, K_d values in soil are dependent upon various geochemical characteristics of the soil and its porewater. Likewise for surface water systems– the K_d for a particular metal depends on the nature of suspended solids or sediment and key geochemical parameters of the water. Geochemical parameters that have the greatest influence on the magnitude of K_d include the pH of the system and the nature and concentration of sorbents associated with the soil or surface water. In the subsurface beneath a waste management facility, the concentration of leachate constituents may also influence the metal K_d through competition for sorption sites.

The metals of interest in HWIR modeling are 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 3MRA 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 sediment 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 3MRA modeling scenario also 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 (first-phase) 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 studies. This includes the collection of published partition coefficients for any of the metals in any of the environmental media of interest, or our 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 concentration, etc.) when these were reported. We anticipated that the literature search would not supply needed partition coefficients for all of the metals in all of the environmental media of interest. Therefore, in the second-phase effort, statistical methods, geochemical speciation modeling, and expert judgement were used to provide reasonable estimates of those partition coefficients not obtained from our literature search and data processing.

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 as well as 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, that 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 our 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.

2.1 SELECTION CRITERIA FOR PARTITION COEFFICIENTS

The following criteria and guidelines were followed in the selection of partition coefficient values from journal articles. Values were accepted from studies characterized by:

- Use of "whole" natural media for determination of partition coefficients in natural media systems (e.g., reject values from studies using pure mineral phases or treated soils)
- In soil systems, use of an extractant having low ionic strength ($\leq$ 0.1 M); in surface water systems, low salinity (freshwater preferred, salinity up to 10 parts per thousand acceptable)
- Use of low total metal concentrations (i.e., if coefficients were determined at multiple total metal concentrations, choose the coefficient corresponding to the lowest concentration where K_d is less likely to depend on metal concentration)
- pH values in the natural range (4 to 10)
- No organic chelates in the extractant (e.g., EDTA)
- One partition coefficient per system studied
- Where multiple partition coefficients are presented for a system due to experimental variation of pH or other parameters, select the partition coefficient corresponding to the conditions most closely approximating natural conditions.
- Batch leaching tests (preferred over column tests if both are available for the same study and soil, but column tests acceptable).

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 parameters are pH, total concentrations of metal in solution and sorbed, and concentrations of important metal complexing agents (including DOC), and weight fraction of particulate organic matter and other sorbing materials. Physical parameters necessary to convert sorbed concentration (mg/kg) over dissolved concentration (mg/L) to partition coefficients in liters per kilogram (L/kg), i.e., porosity, water content, and bulk density, were also recorded when reported in the articles. Equations and relationships presented in journal articles that present K_d as a function of pH or other parameters were recorded in a remark field in the spreadsheet.

2.2 RESULTS OF THE LITERATURE SURVEY

Approximately 245 articles and reports were copied and reviewed. A total of 1170 individual K_d values were obtained from these sources, either 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 these 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 we 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 rejected, but some data from estuaries were included if reported as corresponding to low salinity.) The second most frequently reported K_d values pertained to partitioning in soil. Suspended matter and soil K_d's together totaled 68% of the reported data. Table 1 shows the median and range of K_d values retrieved in our literature search for natural media. (Values shown are log K_d values). For some combinations of metal and media type, too few partition coefficients were found in the literature to state a median or even a reasonable range. In some of these cases, mean or median values were available from previous compilations of partition coefficients. In Table 1, blank spaces in the table correspond to no data found. Values in bold are from previous compilations.

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 metal 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 actual 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 (i.e., a leachate extraction test). Section 3.2 presents further findings with regard to leach tests and appropriate metal partition coefficients for waste systems.

Table 1
Partition coefficients (log K_d in L/kg) from the literature search. Median values listed in boldface are from a previous compilation. Blank spaces represent instances for which no data was found or too few values were 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		
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		
range	1.7 - 4.1	2.8 - 6.8		
N	2	17		
Cd median	2.9	4.7	3.6	5.2
range	0.1 - 5.0	2.8 - 6.3	0.5 - 7.3	3.4 - 5.5
N	41	67	21	4
Co median	2.1	4.7	3.3	4.5
range	(-1.2) - 4.1	3.2 - 6.3	2.9 - 3.6	2.9 - 4.8
N	11	29	3	2

Table 1
Partition coefficients (log K_d in L/kg) from the literature search. Median values listed in boldface are from a previous compilation. Blank spaces represent instances for which no data was found or too few values were found to provide meaningful statistics.

Metal	Soil/Water	Suspended Matter /Water	Sediment/ Water	DOC/Water
Cr(III) median	3.9	5.1	***4.5***	
range	1.0 - 4.7	3.9 - 6.0		
N	43	25		
Cr(VI) median	1.1			
range	(-0.7) - 3.3			
N	24			
Cu median	2.7	4.7	4.2	5.5
range	0.1 - 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	5.3
range	2.2 - 5.8	4.2 - 6.9	3.8 - 6.0	5.3 - 5.6
N	17	35	2	3
CH_3Hg median	2.8	5.4	3.6	
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			

Table 1

Partition coefficients (log K_d in L/kg) from the literature search. Median values listed in boldface are from a previous compilation. Blank spaces represent instances for which no data was found or too few values were found to provide meaningful statistics.

Metal	Soil/Water	Suspended Matter /Water	Sediment/ Water	DOC/Water
Ni median	3.1	4.6	***4.0***	5.1
range	1.0 - 3.8	3.5 - 5.7		4.7 - 5.4
N	18	30		4
Pb median	4.2	5.6	5.1	5.0
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			3	
Se median	1.0		***3.6***	
range	-0.3 - 2.4	3.1 - 4.7		
N	23			
Sn median	**2.9**	5.6	***4.7***	
range	2.1 - 4.0	4.9 - 6.3		
N		3		
Tl median			3.2	
range			3.0 - 3.5	
N			6	

Table 1
Partition coefficients (log K_d in L/kg) from the literature search. Median values listed in boldface are from a previous compilation. Blank spaces represent instances for which no data was found or too few values were found to provide meaningful statistics.

Metal	Soil/Water	Suspended Matter /Water	Sediment/ Water	DOC/Water
V median				
range	1.1 - 2.7			
N				
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 our spreadsheet, nor were they included in the statistical summary of K_d values obtained from the literature as reported herein.

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 and/or median value for the partition coefficient for all metals in all media-types. Therefore, 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 of K_d for each metal in each media-type. Statistical analysis of retrieved data, geochemical modeling, and expert judgement were all used to develop these partition coefficient values. The nature of the available data for natural media and waste systems was different to the extent that it seemed best to consider these two categories separately.

3.1 DEVELOPMENT OF PARTITION 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 eight 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, in cases where K_d associated with multiple pH values were presented, the K_d associated with the pH value closest to the ambient soil pH was chosen. If the ambient soil pH was not specified, then a single K_d value was picked randomly from among those presented and the other K_d values for the soil were discarded. In this fashion, the sample of literature data for each metal and media-type was edited before attempting to identify the underlying probability distribution for K_d.

Statistical tests were performed to determine the shape of the frequency distribution of K_d for each metal and media-type. These tests employed widely recognized techniques available in the statistical package Analyze-It (version 1.32), an add-on module for Microsoft EXCEL 97. The Shapiro-Wilk test and the Kolmogorov-Smirnov test were used to test the 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 only a few cases were the data sufficient to identify the underlying distribution with any degree of certainty. Many of the sample sets (including the most complete (largest) sample sets), 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.

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 method 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 a progression of decreasing affinity for sorption material in the order suspended matter > sediment > soil. In other words, comparison of mean K_d values for particular metals showed the result that $K_{d,\,SPM} > K_{d,Sediment} > K_{d,Soil}$. In two other cases where at least two of the K_d types could be characterized from the literature data, both conformed to this same pattern. In addition, a somewhat consistent progression in K_d magnitude for metals within the three natural media was noted. For the best represented metals, the following patterns of decreasing K_d were observed (based on ordering the mean K_d values from highest to lowest magnitude for each medium):

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 was some shuffling about of the K_d magnitude ordering among these media-types, as might be expected for a data set that is undoubtedly incomplete. The most obvious inconsistency in the progression of K_d magnitude is for As. 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), however, Pb and Hg have greater affinities than HSAB predicts. Certainly, there are multiple adsorption 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 reason, it appears feasible to exploit these trends to provide an estimate of K_d for a given metal in one medium if its value in another medium is available. For example, the literature data provided a reasonable number of K_d values 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 value 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. The regression equation was then used 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. 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 of K_d values for a particular metal 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. The standard deviation was also estimated using the mean and maximum values rather than mean and minimum. 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 upon which each equation is based, the correlation coefficient (r^2), and the 95% confidence interval for the slope and intercept. Scatter plots showing the regressed data points and straight line regressions are shown in Appendix B.

Table 2
Linear regression equations used to estimate mean log K_d values (L/kg) in natural media.

Used to Estimate	Independent 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 soil	mean log K_d suspended matter	0.969 (1.136)	-1.903 (5.703)	0.37	9

The regression 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 as discussed in the next section.

3.1.2 Estimation From Geochemical Speciation Modeling

Geochemical speciation modeling was used to estimate soil/water partitioning if data-based 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 were developed from various sources as presented in the following sections.

MODELING DETAILS AND INPUT DATA FOR SOIL PARTITION COEFFICIENTS

The concentrations of major ions used in geochemical speciation modeling for soils 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 on results of doing so was significantly less than the effect of variability in other important parameters. Model input values for several of the most significant "master" variables affecting K_d were varied over reasonable ranges in order to capture the expected range of K_d values. 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 master variables was characterized by low, medium, and high assigned 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 assigned POC concentration values were obtained from analysis of data in a database for shallow, silt-loam soils (Carsel et al., 1988 and R. Parrish, personal communication). The low, medium, and high values corresponded to the 10th, 50th, and 90th percentiles, respectively, for particulate organic matter concentration (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 initially 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 various aquifers and soils. The mean K_d for Cd, Cu, Ni, Pb, and Zn were computed using these values in MINTEQA2. These computed K_d values were compared with mean K_d values for these same metals in soil obtained from our 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 assigned values 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 setting of POC; the medium settings of pH, DOC, and HFO, and the medium setting of POC; and the medium settings of pH, DOC, and HFO, and the high setting of POC.) Appendix C shows a typical MINTEQA2 input file used in estimating K_d for soil/water.

The minimum and maximum K_d values were established by combining the available literature data and MINTEQA2 results. Again, 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 previously described regression equations based on our literature analysis process were used to estimate the mean K_d values for sediment and suspended matter if these were lacking from the literature data. The standard deviation was estimated as described previously for the linear regression estimates.

MODELING DETAILS AND INPUT DATA 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 known 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 against the binding constants for humic- and fulvic acid (HA and FA, respectively) reported by Tipping (1994). The metals Cd, Cu, Ni, Pb, and Zn were also represented in the database of HA and FA binding constants, so these data were used to develop the regression relationship shown in Equation (2).

$$mean\ \log K_{DOC,Hg} = -\ 0.610 \log K_{HA,Hg} + 4.206 \log K_{FA,Hg} - 3.645 \qquad \textbf{(2)}$$

As derived, Equation (2) has a correlation coefficient (r^2) of 0.95, and produces an estimate of 9.0 for the mean log K for Hg^{2+} binding with DOC (mean log $K_{DOC,Hg}$). (NOTE: This equation gives the mean log K_{DOC}, a formation constant for use in the MINTEQA2 speciation model for the chemical reaction between DOC and Hg. It is not the same as the mean K_d for Hg binding with DOC. The latter is always designated K_d; the objective of the MINTEQA2 modeling is to estimate the K_d for those metals for which literature data is lacking.)

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

$$mean\ \log K_{DOC} = 0.3595 \log K_{OH} + 0.6932 \log K_{Acet} + 0.7974 \qquad \textbf{(3)}$$

The correlation coefficient (r^2) for Equation (3) is 0.98. Equation (3) was used to estimate the mean log K_{DOC} values for Ag^+, Co^{2+}, Sn^{2+}, and Tl^+ for use in MINTEQA2 modeling. The mean log K_{DOC} values estimated for these metals were 2.0, 3.3, 6.6, and 1.0, respectively.

The estimation procedures outlined previously in this section cannot reliably be extended to anions. However, anions are typically not as strongly bound to organic matter. Therefore, we used MINTEQA2 to estimate K_d values for binding to DOC for cationic metals only, and included conservative estimates of K_d values for the anions based on judgement alone.

The concentrations of major ions used in estimating metal-DOC binding with 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 assigned 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 concentrations of 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 K_d value for each cation was specified as that value computed by MINTEQA2 when the pH and DOC concentration were set to their reported mean values in surface water. A typical MINTEQA2 input file used to estimate metal partitioning to DOC is shown in Appendix D.

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 was not possible to establish the shape of the K_d frequency distribution curve 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 a needed mean log K_d, the mean value was estimated subjectively using expert judgement. Factors considered in this process included any values obtained from our 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 also used if reasonable values were available. Otherwise, the extremes in K_d were also estimated by expert judgement. In either case, the standard deviation was estimated as described previously above for linear regression in Section 3.1.1.

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 our 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 involved were assigned a *CL* of 4. Many values were determined in circumstances that warranted 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 latter circumstances could be combined with estimates from modeling, etc.). In these cases, a *CL* of 2 or 3 was assigned as seemed appropriate.

The final values we assigned to the metal partition coefficients for soil, sediment, suspended matter, and DOC are presented in Tables 3, 4, 5, and 6, respectively. The method used to arrive at each assigned value (use of all or a subset of the collected literature K_d values, use of regression equations, modeling results, or expert judgement) is indicated for each metal and media-type, as is the subjectively assigned confidence level.

Table 3

Metal partition coefficients (log K_d) in L/kg for soil/soil water. Values in italics were estimated by regression or from MINTEQA2 results. An entry of "log-normal" 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 assumed" 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). An entry of "---" for the median occurs where regression equations were used to estimate the mean, minimum, and maximum values and no estimate was made for the median.

Metal	Median	Mean	Std. Dev.	Min	Max	Comments
Ag (I)	2.6	2.6	0.8	1.0	4.5	From literature data (raw, n=21); log-normal; *CL*=1
As[a]	3.4	3.2	0.7	0.3	4.3	From literature data (raw, n=21); (log-normal assumed); oxidation state usually not specified in literature; *CL*=2
Ba(II)	---	*2.0*	*0.7*	0.7	3.4	Suspended matter K_d regression equation for mean; (log-normal assumed); *CL*=2
Be(II)	---	*2.2*	*1.0*	1.7	4.1	Suspended matter K_d regression equation for mean; (log-normal assumed); *CL*=3
Cd(II)	2.9	2.7	0.8	0.1	5.0	From literature data (edited, n=37); log-normal; *CL*=1
Co(II)	2.1	2.1	1.2	-1.2	4.1	From literature data (raw, n=11); log-normal; *CL*=1
Cr(III)	3.9	3.8	0.4	1.0	4.7	From literature data (raw, n=22); log-normal; *CL*=2
Cr(VI)	1.1	0.8	0.8	-0.7	3.3	From literature data (raw, n=24); (log-normal assumed); *CL*=2
Cu(II)	2.7	2.5	0.6	0.1	3.6	From literature data (raw, n=20); log-normal; *CL*=1

Table 3
Metal partition coefficients (log K_d) in L/kg for soil/soil water. Values in italics were estimated by regression or from MINTEQA2 results. An entry of "log-normal" 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 assumed" 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). An entry of "---" for the median occurs where regression equations were used to estimate the mean, minimum, and maximum values and no estimate was made for the median.

Metal	Median	Mean	Std. Dev.	Min	Max	Comments
Hg(II)	3.8	3.6	0.7	2.2	5.8	From literature data (raw, n=17); log-normal; *CL*=1
MeHg	2.8	2.7	0.6	1.3	4.8	From literature data (raw, n=11); log-normal; *CL*=2
Mo(VI)	1.1	1.3	0.6	-0.4	2.7	From literature data (raw, n=5); (log-normal assumed); oxidation state not always specified in literature data; *CL*=3
Ni(II)	3.1	2.9	0.5	1.0	3.8	From literature data (raw, n=19); log-normal; *CL*=1
Pb(II)	4.1	3.7	1.2	0.7	5.0	From literature data (edited, n=31); (log-normal assumed); *CL*=2
Sb[b]	---	2.3	1.1	0.1	2.7	From literature data (mean is the average of several reported mean values, n=5); (log-normal assumed); *CL*=4
Se(IV)[c]	1.4	1.3	0.4	-0.3	2.4	From literature data (edited, n=11); (log-normal assumed); *CL*=2

Table 3
Metal partition coefficients (log K_d) in L/kg for soil/soil water. Values in italics were estimated by regression or from MINTEQA2 results. An entry of "log-normal" 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 assumed" 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). An entry of "---" for the median occurs where regression equations were used to estimate the mean, minimum, and maximum values and no estimate was made for the median.

Metal	Median	Mean	Std. Dev.	Min	Max	Comments
Se(VI)	---	*-0.2*	*1.1*	*-2.0*	*2.0*	Mean estimated from MINTEQA2 result; (log-normal assumed); min, max from expert judgement; *CL*=4
Sn(II)	---	2.7	0.7	2.1	4.0	From literature data; (log-normal assumed); *CL*=3
Tl(I)	---	*0.5*	*0.9*	*-1.2*	*1.5*	Estimated from MINTEQA2 result; (log-normal assumed); *CL*=4
V(V)	---	*1.7*	*1.5*	*0.5*	*2.5*	Mean, min, max from suspended matter K_d regression equation; (log-normal assumed); *CL*=4
Zn(II)	3.1	2.7	1.0	-1.0	5.0	From literature data (raw, n=21); (log-normal assumed); *CL*=1
CN-	---	*0.7*	*1.6*	*-2.4*	*1.3*	Estimated from MINTEQA2 result; (log-normal assumed); *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 L/kg for sediment/porewater. Values in italics were estimated by regression or from MINTEQA2 results. An entry of "log-normal" 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 assumed" 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). An entry of "---" for the median occurs where regression equations were used to estimate the mean, minimum, and maximum values and no estimate was made for the median.

Metal	Median	Mean	Std. Dev.	Min	Max	Comments
Ag(I)	---	*3.6*	*1.1*	2.1	5.8	Mean from soil K_d regression equation; (log-normal assumed); min, max from literature data; *CL*=3
As[a]	2.2	2.4	0.7	1.6	4.3	From literature data; log-normal; oxidation state not specified in literature data; *CL*=2
Ba(II)	---	*2.5*	*0.8*	*0.9*	*3.2*	Mean, min, max from suspended matter K_d regression equation; (log-normal assumed); *CL*=3
Be(II)	---	*2.8*	*1.9*	*0.8*	6.5	Mean, min, max from suspended matter K_d regression equation; (log-normal assumed); *CL*=3
Cd(II)	3.7	3.3	1.8	0.5	7.3	From literature data (n=14, edited); log-normal; *CL*=1
Co(II)	---	*3.1*	*1.0*	2.9	3.6	Mean from soil K_d regression equation; (log-normal assumed); min, max from literature data; *CL*=3
Cr(III)	---	*4.9*	*1.5*	*1.9*	*5.9*	Mean, min, max from soil K_d regression equation; (log-normal assumed); *CL*=4

Table 4

Metal partition coefficients (log K_d) in L/kg for sediment/porewater. Values in italics were estimated by regression or from MINTEQA2 results. An entry of "log-normal" 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 assumed" 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). An entry of "---" for the median occurs where regression equations were used to estimate the mean, minimum, and maximum values and no estimate was made for the median.

Metal	Median	Mean	Std. Dev.	Min	Max	Comments
Cr(VI)	---	*1.7*	*1.4*	*0.0*	*4.4*	Mean, min, max from soil K_d regression equation; (log-normal assumed); *CL*=4
Cu(II)	4.1	3.5	1.7	0.7	6.2	From literature data (raw, n = 12); log-normal; *CL*=1
Hg(II)	---	4.9	0.6	3.8	6.0	From literature data (raw, n=2); (log-normal assumed); *CL*=2
MeHg	---	3.9	0.5	2.8	5.0	From literature data (edited, n=2); (log-normal assumed); *CL*=2
Mo(VI)	---	2.5	*0.8*	*0.4*	*3.7*	Mean from literature data (reported mean value with oxidation state not specified); (log-normal assumed); min, max from soil K_d regression equation; *CL*=4
Ni(II)	---	*3.9*	*1.8*	0.3	4.0	Mean from soil K_d regression equation; (log-normal assumed); min, max from literature data; *CL*=3
Pb(II)	5.1	4.6	1.9	2.0	7.0	From literature data (edited, n=14); log-normal; *CL*=1

Table 4

Metal partition coefficients (log K_d) in L/kg for sediment/porewater. Values in italics were estimated by regression or from MINTEQA2 results. An entry of "log-normal" 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 assumed" 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). An entry of "---" for the median occurs where regression equations were used to estimate the mean, minimum, and maximum values and no estimate was made for the median.

Metal	Median	Mean	Std. Dev.	Min	Max	Comments
Sb[b]	---	3.6	1.8	0.6	*4.8*	From literature data (reported mean value); (log-normal assumed); *CL*=4
Se(IV)	---	3.6	*1.2*	*1.0*	*4.0*	Mean from literature data (reported mean value); (log-normal assumed); min, max from expert judgement; *CL*=4
Se(VI)	---	*0.6*	*1.2*	*-1.4*	*3.0*	Mean, min, max from soil K_d regression equation; (log-normal assumed); *CL*=4
Sn(II)	---	*3.7*	*0.7*	*3.1*	*5.1*	Mean, min, max from soil K_d regression equation; (log-normal assumed); *CL*=3
Tl(I)	---	*1.3*	*1.1*	*-0.5*	3.5	Mean, min from soil K_d regression equation; (log-normal assumed); max from literature data; *CL*=4
V(V)	---	*2.1*	*0.9*	*0.4*	*3.2*	Mean, min, max from suspended matter K_d regression equation; (log-normal assumed); *CL*=4
Zn(II)	4.8	4.1	1.6	1.5	6.2	From literature data (edited, n=13); (log-normal assumed); *CL*=1

Table 4

Metal partition coefficients (log K_d) in L/kg for sediment/porewater. Values in italics were estimated by regression or from MINTEQA2 results. An entry of "log-normal" 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 assumed" 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). An entry of "---" for the median occurs where regression equations were used to estimate the mean, minimum, and maximum values and no estimate was made for the median.

Metal	Median	Mean	Std. Dev.	Min	Max	Comments
CN-	---	*1.6*	*1.7*	*-1.8*	*2.2*	Mean, min, max from soil K_d regression equation; (log-normal assumed); *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 L/kg for suspended matter/water. Values in italics were estimated by regression or from MINTEQA2 results. An entry of "log-normal" 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). An entry of "---" for the median occurs where regression equations were used to estimate the mean, minimum, and maximum values and no estimate was made for the median.

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

Table 5

Metal partition coefficients (log K_d) in L/kg for suspended matter/water. Values in italics were estimated by regression or from MINTEQA2 results. An entry of "log-normal" 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). An entry of "---" for the median occurs where regression equations were used to estimate the mean, minimum, and maximum values and no estimate was made for the median.

Metal	Median	Mean	Std. Dev.	Min	Max	Comments
MeHg	---	*4.9*	*0.7*	4.2	6.2	Mean from soil K_d regression equation; (log-normal assumed); min, max from literature data; *CL*=3
Ni(II)[b]	4.3	4.4	0.4	3.5	5.7	From literature data (edited, n=25); log-normal; *CL*=1
Mo(VI)	---	*4.4*	*1.0*	*3.7*	*4.9*	Mean, min, max from soil K_d regression equation; (log-normal assumed); *CL*=4
Pb(II)[c]	5.7	5.7	0.4	3.4	6.5	From literature data (edited, n=38); (log-normal assumed); *CL*=1
Sb[d]	---	*4.8*	*0.5*	*3.9*	*4.9*	Mean, min, max from soil K_d regression equation; (log-normal assumed); *CL*=4
Se(IV)	---	*4.4*	*0.4*	*3.8*	*4.8*	Mean, min, max from soil K_d regression equation; (log-normal assumed); *CL*=4
Se(VI)	---	*3.8*	*1.0*	*3.1*	*4.6*	Mean, min, max from soil K_d regression equation; (log-normal assumed); *CL*=4
Sn(II)	---	*4.9*	*0.8*	*4.7*	6.3	Mean, min from soil K_d regression equation; (log-normal assumed); max from literature data; *CL*=4

Table 5

Metal partition coefficients (log K_d) in L/kg for suspended matter/water. Values in italics were estimated by regression or from MINTEQA2 results. An entry of "log-normal" 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). An entry of "---" for the median occurs where regression equations were used to estimate the mean, minimum, and maximum values and no estimate was made for the median.

Metal	Median	Mean	Std. Dev.	Min	Max	Comments
Tl(I)	---	*4.1*	*1.0*	*3.0*	*4.5*	Mean from soil K_d regression equation; (log-normal assumed); other parameters from expert judgement; *CL*=4
V(V)	---	3.7	0.6	*2.5*	*4.5*	Mean from literature data (raw, n=5); (log-normal assumed); min, max from expert judgement; oxidation state not always specified in literature; *CL*=3
Zn(II)	5.1	5.0	0.5	3.5	6.9	From literature data (edited, n=47); log-normal; *CL*=1
CN-	---	*4.2*	*0.6*	*3.0*	*4.4*	Mean, min, max from soil K_d regression equation; (log-normal assumed); *CL*=4

[a] Positive result for Shapiro-Wilk test for normality of data not log-transformed. 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 L/kg 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	Mean	Std. Dev.	Min	Max	Comment
Ag(I)	*2.5*	*1.0*	*1.5*	*4.5*	Mean estimated from MINTEQA2 results; other parameters from expert judgement; (log-normal assumed); *CL*=3
As	*2.0*	*1.0*	*0.0*	*3.0*	No data, values from expert judgement (conservative); (log-normal assumed); (log-normal assumed); *CL*=4
Ba(II)	*3.6*	*1.0*	*2.5*	*4.0*	Mean estimated from MINTEQA2 results, values for other parameters from expert judgement; (log-normal assumed); *CL*=3
Be(II)	*2.1*	*1.0*	*1.1*	*3.8*	All parameters estimated from MINTEQA2 results; *CL*=3
Cd(II)	*3.8*	*0.9*	*2.0*	*5.5*	Mean estimated from MINTEQA2 results; min, max from expert judgement; *CL*=3
Co(II)	*3.8*	*0.9*	*2.0*	*5.5*	Mean estimated from MINTEQA2 results; min, max from expert judgement; *CL*=3
Cr(III)	*1.1*	*1.6*	*-0.6*	*4.3*	Mean estimated from MINTEQA2 results; min, max from expert judgement; *CL*=4
Cr(VI)	*2.0*	*1.0*	*0.0*	*3.0*	No data, values from expert judgement (conservative); (log-normal assumed); *CL*=4
Cu(II)	5.4	1.1	2.5	7.0	From literature data (raw, n=17); (log-normal assumed); *CL*=2
Hg(II)	5.4	*1.2*	*3.0*	*6.0*	Mean from literature data (raw, n=3); (log-normal assumed); min, max from expert judgement; *CL*=4

Table 6

Metal partition coefficients (log K_d) in L/kg 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	Mean	Std. Dev.	Min	Max	Comment
MeHg	*5.0*	*1.1*	*2.8*	*5.5*	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; (log-normal assumed); *CL=4*
Ni(II)	*3.7*	*0.9*	*1.9*	*5.4*	Mean estimated from MINTEQA2 results; min, max from expert judgement; (log-normal assumed); *CL*=3
Mo(VI)	*2.0*	*1.0*	*0.0*	*3.0*	No data, values from expert judgement (conservative); (log-normal assumed); *CL*=4
Pb(II)	4.9	*0.5*	3.8	5.6	From literature data (raw, n=9); (log-normal assumed); *CL*=2
Sb	*2.0*	*1.0*	*0.0*	*3.0*	No data, values from expert judgement (conservative); (log-normal assumed); *CL*=4
Se(IV)	*2.0*	*1.0*	*0.0*	*3.0*	No data, values from expert judgement (conservative); (log-normal assumed); *CL*=4
Se(VI)	*2.0*	*1.0*	*0.0*	*3.0*	No data, values from expert judgement (conservative); (log-normal assumed); *CL*=4
Sn(II)	*2.0*	*1.0*	*0.0*	*3.0*	No data, values from expert judgement (conservative); (log-normal assumed); *CL*=4
Tl(I)	*1.6*	*1.0*	*0.0*	*3.0*	Mean estimated from MINTEQA2, values for other parameters from expert judgement; (log-normal assumed); *CL*=4

Table 6
Metal partition coefficients (log K_d) in L/kg 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	Mean	Std. Dev.	Min	Max	Comment
V(V)	*2.0*	*1.0*	*0.0*	*3.0*	No data, values from expert judgement (conservative); (log-normal assumed); *CL*=4
Zn(II)	*5.1*	*0.7*	*4.6*	*6.4*	From literature data (raw, n=9); (log-normal assumed); *CL*=3
CN-	*2.0*	*1.0*	*0.0*	*3.0*	No data, values from expert judgement (conservative); (log-normal assumed); *CL*=4

3.2 DEVELOPMENT OF PARTITIONING COEFFICIENTS FOR WASTE SYSTEMS

The multimedia, multi-pathway risk assessment for 3MRA 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 leachate extraction test results for specific wastes. Our 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 leachate extraction test data to predict the leachate composition exiting landfills (U.S. EPA, 1991). The U.S. EPA Toxicity Characteristic Leaching Procedure (TCLP) was specifically designed to characterize leachate compositions produced by specific wastes co-disposed with municipal solid waste. Recent papers suggest 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). In the first regime, the leachate composition is controlled by initial wash-off of loosely adhered contaminant; in the second, the leachate composition is controlled by dissolution of primary materials and perhaps re-precipitation of more stable phases; and in the third, the leachate composition is controlled by the diffusion of waste constituents from the interior of waste particles to the particle surface. The time of onset and duration of these regimes are highly variable, and depend on the life-cycle of the specific waste system (acetogenesis, methanogenesis, etc.). The overall chemical composition (major ion concentration and concentration of metal-complexing organic ligands) is also important in determining the metal leachate concentration that will be observed in any particular case. In general, it would seem that the highest metal leachate concentrations would be 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 3MRA as used for HWIR rulemaking? Since the 3MRA model does not allow a time-variable partition coefficient, it would seem that an aggregate partition coefficient that represents an average over an appropriate exposure or waste management unit lifetime 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 leachate 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 more specific modeling or other estimating techniques.

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

Adopting these simplifications, it is only necessary to derive separate estimates of metal partition coefficients specifically for waste piles and landfills. The following sections detail how these latter two sets of waste management unit coefficients have been estimated from available TCLP and similar leachate extraction tests that characterize both the solid phase and the corresponding leachate metal concentrations. We have also 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 the leachability of metals from incinerator ash, with the aim of investigating the suitability of the ash materials for disposal or for use in construction. Unfortunately, leachate extraction test results (metal leachate concentrations) often are reported without the corresponding concentration in the solid phase. This omission makes those data useless in estimating expected metals partitioning. Our literature survey produced 203 leach test results for which both leachate and solid phase data were presented. Table 7 shows the range and mean values of effective partition coefficients calculated 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 concentration in the solid phase to that in the solution phase as represented in the leach test results. These coefficients 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. For example, the authors cite possible Cd complexation with chloride that they investigated using MINTEQA2. They found that an increased leachability of Cd in some of the ash materials was correlated with increased 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 metals 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 metals partitioning affinity relationships noted in Section 3.1.1 and the similarities noted by these latter 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 in 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 combining with 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 for use with metals for which little or no data was found. We chose to use soil K_d as the predictor because a comparison of K_d values for soils, sediments and suspended matter suggested that the solid to liquid concentration ratio is important in determining the magnitude of K_d. (This apparent dependence of K_d on solid to liquid ratio has been noted in other studies and is sometimes referred to as the “particle concentration effect.") This solid to liquid concentration ratio for landfills and waste piles is probably more similar to that of soils than to 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 our regression 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:

$$\log K_{d,waste} = 0.7 \log K_{d,soil} + 0.3 \qquad \textbf{(4)}$$

This relationship has a rather low correlation coefficient (r^2) of 0.4 implying that only 40% of the variation in log $K_{d,waste}$ from the leach test data is accounted for. The implication is that log K_d values predicted by means of this equation must be regarded as highly uncertain. Appendix B shows the scatter plot of data from which this relationship was developed.

3.2.2 Estimation from Geochemical Speciation Modeling

The MINTEQA2 geochemical speciation model was used to investigate the possible range of metal partition coefficients for landfills. The input requirements of the model for estimating metal partitioning include the concentrations of major solute 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 solute ions, the DOC concentration, the POC concentration, and the pH. These 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 the various waste management 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 likely that solid 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 (HFO) 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 our 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 our modeling for the four landfill 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 (9.0, 10.0, 11.0) 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 E.

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]
Ionic Strength (M)	0.1[c]	0.1[c]	0.1[c]	0.1[c]
Ca (mg/L)	6000[d]	975[d]	1,700[b]	2850[f]
Mg (mg/L)	625[d]	500[d]	10[b]	10[f]

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
Na (mg/L)	1350[e]	1350[e]	300[b]	300[f]
K (mg/L)	1100[e]	1100[e]	380[b]	400[f]
CO_3 (mg/L)	500[c]	250[c]	50[c]	50[f]
Cl (mg/L)	2100[e]	2100[e]	1,200[b]	380[f]
Fe (mg/L)	780[e]	0	0	0
SO_4 (mg/L)	500[d]	80[d]	1,400[b]	630[f]
DOC (mg/L)	100[c]	50[c]	15[c]	15[c]
POC (mg/L)	100,000[c]	50,000[c]	0	0

[a] Minimum, average, and maximum values reported in Ehrig (1992).

[b] Obtained from analysis of MSWI data obtained in our literature survey.

[c] Reasonable guesses.

[d] Computed from typical dissolved values reported in Ehrig (1992), 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 for selected wastes estimated from the MINTEQA2 modeling exercise for several metals are shown in Table 9. The partition coefficients were calculated as the ratio of the simulated sorbed and dissolved concentrations as expressed in Equation (1). The units of K_d were converted to 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 landfill modeling 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 set of concentration values for the major ambient 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 in Table 9 appear to be related to complexation with chloride that is entered at relatively high ambient concentration in all scenarios.

This effect is in keeping with observations by others (van der Sloot et al., 1996). Another major ambient ion whose concentration level can influence metal partitioning is calcium. At the high concentrations of calcium cations found 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 trace metals whose partitioning is significantly influenced by the concentration level of a major ambient ion such as chloride or calcium, it is expected that this fact alone 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) in waste for selected metals determined from MINTEQA2 modeling.

	Estimated log K_d (L/kg)			
Metal	**MSW Acetogenesis**	**MSW Methanogenesis**	**MSWI Ash Monofill**	**CKD Monofill**
Be	0.8 - 3.9	3.3 - 4.4	(-0.4) - 4.0	(-2.7) - 2.4
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	(-2.5) - 2.3
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	(-2.7) - 1.1

We compared the partition coefficients estimated for wastes using MINTEQA2 with values predicted by the previously discussed regression equation (log $K_{d,waste}$ = 0.7 log $K_{d,soil}$ + 0.3; see Section 3.2.1). The degree of agreement varied among metals. (We defined the measure of "agreement" for a metal to be whether the value predicted by the regression 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 MINTEQA2-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.") In agreement with the literature-reported K_d values for natural media, Pb and Cr(III) tend to have high K_d estimates from the MINTEQA2 waste simulations. In general, the MINTEQA2 results for the acetogenic and methanogenic landfill scenarios agreed more closely with values estimated by the regression relationship based on soil K_d values than for the more alkaline ash and CKD landfill scenarios. It is probable that the lower K_d values in the latter scenarios are due to the combination of higher major ambient ion concentrations that compete with the trace metals for sorbing sites and solubilize the metals by complexation, plus the assumed absence of particulate organic carbon in the model landfill systems.

4.0 DISCUSSION OF RESULTS AND SOURCES OF UNCERTAINTY

Partition coefficients obtained from literature data are subject to numerous sources of uncertainty. Many previous studies have demonstrated that in a variety of soils and for a variety of metals, partition coefficients vary with pH and with the concentration of sorbing phases in the soil matrix (e.g., weight percent organic matter content and weight percent hydrous ferric oxides and corresponding oxides of aluminum and manganese) (Janssen et al., 1997; Hassan and Garrison, 1996; Bangash and Hanif, 1992; Anderson and Christensen, 1988). It is well known that dissolved ligands present in soil porewater (e.g., dissolved organic matter, anthropogenic organic acids) can complex with metals, reducing their propensity for sorption in proportion to the concentration of the ligands (Christensen et al., 1996). In multi-metal systems, competition among metals for sorption sites and the attendant reduction in the partition coefficient in comparison with single-metal systems has also been reported (Jin et al., 1996). Within the population of soils, the natural variability in soil composition and composition of associated soil porewater are such as to result in variation in K_d over orders of magnitude, even for a single metal. For this reason, any comprehensive compilation of K_d values selected from the literature should be expected to present values that define a distribution. In fact, for any particular metal, K_d depends on these and other characteristics of the natural media system (soil, sediment, surface water), and in a nationwide risk assessment it is desirable to sample the national population of such natural media systems to obtain a frequency distribution of K_d.

Unfortunately, the collection of natural media systems chosen for study by various researchers and reported in the literature is almost certainly not representative of the national population of such systems, and collections of K_d values obtained from the literature are almost certainly not representative of the true national frequency distribution of K_d for any particular metal of interest. Furthermore, the degree to which the natural systems reported in the literature are adequately representative of the population of such systems varies greatly among the different metals for which K_d values have been obtained. The manner in which the K_d values obtained in this study were used to develop estimates of the frequency distributions of K_d for the metals of concern were presented in Section 3.0. Statistical tests suggested that the data collected for the most studied metals were consistent with a log normal distribution. In addition, certain consistencies were observed in the magnitude of K_d for a particular metal in different media types, and in the ranked magnitude of K_d for different metals in a particular medium. These facts were used to advantage in developing the K_d frequency distributions for what must be considered a sparse dataset. The use of such patterns to discern the underlying frequency distributions of K_d is subjective, and implies a significant degree of uncertainty in the derived distributions.

Apart from uncertainties in representing the expected variation in K_d that arise from variation in soil/aquifer properties, there are significant uncertainties associated with individual K_d values obtained from the literature. Sources of uncertainty in individual literature K_d values include:

- Detection limits in measuring metal concentrations can result in limiting the observed maximum K_d value.
- Equilibrium conditions may not have prevailed in the experiment when measuring the media concentrations. Most batch experiments are carried-out over a time span of one or two days.

Equilibrium may or may not have been attained, and unaccounted-for non-equilibrium processes may have occurred.

- Some variability in collected K_d values may reflect variability in the different methods of measurement (e.g., batch experiments, measurements from natural soil and associated porewater, calculation from tracer/retardation studies).
- Some variability in collected K_d values may reflect variability in the extractants used in batch tests. Some researchers used soil porewater or groundwater as the extractant. Others used distilled water or a solution of electrolyte. The modeling in which these K_d values are to be used may implicitly prescribe an extractant that is dissimilar to any used in the literature studies that produced the K_d values. For example, landfill leachate may contain high concentrations of organic acids, Ca, Na, Cl, SO_4, and other ions. The presence of these constituents can result in lower K_d values relative to the values reported for more "pristine" systems. Lower K_d values can also result from increased competition for sorption sites or from complexation of the metal with dissolved ligands.
- Some uncertainty in the reported K_d values is associated with uncontrolled or unknown redox conditions during the course of experimental measurements, especially for redox-sensitive metals (e.g., Cr, As, Se). Separate K_d values for different oxidation states of the same metal were obtained whenever reported, but authors frequently did not report the oxidation state. Even when reported, the oxidation state must be regarded as somewhat uncertain— sorption reactions can be intimately associated with oxidation-reduction.
- There is uncertainty in the K_d values due to neglecting the impact of total system metal concentration on the magnitude of K_d. Numerous studies have documented the dependence of K_d on total metal concentration—K_d tends to decrease as the total metal concentration increases. No attempt has been made in this compilation of literature values to investigate or represent the dependence of K_d on total metal concentration. It is assumed that the K_d values compiled here are likely to be more representative of those in systems with low metal concentration than systems with high metal concentration.

Finally, the magnitude of the uncertainty in K_d values presented in this database of literature values should be regarded as having a significant metal-dependent component. As noted already, several metals have been more widely studied (e.g., Cd, As, Pb). For some of the metals of interest in this study, most notably Tl and Sb, there is very little partitioning data available for soil and groundwater systems. In addition, some sources of uncertainty listed above are associated with metal-specific phenomena (e.g., detection limits, redox transformations, propensity for dependence of K_d on metal concentration).

There are great uncertainties inherent in the use of equilibrium speciation modeling to estimate metal partition coefficients in waste systems. Much uncertainty in the model result is due to not having sufficient data to characterize the range of waste compositions, especially the character and concentration of sorption sites. In view of the uncertainty in speciation model estimated values, a possible alternative for representing metal partitioning in waste piles and landfills is to use the regression equation (i.e., Equation (4)) relating K_d in waste and soil (presented in Section 3.2.1). The latter has the advantage of preserving the relative affinities among metals that has been noted to be common to the natural media. However, the speciation 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 equation (Equation (4)) as variables subject to uncertainty that can be represented in the 3MRA monte carlo iterations. In the overall modeling strategy of 3MRA, if the frequency of occurrence of a highly alkaline waste system can be established and used in the monte carlo realizations, the regression equation 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 concentrations of metals in leachate from waste management systems, 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 wastepile/landfill scenarios, 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 and other processes in waste management systems.

5.0 REFERENCES

This reference list includes the complete bibliography of papers, articles, and reports that were copied and reviewed in our literature search. Those articles that 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 RECENT 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	---

Metal	**Risk Assessment**	**Type of Kd**	**Kd(L/kg)**	
			Single Value	**Range**
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	---

Metal	**Risk Assessment**	**Type of Kd**	**Kd(L/kg)**	
			Single Value	**Range**
	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	---
	US EPA Region 6 Combustion [USEPA96b]	sediment /water	3000	---

Metal	Risk Assessment	Type of Kd	Kd(L/kg)	
			Single Value	Range
	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	---

Metal	Risk Assessment	Type of Kd	Kd(L/kg)	
			Single Value	Range
	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
	US EPA Region 6 Combustion [USEPA96b]	suspended matter /water	---	2.2 -18

Metal	Risk Assessment	Type of Kd	Kd(L/kg)	
			Single Value	Range
	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	---

Metal	**Risk Assessment**	**Type of Kd**	**Kd(L/kg)**	
			Single Value	**Range**
	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

SCATTER PLOTS FOR LINEAR REGRESSIONS USED TO ESTIMATE MEAN LOG K VALUES

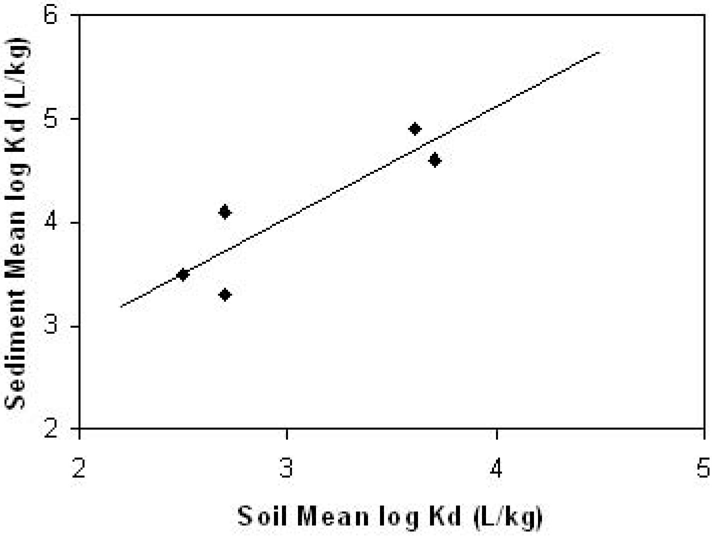

Figure B-1. Data used to develop regression equation to predict sediment K_d from soil K_d.

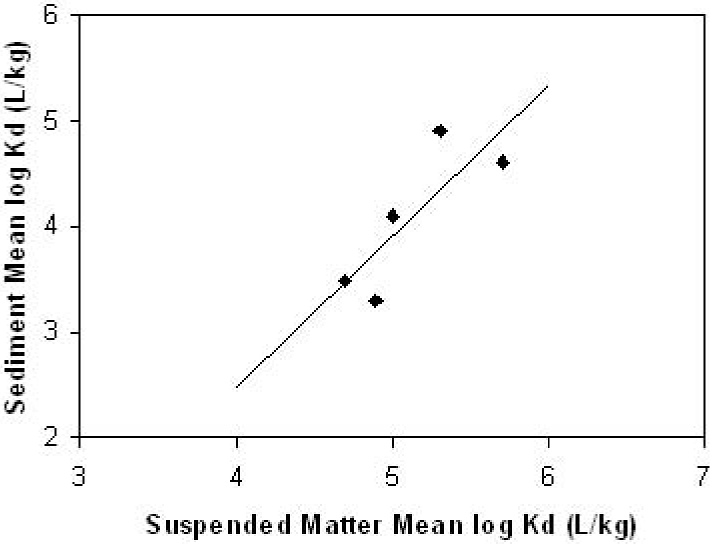

Figure B-2. Data used to develop regression equation to predict sediment K_d from suspended matter K_d.

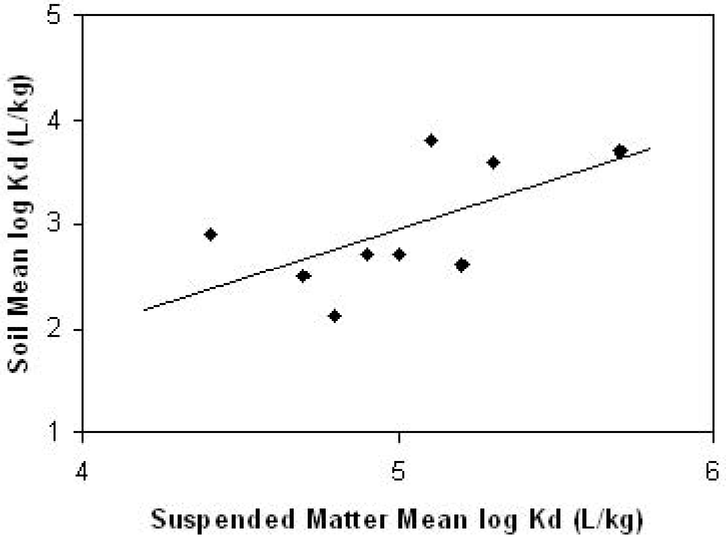

Figure B-3. Data used to develop regression equation to predict soil K_d from suspended matter K_d (and vice versa).

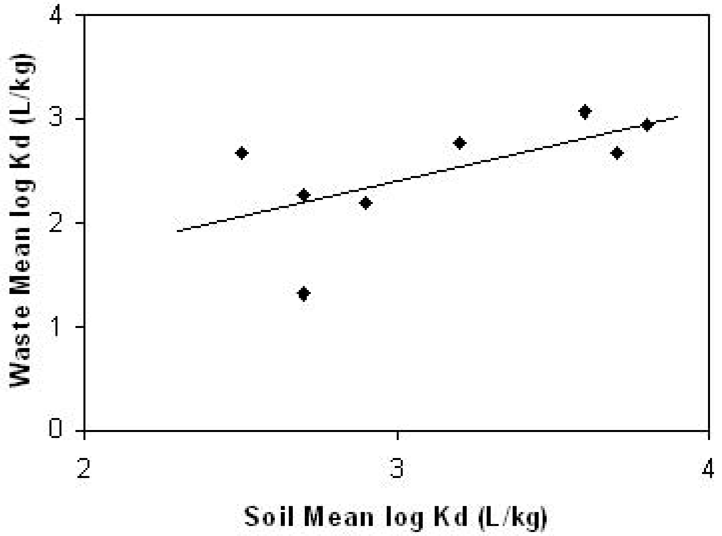

Figure B-4. Data used to develop regression equation to predict waste K_d from soil K_d.

APPENDIX C

EXAMPLE INPUT FILE FOR THE MINTEQA2 MODEL USED TO ESTIMATE METAL PARTITIONING IN SOIL/SOIL WATER SYSTEMS

```
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  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  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  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  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  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  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 =FeOHSO4-2      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 =FeOHSO4-2      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(OH4    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(OH4    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 D

EXAMPLE INPUT FILE FOR THE MINTEQA2 MODEL USED TO ESTIMATE METAL PARTITIONING TO 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 E

EXAMPLE INPUT FILE FOR THE MINTEQA2 MODEL USED TO ESTIMATE METAL PARTITIONING IN WASTE MANAGEMENT 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+02   -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)