BRITISH COLUMBIA MINE:

ION SPECIATION MODEL

MEND Project 4.7.5

This project was funded by Noranda Minerals Inc. and by the British Columbia Ministry of Energy, Mines and Petroleum Resources under the Canada/British Columbia Mineral Development Agreement

August 1992

BRITISH COLUMBIA MINE:
ION SPECIATION MODEL

I **EVALUATION FOR APPLICATION TO ACID MINE DRAINAGE REGULATIONS**

II **OPERATIONS MANUAL**

III **SOFTWARE**

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August 1992

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I EVALUATION OF B.C. MINE FOR APPLICATION TO ACID MINE DRAINAGE REGULATIONS

ACKNOWLEDGEMENT

This study was prepared for the British Columbia Acid Mine Drainage Task Force through funding in part from Noranda Minerals Inc.

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1.0 INTRODUCTION

For many years regulatory agencies have been exploring methodologies to evaluate the harmful effects of anthropogenic activity on the environment. Often times legislation is built on a comparison of available technology, observed environmental effects and requirements for industrial growth. In recent years, goals have been set by most agencies for sustainable industrial development, but often without reliable long term environmental impact information.

In this report, a model is presented that is intended to predict trace metal speciation in the environment. It is felt that it may be a useful tool in helping to regulate the release of acid mine drainage (AMD). AMD has been the subject of much review and research in recent years (e.g., Nolan, 1987; Pain 1987; Morin and Cherry, 1988; and Morin et al., 1988).

Regulatory agencies have historically been monitoring total metal levels for permitting criteria and they have attempted to correlate these levels with observed environmental biological effects. Our own activity with the B.C. Government has established subcellular techniques that can establish the effect that a given effluent may have on, for example, the metal metabolism of fish.

In this report a number of concepts have been used that may not be familiar to all readers. To aid in the understanding of the contents of this report, definitions of some terms used are provided.

Free Metal Ion

This refers to the fraction of the disclosed metal concentration that is in the free cation of hydrate form, e.g.,

$$\underset{\text{Free Metal Ion}}{Cu^{2+}} + \underset{\text{Ligand}}{L^{2-}} \rightleftharpoons \underset{\text{Metal Ligand Complex}}{CuL}$$

Hydrate forms such as $Cu(OH)_2$ may also be regarded as "free metal ions" from the point of view of this report as their dissociation is very rapid on interaction with biological membranes. Other complexes such as $CuCO_3$, for example, would not be included in this term.

Ion Speciation Model

This term refers to the type of model used in this report. In the model, specific ionic species are evaluated and the interactions of each catonic species with each anionic species is considered. Through an interactive process of balancing, each reaction is determined within the parameters of known redox and thermodynamic process,

Bioloaicallv Available

This term is used to describe the cumulative fraction of a specific element species that are able to be taken up by biological membranes. This term is somewhat subjective as several mechanisms of metal uptake can occur both in the dissolved phase (both active and passive) and in some cases by pinocytosis (partial uptake) (George *et al.*, 1976, 1977).

Equilibrium Constant

Consider the reaction

$$Cu + L \rightleftharpoons CuL.$$

At the equilibrium, the formation constant *or* the rate of formation of CuL is equal to the rate of dissociation of CuL to its constituents. The equilibrium constant for the above reaction may be defined as

$$K^1 = \frac{[Cu]\ [L]}{[CuL]}$$

Single Ion Activity Coefficient

Single ion activity coefficients are constants that greatly simplify calculations. They are not measurable individually; only ratios or products of ionic activity coefficients are measurable. These theoretical expressions are usually based on the Debye-Hinckel Limiting Law (see Stumm and Morgan, 1970). Other empirical relationships can also be used. For a *more* detailed explanation, see Stumm and Morgan, 1970.

It has been clear since the 1970's (Sunda and Guillard, 1976) that the free metal ion is the predominant metal species that is biologically available. For some biological systems, specific pathways of metal membrane transfer and partitioning are well established {Florence, et *al., 1984).*

In this proposal we have used an ion speciation model to calculate, from tke total concentration of parameters usually collected by the government agencies, the environmental concentration ranges 0% free metals.

The use of such procedures as a predictive tool is assessed in several stages:

- first, the model has been adapted to best fit with existing Tsolum River data
- second, the model is amended with data to allow for the organic bonding observed at this location to be evaluated
- third, the model predictions for this site are compared with determined metal species
- fourth, the accuracy of prediction is assessed by comparing model data and determined species.

In an attempt to evaluate the effectiveness of the model, the major parameters affecting speciation and its potential usefulness to regulators are discussed.

2.0 DEVELOPMENT OF B.C. MINE 1.2

A number of mathematical models have been developed to determine the chemical speciation of anions and cations in the environment. Some of these have been based on equilibrium constant data and some using kinetic effects.

The MINEI.2 model is an equilibrium model based on a specific ion interaction. The methodology for the model was first introduced by Francois Morel of M.I.T. in 1979. The principle of this model is that a single ion activity coefficient can be determined by considering specific ion interactions. That is the interaction of each anion with each and every cation.

In our model, this process is repeated for each cation and each anion.

In order to allow for kinetic effects that may impact the observed free metal ion activities, the stability constants of some ligands have been amended to allow for the observed effects. These new values have been termed "apparent stability constants".

An example of such effects would be the release of lead from particles and colloids. These reactions often cannot be described just in terms of the thermodynamic equilibrium. The release of lead from many natural surfaces is slow and thus the apparent "stability constant" is different from the theoretically predicted value. Such variations can be accounted for by using an experimentally derived "stability constant" number which is referred to as the "conditional stability constant". These "constants'* are operationally defined but can be used to improve the ability of the model to fit observed data.

The operation of MINE 1.2 is fully described in the manual (Mine 1.2, CBR 1992). Several alternate calculations are available, and are described in tha manual.

Options now exist for both input and output data to be selected. The output data has been reorganized in an attempt to clarify the data obtained.

An example of output data is shown in Appendix 1.

The output data tabulates input concentrations and calculated equilibrium values. The percentage contribution to the dissolved phase is also calculated together with the Concentration of each species. The partitioning between the particulate and dissolved phases axe based on redox eguilibrium'phase considerations. The output has been divided into three categories, each of which may be selected in the program using an on-off toggle.

In addition, the format of the output has been improved to more clearly show the results of the model predictions.

3.0 EVALUATION OF MINE 1.2 FOR TSOLUM RIVER

3.1 TSOLUM RIVER DATA FILES

Information on the chemical characterization of the Tsolum River was provided by John Deniseger, B.C. Ministry of Environment (BCMOE). From this data, nine data files were prepared. The first three files were prepared for minimum, maximum and average data from the Tsolum River, Farnham Bridge site. In all cases where total and dissolved concentrations were presented, total concentrations were used for the initial input data. Case measurements for the Farnham Bridge were provided by the BCMOE, and the pH ranged from 6.6 to 7.5 with a mean of 7.04.

The major variables that affect the speciation of metals of natural waters are pH and pE. Data provided by the BCMOE have been used in evaluating the effectiveness of the model. The calculation of pE was performed in a number of ways, using both oxygen data and manganese data provided by the BCMOE, and some assumptions on equilibrium.

The input data of Tsolum River at Farnham Bridge is presented in Tables 3.1, 3.2 and 3.3.

BY selecting files of maximum and minimum recorded concentrations of each parameter at the Farnham Bridge site, it is hoped to evaluate the potential variability of the actual and calculated metal speciation.

Similar files were created for Tsolum River at Duncan Main and Tsolum River at Rossiter. These files were used to evaluate the effect of several variables (section 4) and the variability of the model predictions (section 3).

For the determination of predictive models for all sampling sites, organic ligands were treated as one moiety.

Tsolum farnham

--- Input Data ---

INITIAL CONDITIONS

pE = 13.0
pH = 7.0

Ionic Strength = 3.86E-04

ID#	Analytical Concentration (MOLAR)	Component
1	2.25D-05	CA
2	9.47D-06	MG
4	1.28D-08	K
5	1.61D-04	NA
6	1.25D-06	FE3
8	1.82D-07	MN2
9	3.15D-08	cu2
10	2.19D-07	BA
11	8.90D-08	CD
12	1.53D-07	ZN
13	8.52D-07	NI
19	3.85D-07	CR
20	1.87D-06	AL
50	1.00D-09	H

ID#	Analytical Concentration (MOLAR)	Component
99	1.00D-09	E
101	8.00D-05	co3
102	1.77D-05	so4
103	3.67D-05	a
109	1.05D-06	P04
112	3.00D-07	6103
157	3.04D-06	N03
159	6.40D-07	FA
160	2.40D-07	HA

Table 3.1 Input data for Tsolum River at Farnham (min.)

MINE 1.2

1993 Feb 27 17:08

Tsolum far Max

--- Input Data ---

INITIAL CONDITIONS

pE = 13.0
pH = 7.0

Ionic Strength = 1.81E-03

ID#	Analytical Concentration ---(MOLAR)---	Component
1	1.44D-04	CA
2	5.68D-05	MG
4	1.28D-10	K
5	1.61D-04	NA
6	6.06D-05	FE3
8	2.37D-06	MN2
9	1.73D-06	cu2
10	2.19D-07	BA
11	8.90D-08	CD
12	4.59D-07	ZN
13	8.52D-07	NI
19	3.85D-07	CR
20	6.61D-05	AL
50	0.00D+00	H

ID#	Analytical Concentration --- (MOLAR) ---	Component
w-1--		
99	0.00D+00	E
101	8.00D-05	co3
102	2.72D-04	so4
103	7.05D-05	CL
109	1.05D-06	P04
112	3.00D-07	SI03
157	3.04D-06	N03
159	1.28D-06	FA
160	3.20D-08	HA

Table 3.2 Input data for Tsolum River at Farnham (max.)

MINE 1.2 1993 Feb 27 17:10

Tsolum far Average

--- Input Data ---

INITIAL CONDITIONS

pE = 13.0
pH = 7.0

Ionic Strength = 6.55E-04

ID#	Analytical Concentration (MOLAR)	Component
1	1.87D-05	CA
2	3.27D-05	MG
4	1.28D-10	K
5	1.61D-04	NA
6	4.34D-06	FE3
8	6.48D-07	MN2
9	2.61D-07	cu2
10	2.19D-07	BA
11	7.83D-13	CD
12	2.78D-07	ZN
13	8.52D-07	NI
19	3.85D-07	CR
20	3.73D-05	AL
50	1.00D-09	H

ID#	Analytical Concentration (MOLAR)	Component
99	0.00D+00	E
101	8.00D-05	co3
102	4.18D-05	so4
103	5.45D-05	CL
109	1.05D-06	P04
112	3.00D-07	6103
157	3.04D-06	NO3
160	1.61D-07	HA

Table 3.3 Input data for Tsolum River at Farnham (average)

In using the model, pH and pE have to be input as major variables. The determination of pH is usually performed on site. For pE, however, values must be calculated.

[N.B. In the previous model MINE 1.1, an error exists in the input file. pE is incorrectly termed Eh.]

In the remainder of this section, the considerations use to calculate pE are explained. Eh can be measured directly by using an approximate conductivity meter and it is suggested that this be done when predicting base data for such models. However, this ratio can be calculated. The log of this concentration pE has been estimated making a number of assumptions.

To calculate pE, the redox reactions must be considered. The speciation of oxygen in natural waters has been well established, as has the importance of control redox variables such as iron species and manganese species.

TO calculate the pE pertaining to the Tsolum River system at Farnham Bridge, the data from the average file was used.

To determine pE, the following equilibria were considered:

1. First the oxygen equilibrium was considered.

$$O_{2(g)} + 4H^+ + 4e^- = 2H_2O_{(L)} \quad (1)$$

If the water sample was at equilibrium with atmosphere:

the partial pressure of O_2 gives $P_{02} = 0.21$ atm.

From equation 1, $k = \dfrac{1}{P^{\frac{1}{2}}O_2[H^+]^2[e^-]^2} = 41.55$

From the Nernst equation:

$$pE = 20.78 + \tfrac{1}{4} \log(P^{\frac{1}{2}}_{O2}[H^+]^2), \quad (2)$$

$$pE = 20.45 - pH \text{ at } 25°C \text{ and } 0.21 \text{ atm } P_{O2}$$

From Henry's Law $[O_2] = \frac{P_{O2}}{RT}$ with $[O_2]$ at 10 mg/L

$P_{O2}^{\frac{1}{2}} = 0.15$ at 7-C

From equation 1 and 2 above, at 7°C the calculated value for pE:

$$pE = 13.26$$

2. Secondly, the manganese equilibrium was considered:

$$pE = 20.42 + \tfrac{1}{2} \log \frac{[H^+]^4}{[Mn^{++}]}$$

Again, by substitution in.equation 1:

$$pE = 20.42 + 2pH + \tfrac{1}{2} \log[M^{++}]$$

Using the mean pH data from Tsolum River at Farnham and the mean manganese concentration:

i.e., For pH of 7.04 and Mn of, 2.2 10^{-6} molar

$$pE = 12.94$$

The values obtained from both of these calculations were considered and concentrations of pH at 7.0 and of pE at 13.0 were used in the further evaluation of the model.

3.2 ORGANIC LIGAND CONCENTRATIONS

One of the principle variables controlling metal speciation in natural waters is the concentration of organic ligands that bind specific metals. The degree to which a given metal will be bound will depend on competition reactions with other ligands and the individual metal's affinity to those ligands.

In the organic rich river systems of British Columbia, often a considerable portion of the humic material is involved in associations with copper. This element has the highest affinity with the binding sides of humic materials. Because of the controlling influence of humics on metal speciation, humic determinations were made at a number of sites in this project. These data are presented in Table 3.4.

The concentration of humics in the Tsolum River at Farnham was then used in our average model data set. An average molecular weight of 1000 was used for calculation of humic acid concentrations. The model was run at pH 7 and pE of 13. The printout from the model is presented in Appendix 1. From this determination, free cupric ion activity was estimated at equilibrium to be 7.8×10^{-10} molar. While some copper carbonate complexes appeared at dissolved solids type 5 species, over 82% of the dissolved copper species were bound to humic material. Using the same model, but adjusting the humic acid concentration to 1.61 milligrams per litre, the calculated percentage binding of copper humic material was 58% of the total dissolved copper. Clearly the concentration of humic material is critical in this determination of freely available copper species in this system.

3.3 COMPLEXING CAPACITY AND STABILITY CONSTANT DATA

In order to evaluate the effectiveness of the MINE 1.2 model of the Tsolum River system, the predicted metal speciation was ground-proofed by performing speciation determinations from that river system. Speciation determinations were performed two separate ways.

Table 3.4 Concentration of Humic Substances

LOCATION	DATE	HUMIC ACID CONCENTRATION (MOLAR)*	pH
Murex Creek at Rossiter	10/22/91	1.20	6.42
Tsolum River at Duncan Main	10/22/91	4.50	6.50
Tsolum River at Farnham	10/22/91	2.40	6.77
Benson Mine adit	11/14/91	0.96	7.69
Quatze River	12/11/91	8.70	6.33
Benson Mine adit	11/27/91	0.96	7.81
Quatze River	11/14/91	8.00	7.48
Quatze River	11/14/91	8.50	6.89
Murex Creek	11/05/91	1.45	6.56
Tsolum River at Duncan Main	11/05/91	3.15	6.20
Tsolum River at Farnham	11/05/91	1.61	8.40

* Assumes molecular weight of 1000

In the first method, the metal ligand assemblage was titrated 'with the addition of cupric, cadmium, lead, and zinc ions and titration curves were performed for all of these metals.

From this data, complexing capacities were determined, as was the initial concentration of metal bound to ligand. In all cases, only one major break in the titration curve was observed. Establishing that the ligand assemblages in terms of analytical protocol act as a single unit, the metal complexing capacity data and the associated stability constants are presented in Table 3.5 and 3.6.

In all cases, stability constant data was calculated by the methods of Chau et *al.* (1974), Ruzic (1982) and Matson (1984). The tables represent mean determinations of these three methods. The conditional stability constants calculated are average operationally defined "constants" forthetotal ligand assemblage.

Theoretically, from the complexing capacity titration curves, it is possible to calculate the free metal ion activity in the initial sample. This is performed by transposing the gradient of the free metal titration curve, i.e. after the complexing capacity has been exceeded, through the initial starting point on the intersect on the x axis, thus giving you the concentration of free metal ion.

Due to the errors experienced in the first data points of the titration process and the binding affinity of the organic ligands in this system, it was not possible to calculate the free metal ion activity accurately from the titration curves obtained. Consequently, it was important to determine the organically bonded calculation of metals by direct measurement.

The second method involves the direct determination of metal species, analytically. This poses a difficult task in that at any stage inorganic metal contamination can greatly change the data obtained.

Table 3.5 Average Complexing Capacity and Stability Constant Data from the Tsolum River System

SAMPLE I.D.	pH	METAL	TOTAL DISSOLVED METAL ($mx10^{-8}$)	AVERAGE METHOD C_L ($mx10^{-8}$)	STAB. CONST. log
Murex Creek at Rossiter E206686	6.42	Cadmium	[illegible]	[illegible]	[illegible]
		Copper	[illegible]	[illegible]	[illegible]
Tsolum River at Duncan Main E206513		Zinc	3.57	--	- 0
		Cadmium	<0.05	--	--
		Lead	<0.009	70.0	9.75
		Copper	2.41	181	7.56
Tsolum River at Farnham 0127620	6.77	Zinc	3.91	--	--
		Cadmium	<0.05	--	--
		Lead	1.99	363	9.69
		Copper	5.66	815	7.36
Murex Creek at Rossiter E208668	6.58	Zinc	2.59	--	--
		Cadmium/	so.05	--	--
		Copper	29.8	--	-0
		Lead	1.19	--	--
Tsolum River at Duncan Main E208519	6.20	Zinc	3.34	--	- 0
		Cadmium	593	--	--
		Lead	0.03	1280	8.41
		Copper	1.44	2470	7.18
Tsolum River at Farnham 0127620	6.40	Zinc	3.13	--	- 0
		Cadmium	1.41	19.9	8.72
		Lead	0.689	1.36×10^{-8}	22.16
		Copper	9.51	25.8	a.54

Table 3.6 Average Complexing Capacity and Stability Constant Data from B.C. River Water

SAMPLE I.D.	METAL	TOTAL METAL moles $x10^{-8}$	AVERAGE METHOD moles $x10^{-8}$	STAB. CONST. log
Benson Mine Adit 91/11/14	Zinc	32.9	--	--
	Cadmium	1.12	--	--
	Lead	0,117	8.25	8.68
	Copper	59.9	17.6	7.49
Quatze River 0126360 91/11/14	Zinc	3.82	--	--
	Cadmium	--	--	--
	Lead	0.166	697	8.81
	Copper	6.92	64.5	8.44
Benson Mine Adit 91/11/27	Zinc	41.6	--	--
	Cadmium	--	-0	--
	Lead	3.26	13.5	9.57
	Copper	76.3	32.5	6.60
Quatze River 0126360 91/11/27	Zinc	12.6	--	--
	Cadmium	--	57.5	6.88
	Lead	--	17.2	9.19
	Copper	513	93.5	8.52
Quatze River 91/12/11	Zinc	240	--	--
	Cadmium	126	--	--
	Lead	0.330	1.82	8.96
	Copper	$76.3x10^{-7}$	--	--

For this study, a combination of photo-oxidation and Chelex 100 resin extraction was used. Accordingly, cleaning techniques were used through this study (including the use of our class 100 clean room) to reduce the risk of contamination.

In this method "available" metal was extracted on a chelex resin and washed off into acid solution. The metal content of this solution was then determined by atomic absorption spectrometry. This process was then repeated with a further aliquot of sample that had first been photo oxidised by radiation to break down the organic ligands in the sample. The total concentration of metal bound to the organic fraction was then determined by the difference.

These data for several locations in B.C. rivers are presented in Table 3.7.

Table 3.7 Determined Concentrations of Dissolved Copper Speciation by Extraction and Photo-Oxidation

SITE/LOCATION	DATE	TOTAL COPPER moles ($x10^{-8}$m)	FREE COPPER moles ($x10^{-8}$)	BOUND COPPER moles ($x10^{-8}$)
Tsolum River/Farnham	91/11/05	9.51	1.77	7.7
Tsolum River/Farnham	91/10/22	5.66	1.27	4.4
Quatze River	91/11/14	8.92	0.001	8.9
Quatze River	91/11/27	5.19	0.001	5.23
Quatze River	91/12/11	7.69	0.001	7.7
Benson Mine Adit	91/11/27	76.9	16.4	60.5
Benson Mine Adit	91/11/14	59.9	14	4.59
Tsolum River/Duncan		2.9	0.5	2.4
Tsolum River/Rossiter		8.5	5.4	3.1

4.0 COMPARATIVE ANALYSIS OF COPPER SPECIATION FROM MODEL AND LABORATORY DETERMINATIONS

In order to evaluate the effectiveness of the model, an average data file for the Tsolum River at Farnhamwas created, (Appendix 1). This data was then compared with data from ion speciation provided by our laboratory determinations.

Comparative data for dissolved copper species in percentage terms was collected. Model data using BCMOE data and our determined humic concentrations was calculated for average data files from three locations (see Appendix II and III):

Tsolum River at Farnham
Tsolum River at Duncan Main
Murex Creek at Rossiter.

These data were then compared with experimental data (Table 4.1) for the Tsolum River site at Farnham. The percentage contribution of organically bound copper by the two methods was within 2.5%. This was despite the fact that total copper concentrations in both our data and that from the BCMOE varied considerably. From the lab data these correspond to "free dissolved metal" concentrations of:

1.77×10^{-8} molar dissolved copper on the 05/11/91 and,
1.27×10^{-8} molar dissolved copper on the 27/11/91.

The model predicted 1.46×10^{-8}. Laboratory data average is 1.52×10^{-8} comparison to 1.46×10^{-8} (dissolved copper) from the model.

In percentage terms, the Tsolum River site at Duncan also showed similar results. The Rossiter data, however, showed a discrepancy of approximately 10%. This inaccuracy corresponds to an actual concentration variable of 0.8×10^{-8} molar copper or 0.5 µg/L total copper or 0.15 µg/L free copper.

Table 4.1 Comparison of Contribution (%) of Organically Bound Copper by Direct Determination and Calculation

SITE/LOCATION	% ORGANICALLY BOUND DISSOLVED COPPER		
	DATE	LAB	MODEL
Tsolum Farnham	91/10/05	81.0%	82.1%
	91/10/22	78.0%	--
Quatze River	91/11/14	99.0%	--
	91/11/27	99.0%	--
	91/12/11	99.0%	--
Benson	91/11/27	78.0%	--
	91/11/14	76.0%	--
Duncan Main	91/11/14	82.7%	86.7%
Rossiter	91/10/27	36.5%	45.8%

5.0 EFFECT OF MAJOR VARIABLES ON COPPER SPECIATION

In order to review the effects of major variables on the data provided by the model, data from the Tsolum River at Farnham were used. The variables considered were: **pH, pE,** manganese concentration, **humic** acid concentration and general metal concentrations. Variations in each of these parameters are discussed below.

In order to evaluate the effects of each parameter, the model was run with simulated data from the Rossiter site but with one variable changing. This required more than 50 runs. The results of each group of runs has been presented in terms of changes in the concentration of specific copper forms or in terms of the percentage contribution of organically bound copper. Those forms that were determined by the model to be dissolved solids (see manual) have not been included in the calculation of percentage of each dissolved copper species.

5.1 VARIATION IN pH

All of the samples collected were in a relatively narrow **pH** range of 6.0 to 7.4 **pH** units. Runs to evaluate **pH** were performed with only this variable changing and with **pE** remaining constant. While this evaluation was performed for simplicity, it was, of course, realized that **pH** effects the **pE** value and it might be more appropriate to calculate **pE** for each **pH** used.

Nevertheless, the model was run at constant **pE** of 12.

The effect of **pH** variation on the percentage of organically bound dissolved copper and the concentration of free dissolved copper is shown in Figure 5.1.

In the range 6.2 to 7, the percentage change due to **pH** is less than 10% at **pH** 8.

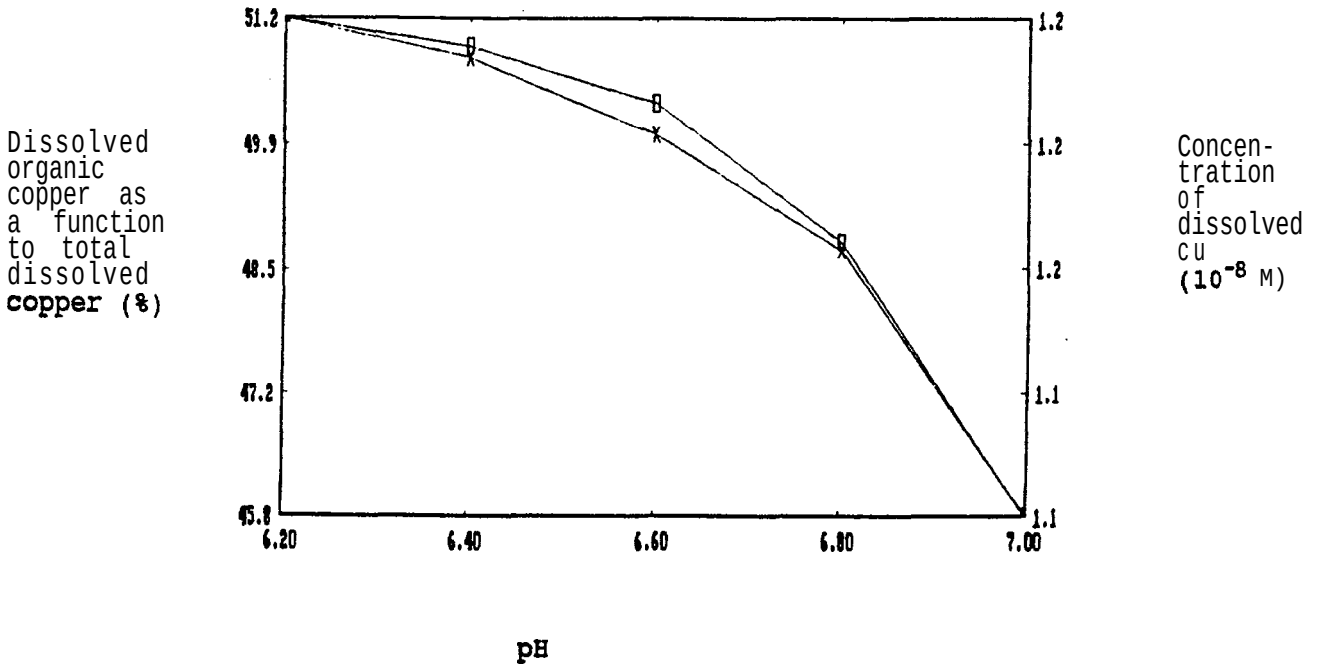

Figure 5.1 Variation of Organically-Bound Dissolved Copper with pH

5.2 EFFECT OF pE VARIATION ON COPPER SPECIATION

The value for pE was varied from 11.8 to 18.8 for Rossiter samples and was found to have no effect on the percentage of organically bound copper.

5.3 MANGANESE CONCENTRATION

The concentration of manganese was examined as it influence over pE is important. However, the model operates by setting the pE value at the beginning of each run. Then the model sets the dissolved manganese concentration based on that data. The determination of dissolved available manganese would, however, be an important tool in determining the pE for a given system.

5.4 CONCENTRATION OF HUMIC MATERIAL

The data for Rossiter was run on the model at a pH of 7 and pE of 13. Humic acid concentrations were varied from $1.0x10^{-7}$ m to 12x10" m.

These variations were shown to have a substantial effect on the percentage of copper bound to organic ligand and the concentration of free dissolved copper. This data is presented in Table 5.1 and in Figure 5.2.

From this data, it is clear that the major effect on copper speciation is the concentration of organic ligands and the concentration of metals in solution.

5.5 COPPER CONCENTRATIONS

To further examine the relationship of copper to organic ligand, the concentrations of total copper were changed. These data are shown in Figure 5.3. Once the organic ligand assemblage (humic acid) is saturated with copper, the amount of organic binding is reduced to a few percent. This has important. implications in the determination of biologically active copper.

Table 5.1 Effect of Humic Acid Concentration on Copper Speciation at Rossiter

pH 6.5 pE 12.5 HUMIC ACID (10^{-7} m)	ORGANICALLY BOUND Cu (%)	FREE COPPER (10^{-7} m)
1.0	36.2	1.36
1.5	52.1	1.02
2.0	65.5	0.74
4.0	89.3	0.23
8.0	96.3	0.08
12.0	97.8	0.05

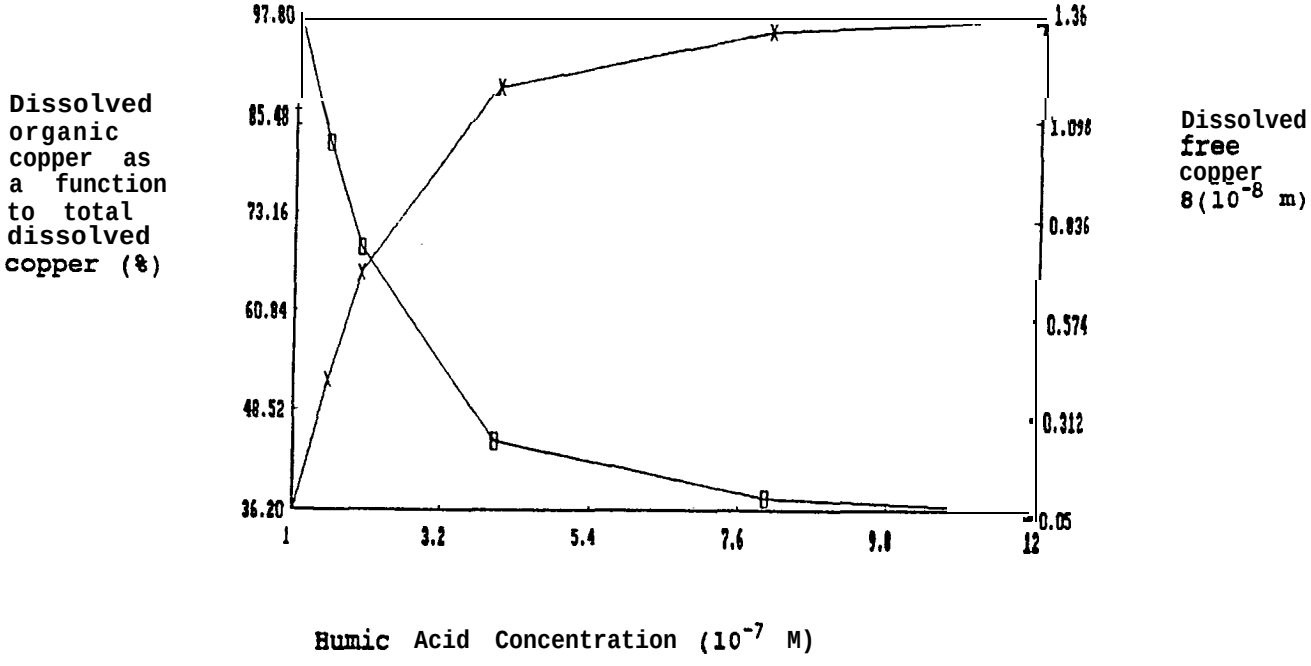

Figure 5.2 Effect of the Variation of Humic Acid on organic copper Binding.

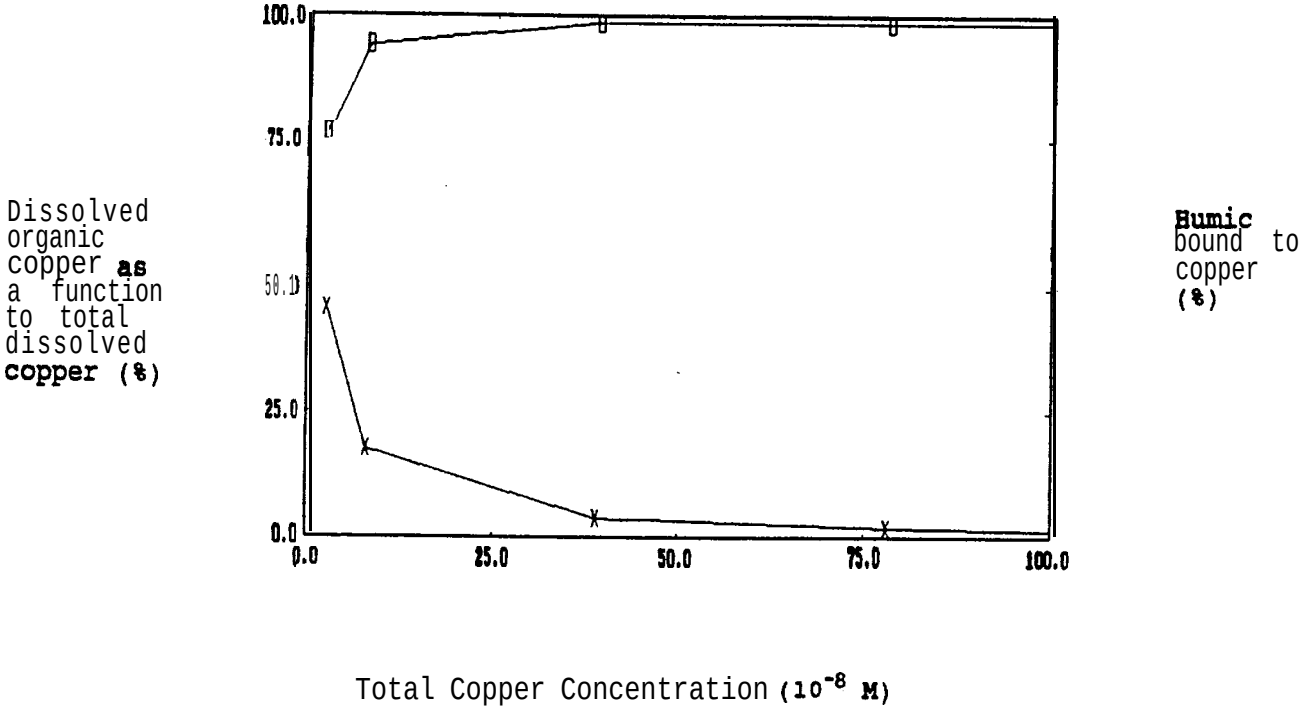

Figure 5.3 Variation of Organically Bound Copper with changing Copper concentration

6.0 RECOMMENDATIONS OF PARAMETERS REQUIRED FOR ACCURATE PREDICTIVE MODELLING

Evaluations of the effects of major variables on copper speciation has been shown in Section 5.0. This data is used for both background determinations, at proposed mining sites and for ongoing monitoring at operational sites as criteria for compliance with environmental permits.

From the data presented in this report, it appears that the MINE model could be a useful tool in monitoring. To ensure accurate predictions, some additional data to the data already collected by the BCMOE should be considered. The main parameter currently not measured, but which has dramatic effect on metal speciation, is that of the humic acid component.

In order to produce an accurate predictive model at each MINE site or potential MINE site in B.C., the following criteria are required:

1. Determination of total cation and anion species.

   Much of this data is obtained from the routine monitoring currently performed by BCMOE. It is important that these routine determinations be accurately performed and that cations and anions concentrations be established.

2. Determination of humic acid content.

   The determination of combined humic and fulvic acids at each site appears to be critical in determining the proportion of metal that is available for binding. As shown in Section 5.0, organic ligand concentration is the single most important parameter in determining the amount of free metal available for biological systems.

3. Determination of pH.

The determination of pH is a critical criteria in these systems. More importantly, the range of pH to be experienced in any one environment is of critical importance in looking at release and uptake of metals by natural ligands and particulates.

4. Determination of Metal Speciation.

Determination of metal speciation on an occasional basis and during the initial setup of models for a specific system is suggested. The model should be ground-proofed by independent determination of metal speciation. This should not be done electrochemically using the intersect point but rather done separately using a combination of extraction procedures and photo-oxidation. These data, while suffering from the problems of requiring clean techniques to perform, produce more reliable data for the determination of speciation. It is felt that this is a necessary step to ensure the quality and predictive capability of the model for a specific system.

7.0 IMPLICATIONS OF B.C. MINE AND COMPLEXING CAPACITY TO REGULATORY CONSIDERATIONS

The model described in this report appears to give reasonably accurate projections of metal speciation at any one point in time from a given location. In order to be able to use this data in a regulatory sense, it is important to determine under what considerations metal bound to organic material would become available to biological systems. In this regard, some historical data on the specific site in question or general data showing variations specifically in pH and Eh for that area are important. This information, combined with total metal levels, provide the basis for using predictive modelling as part of the regulatory process. Models that have been calibrated with specific data and showing actual metal speciation appear to produce accurate determinations of metal species.

The stability constant data used in our model for specific ligand interactions appear to be generally applicable in each of the cases studied. No changes were made to those stability constants after the initial setup of the model, despite material being taken from varying sites.' While the model provides a clear predictive capability to determine speciation at any one time, it is important to look at the metal buffering capacity of each environmental receiving system. This can be determined when measuring the complexing capacity of that system.

While more limited information is gained from the determination of complexing capacity for lead, zinc and cadmium, cupric complexing capacity is a useful parameter in determining the buffering capacity of 'that system. The binding affinities of other metals to organics are well known and published in the literature. The relative binding of Pb, -Cd and Zn can therefore, be calculated from the copper data. In our view, by determining the concentration of copper that can be bound by organics in a given system may be the basis

for providing regulatory information in terms of increased copper that can be received to that environment without undue effect on the relative biota. In addition, some elements such as cadmium physical binding to other components such as clays, should be considered.

In summary, the following recommendations are made to improve the basis of regulatory decision-making in evaluating the effect of increased metal loading to a given environment.

1. Determination of cupric complexing capacity.

   This gives an estimate of the metal buffering capacity in that system.

2. Determination of total metal levels in major anions and pH.

   These parameters allow the determination of metal available as well as providing information on total metal loading.

3. Measurement of metal speciation, i.e., the determination of ion bound and bound metal forms:

   This measurement provides information on actual available metal at that time. Measurement of this parameter allows the accurate use of MINE 1.2 and also provides an estimate in terms of concentration of metal available to biological systems.

4. Variation in pH.

   The total expected variation in pH is critical to worst possible case situation for metal availability.

5. MIMS Bioassays.

   The use of bioassay in *situ* or in the lab and the determination of molecular indications of metal stress allow actual biological effects of increased metal loading to be established (Imber et al., 1992).

8.0 CONCLUSIONS

The latest version of the **MINE** 1.2 has hopefully made the model sufficiently user-friendly so that scientists who do not have specific expertise in speciation modelling can safely use the model as a predictive tool for metal speciation.

The model appears to be accurately predictive, provided specific background information on the locality is available. To improve the criteria for regulating new operations, particularly in **areas** of high background metal levels, it may be appropriate to incorporate some fraction of **complexing** capacity measurements in the determination of the increased loading allowable to the receiving environment. Such an approach using metal speciation rather than total metal levels in the calculation of regulations allow a scientifically defensible position in the determination of a concentration level for specific elements.

With the information provided, in terms of organic binding and free metal ion activity, it is possible to safely provide, in some cases, increased metal into the system before biological impact is observed. In addition to these approaches, metal metabolism of indicator organisms as a controlling system may well be an important part in the regulatory process.

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APPENDIX I

NINE 1.2 DETERMINATION OF METAL SPECIES
AT THE TSOLUM RIVER SYSTEM AT FARNHAM BRIDGE

TSOLUM RIVER AT FARNHAM
USING 2.400 MG/L HUMIC MATERIAL

MINE 1.2 1993 Feb 28 09:42

Tsolum far Average

--- Output Data ---

FINAL CONDITIONS

Number of iterations = 59

pE = 13.0
pa = 7.0 Ionic Strength = 6.55E-04

ID# 1-w-1	Concentration (MOLAR) I----- Equilibrium	Analytical	Remainder	Component
1	1.86D-05	1.87D-05	1.72D-14	CA
2	3.24D-05	3.27D-05	3.77D-14	MG
4	1.28D-10	1.28D-10	8.36D-21	K
5	1.61D-04	1.61D-04	4.19D-15	NA
6	2.58D-15	4.34D-06	-7.14D-21	FE3
8	8.92D-13	6.48D-07	0.00D+00	MN2
9	1.46D-08	2.61D-07	1.34D-17	cu2
10	1.92D-07	2.19D-07	-5.89D-12	BA
11	7.66D-13	7.83D-13	-7.07D-28	CD
12	2.52D-07	2.78D-07	2.33D-16	ZN
13	8.31D-07	8.52D-07	7.68D-16	NI
19	1.24D-27	3.85D-07	1.81D-21	CR
20	2.98D-14	3.73D-05	0.00D+00	AL
50	1.00D-07	1.00D-09	0.00D+00	H
99	1.00D-13	0.00D+00	0.00D+00	E
101	4.75D-08	8.00D-05	-2.68D-20	co3
102	4.14D-05	4.18D-05	0.00D+00	so4
103	5.45D-05	5.45D-05	-4.79D-20	CL
109	1.22D-12	1.05D-06	-2.53D-21	PO4
112	7.09D-16	3.00D-07	-4.61D-22	6103
157	3.04D-06	3.04D-06	4.66D-21	NO3
160	1.85D-08	2.40D-07	-6.56D-21	HA

MINE 1.2 1993 Feb 28 09:42

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--- Output Data ---

TYPE I: COMPONENTS

ID# --a--	Equilibrium Concentration ---(MOLAR)---	LogK --e--w--	Species (Name:Stoichiometric Coeff)	
2	3.24D-05	.00	MG	1
4	1.28D-10	.00	K	1
5	1.61D-04	.00	NA	1
6	2.58D-15	.00	FE3	1
8	8.92D-13	.00	MN2	1
9	1.46D-08	.00	cu2	1
10	1.92D-07	.00	BA	1
11	7.66D-13	.00	CD	1
12	2.52D-07	.00	ZN	1
13	8.31D-07	.00	NI	1
19	1.24D-27	.00	CR	1
20	2.98D-14	.00	AL	1
101	4.75D-08	.00	co3	1
102	4.14D-05	.00	so4	1
103	5.45D-05	.00	CL	1
109	1.22D-12	.00	PO4	1
112	7.09D-16	.00	S103	1
157	3.04D-06	.00	NO3	1
160	1.85D-08	.00	HA	1

MINE 1.2 1993 Feb 28 09:42

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--- Output Data ---

TYPE II: COMPLEXES

ID#	Equilibrium Concentration ---(MOLAR)---	LogK ---I---	Species (Name:Stoichiometric Coeff)					
1	1.86D-05	.00	CA	1				
1000	7.02D-10	2.90	CA	1	co3	1		
1010	2.79D-08	11.50	CA	1	co3	1	H	1
1020	1.22D-07	2.20	CA	1	so4	1		
1080	6.02D-10	14.43	CA	1	PO4	1	H	1
1200	1.80D-09	3.72	CA	1	HA	1		
1350	1.11D-10	-12.22	CA	1	H	- 1		
1360	1.94D-09	3.10	MG	1	co3	1		
1370	4.88D-08	11.50	MG	1	co3	1	H	1
1380	2.68D-07	2.30	MG	1	so4'	1		
1440	3.32D-09	14.93	MG	1	PO4	1	H	1
1580	1.90D-09	3.50	MG	1	HA	1		
1740	1.93D-09	-11.22	MG	1	H	-1		
1960	5.94D-14	1.05	K	1	so4	1		
1995	5.30D-16	2.35	K	1	HA	1		
2000	1.08D-10	1.15	NA	1	co3	1		
2010	2.98D-08	.65	NA	1	so4	1		
2060	3.34D-09	3.05	NA	1	HA	1		
2070	1.20D-15	4.05	FE3	1	so4	1		
2080	1.11D-18	5.40	FE3	1	so4	2		
2090	2.98D-18	1.33	FE3	1	CL	1		
2100	7.26D-22	1.98	FE3	1	CL	2		
2110	5.92D-27	1.15	FE3	1	CL	3		
2170	9.39D-14	20.48	FE3	1	PO4	1	H	1
2190	4.34D-14	23.38	FE3	1	SI03	1	H	1
2666	3.38D-16	6.85	FE3	1	HA	1		
2670	4.59D-10	-1.75	FE3	1	H	-1		
2680	4.33D-06	-4.77	FE3	1	H	-2		
2690	1.73D-14	-20.17	FE3	1	H	-3		
2700	7.27D-09	-21.55	FE3	1	H	-4		
2710	3.33D-18	-2.30	FE3	2	H	-2		
3290	4.25D-15	12.00	co3	1	MN2	1	H	1
3300	5.86D-15	2.20	MN2	1	so4	1		
3310	5.46D-16	1.05	CL	1	MN2	1		
3320	2.81D-20	1.03	CL	2	MN2	1		
3330	4.85D-25	.53	CL	3	MN2	1		
3360	1.15D-15	16.03	PO4	1	MN2	1	H	1
3900	6.69D-16	-10.12	MN2	1	H	-1		
3910	5.63D-26	-34.20	MN2	1	H	-3		
3920	2.76D-09	6.60	cu2	1	co3	1		
3930	2.08D-13	9.80	cu2	1	co3	2		
3932	1.10D-10	12.20	cu2	1	co3	1	H	1
3940	9.56D-11	2.20	cu2	1	so4	1		
3950	2.82D-12	.55	cu2	1	CL	1		

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--- Output Data ---

TYPE II: COMPLEXES (cont'd)

ID#	Equilibrium Concentration ---(MOLAR)---	LogK	Species (Name:Stoichiometric Coeff)					
3960	9.16D-17	.33	cu2	1	CL	2		
4010	4.72D-11	16.43	CU2	1	PO4	1	H	1
4813	2.14D-07	8.90	cu2	1	HA	1		
4840	1.73D-09	-7.92	cu2	1	H	-1		
4842	2.74D-08	-13.72	cu2	1	H	-2		
4844	2.31D-14	-26.80	cu2	1	H	-3		
4846	2.05D-20	-39.85	cu2	1	H	-4		
4850	1.00D-12	-10.32	CU2	2	H	-2		
4912	2.82D-11	3.90	BA	1	HA	1		
5060	2.87D-13	-12.82	BA	1	H	-1		
5070	4.59D-17	3.10	CD	1	co3	1		
5072	5.78D-15	12.20	CD	1	co3	1	H	1
5090	3.73D-15	1.95	CD	1	CL	1		
5100	9.62D-19	2.63	CD	1	CL	2		
5110	1.32D-23	2.03	CD	1	CL	3		
5270	5.25D-21	3.75	CD	1	PO4	1		
5930	7.24D-15	-9.02	CD	1	H	-1		
5940	5.75D-18	-19.12	CD	1	H	-2		
5950	3.05D-22	-30.40	CD	1	H	-3		
5954	1.91D-09	5.20	ZN	1	co3	1		
5956	1.91D-09	12.20	ZN	1	co3	1	H	1
5960	1.66D-09	2.20	ZN	1	so4	1		
5970	3.88D-12	-.55	ZN	1	CL	1		
5980	6.33D-17	-1.07	ZN	1	CL	2		
5990	3.45D-20	-.07	ZN	1	CL	3		
6060	1.03D-10	15.53	ZN	1	PO4	1	H	1
6733	3.71D-10	4.90	ZN	1	HA	1		
6740	7.54D-10	-9.52	ZN	1	H	-1		
6745	1.89D-08	-15.12	ZN	1	H	-2		
6750	1.27D-13	-27.30	ZN	1	H	-3		
6760	1.42D-19	-40.25	ZN	1	H	-4		
6770	5.46D-09	2.20	NI	1	so4	1		
6780	1.28D-10	.45	NI	1	CL	1		
7590	1.57D-08	-8.72	NI	1	H	-1		
9890	2.90D-27	4.75	CR	1	so4	1		
10000	5.56D-24	-3.35	CR	1	H	-1		
10010	1.66D-22	-8.87	CR	1	H	-2		
10020	1.76D-23	-23.85	CR	1	H	-4		
10030	1.39D-15	3.05	AL	1	so4	1		
10040	2.04D-18	4.60	AL	1	so4	2		
10102	2.17D-25	7.78	PO4	1	H	1	AL	1
10104	2.29D-37	2.80	PO4	1	H	2	AL	1
10340	8.41D-12	-4.55	H	-1	AL	1		
10342	1.26D-09	-9.37	H	-2	AL	1		

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--- Output Data ---

TYPE II: COMPLEXES (cont'd)

ID#	Equilibrium Concentration ---(MOLAR)---	LogK	Species (Name:Stoichiometric Coeff)					
10344	2.51D-08	-15.07	H	-3	AL	1		
10350	2.11D-09	-23.15	H	-4	AL	1		
10352	1.77D-21	-7.70	H	-2	AL	2		
10354	3.53D-27	-13.88	H	-4	AL	3		
12530	6.72D-05	10.15	co3	1	H	1		
12540	1.27D-05	16.43	co3	1	H	2		
12550	5.85D-10	2.15	H	1	so4	1		
12600	3.24D-07	12.43	PO4	1	H	1		
12610	7.25D-07	19.78	PO4	1	H	2		
12620	6.85D-12	21.75	PO4	1	H	3		
12710	7.96D-10	13.05	6103	1	H	1		
12720	2.99D-07	22.63	S103	1	H	2		
13595	1.06D-07	-13.98	H	-1				
13600	5.42D-13	******	CR	2	H	-14	E	-6
13610	7.38D-08	-68.23	CR	1	H	-7	E	-3
13620	3.11D-07	-74.60	CR	1	H	-8	E	-3

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--- Output Data ---

TYPE III: FIXED SOLIDS

ID#	Equilibrium Concentration ---(MOLAR)---	LogK	Species (Name:Stoichiometric Coeff)
50	3.15D-05	7.00	H 1
99	2.45D-06	13.00	E 1

TYPE IV: PRECIPITATED SOLIDS

ID#	Equilibrium Concentration --- (MOLAR) ---	LogK	Specie6 (Name:Stoichiometric Coeff)
20520	2.68D-08	11.10	BA 1 so4 1
21180	3.73D-05	-7.47	H -3 AL 1
21470	6.48D-07	-41.95	MN2 1 H -4 E -2

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Tsolum far Average

--- Output Data ---

TYPE V: DISSOLVED SOLIDS

ID#	Equilibrium Concentration --- (MOLAR) ---	LogK	Species (Name:Stoichiometric Coeff)					
20000	1.40D-04	8.20	CA	1	co3	1		
20010	3.06D-05	4.60	CA	1	so4	1		
20030	1.33D-08	44.53	CA	5	PO4	3	H	-1
20040	9.59D-15	47.65	CA	4	PO4	3	H	1
20050	3.02D-05	19.13	CA	1	PO4	1	H	1
20070	5.24D-12	8.60	CA	1	6103	1		
20130	2.21D-13	-21.92	CA	1	H	-2		
20140	3.08D-07	5.30	MG	1	co3	1		
20160	5.35D-10	28.03	MG	3	PO4	2		
20200	1.22D-07	-16.42	MG	1	H	-2		
20280	1.18D-01	25.58	FE3	1	PO4	1		
20370	8.47D-10	10.30	co3	1	MN2	1		
20400	2.52D-17	10.60	S103	1	MN2	1		
20430	2.66D-13	-14.52	MN2	1	H	-2		
20438	2.35D-06	9.53	cu2	1	co3	1		
20440	7.57D-04	5.88	cu2	2	co3	1	H	-2
20460	9.68D-11	37.33	cu2	3	PO4	2		
20500	1.37D-02	-8.02	cu2	1	H	-2		
20510	7.25D-05	9.90	BA	1	co3	1		
20570	5.78D-09	11.20	CD	1	co3	1		
20582	1.12D-28	32.23	CD	3	PO4	2		
20620	1.82D-12	-13.62	CD	1	H	-2		
20630	6.02D-04	10.70	ZN	1	co3	1		
20650	5.05D-08	36.33	ZN	3	PO4	2		
20660	4.50D-04	18.40	S103	1	ZN	1		
20700	2.38D-04	-11.02	ZN	1	H	-2		
20710	4.98D-06	8.10	WI	1	co3	1		
20750	6.23D-03	-10.12	NI	1	H	-2		
21140	2.63D-16	-9.67	CR	1	H	-3		
21150	6.85D-04	22.28	PO4	1	AL	1		
21160	1.13D-04	39.40	SI03	2	H	-2	AL	2
21440	1.50D-04	25.33	SI03	1	H	2		
21480	1.42D-16	-61.70	MN2	3	H	-8	E	-2
21490	1.78D-04	-25.70	MN2	1	H	-3	E	-1
21510	3.66D-23	11.40	cu2	1	E	2		

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N---------m-------

--- Output Data ---

TYPE VI: SPECIES NOT CONSIDERED

ID#	Equilibrium Concentration --- (MOLAR) ---	LogK	species (Name:Stoichiometric Coeff)
20310	1.28D+03	-3.30	FE3 1 H -3
21460	5.14D+04	5.48	FE3 3 H -8 E 1
25000	4.00D-04	17.93	co3 1 H 2

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--- Output Data ---

DISTRIBUTION OF COMPONENTS

ID#	Component	Percent Bound in Species (Name:Stoichiometric Coeff)								
		(%)	ID#							
1	CA	99.2	1	CA	1					
2	MG	99.0	2	MG	1					
4	K	100.0	4	K	1					
5	NA	100.0	5	NA	1					
6	FE3	99.8	2680	FE3	1	H	-2			
8	MN2	100.0	21470	MN2	1	H	-4	E	-2	
9	cu2	5.6	9	CU2	1					
		1.1	3920	cu2	1	co3	1			
		82.1	4813	CU2	1	HA	1			
		10.5	4842	CU2	1	H	-2			
10	BA	87.7	10	BA	1					
		12.3	20520	BA	1	so4	1			
11	CD	97.9	11	CD	1					
12	ZN	90.8	12	ZN	1					
		6.8	6745	ZN	1	H	-2			
13	NI	97.5	13	NI	1					
		1.8	7590	NI	1	H	-1			
19	CR	19.2	13610	CR	1	H	-7	E	-3	
		80.8	13620	CR	1	H	-8	E	-3	
20	AL	99.9	21180	H	-3	AL	1			
50	H	1.6	13610	CR	1	H	-7	E	-3	
		7.9	13620	CR	1	H	-8	E	-3	
		27.5	2680	FE3	1	H	-2			
		8.2	21470	MN2	1	H	-4	E	-2	
		354.8	21180	H	-3	AL	1			

Tsolum far Average

--- Output Data ---

DISTRIBUTION OF COMPONENTS

ID#	Component	Percent Bound in Species (%)	ID#	(Name:Stoichiometric Coeff)				
99	E	9.0	13610	CR	1	H	-7	E -3
		38.1	13620	CR	1	H	-8	E -3
		52.9	21470	MN2	1	H	-4	E -2
101	co3	84.0	12530	CO3	1	H	1	
		15.8	12540	CO3	1	H	2	
102	so4	98.9	102	so4	1			
103	CL	100.0	103	CL	1			
109	PO4	30.7	12600	PO4	1	H	1	
		68.9	12610	PO4	1	H	2	
112	SI03	99.7	12720	SI03	1	H	2	
157	NO3	100.0	157	NO3	1			
160	HA	7.7	160	HA	1			
		1.4	2060	NA	1	HA	1	
		89.2	4813	CU2	1	HA	1	

APPENDIX II

EQUILIBRIUM MODEL FOR TSOLUM
RIVER AT DUNCAN MAIN

MINE 1.2 1993 Feb 28 09:59

TSOLUM R at DUNCAN MAIN

--- Output Data ---

FINAL CONDITIONS

Number of iterations = 70

pE = 13.0
pH = 7.0 Ionic Strength = 5.01E-01

ID#	Concentration (MOLAR) Equilibrium	Analytical	Remainder	Component
			I--------	C--------
1	1.06D-04	1.06D-04	-3.47D-20	CA
2	5.16D-05	5.16D-05	3.96D-21	MG
4	1.28D-10	1.28D-10	1.47D-25	K
5	1.61D-04	1.61D-04	2.21D-20	NA
6	3.41D-14	7.78D-06	-2.89D-20	FE3
8	2.35D-13	5.40D-07	0.00D+00	MN2
9	3.39D-09	5.30D-08	-5.24D-23	CU2
10	2.18D-07	2.19D-07	1.17D-22	BA
11	8.82D-08	8.90D-08	1.52D-22	CD
12	1.95D-07	2.04D-07	2.98D-22	ZN
13	1.03D-05	1.04D-05	4.01D-21	NI
19	2.57D-31	1.92D-07	6.90D-15	CR
20	2.20D-13	5.66D-06	9.66D-22	AL
50	l.00D-07	l.00D-09	0.00D+00	H
99	1.00D-13	1.00D+00	0.00D+00	E
101	1.95D-07	8.00D-05	-2.62D-20	CO3
102	1.61D-05	1.61D-05	-1.35D-14	SO4
103	9.03D-05	9.03D-05	-2.85D-20	CL
109	1.83D-11	1.05D-06	2.61D-21	PO4
112	5.22D-15	3.00D-07	1.66D-21	SI03
157	3.04D-06	3.04D-06	4.66D-21	NO3
160	2.45D-07	3.15D-07	-5.00D-22	HA

MINE 1.2 1993 Feb 28 09:59

TSOLUM R at DUNCAN MAIN

--- Output Data ---

TYPE I: COMPONENTS

ID# m-o--	Equilibrium Concentration ---(MOLAR) ---	LogK ----PI--	Species (Name:Stoichiometric Coeff)
1	1.06D-04	.00	CA 1
2	5.16D-05	.00	MG 1
4	1.28D-10	.00	K 1
5	1.61D-04	.00	NA 1
6	3.41D-14	.00	FE3 1
8	2.35D-13	.00	MN2 1
9	3.39D-09	.00	cu2 1
10	2.18D-07	.00	BA 1
11	8.82D-08	.00	CD 1
12	1.95D-07	.00	ZN 1
13	1.03D-05	.00	NI 1
19	2.57D-31	.00	CR 1
20	2.20D-13	.00	AL 1
101	1.95D-07	.00	co3 1
102	1.61D-05	.00	so4 1
103	9.03D-05	.00	CL 1
109	1.83D-11	.00	P04 1
112	5.22D-15	.00	6103 1
157	3.04D-06	.00	N03 1
160	2.45D-07	.00	HA 1

MINE 1.2 1993 Feb 28 09:59

TSOLUM R at DUNCAN MAIN

--- Output Data ---

TYPE II: COMPLEXES

ID#	Equilibrium Concentration ---(MOLAR)---	LogK	Species (Name:Stoichiometric Coeff)					
1000	1.14D-09	1.74	CA	1	CO3	1		
1010	4.53D-08	10.34	CA	1	CO3	1	H	1
1020	1.88D-08	1.04	CA	1	SO4	1		
1080	4.86D-10	12.40	CA	1	PO4	1	H	1
1200	9.45D-09	2.56	CA	1	HA	1		
1350	3.23D-10	-12.51	CA	1	H	-1		
1360	8.82D-10	1.94	MG	1	CO3	1		
1370	2.21D-08	10.34	MG	1	CO3	1	H	1
1380	1.15D-08	1.14	MG	1	SO4	1		
1440	7.51D-10	12.90	MG	1	PO4	1	H	1
1580	2.78D-09	2.34	MG	1	HA	1		
1740	1.58D-09	-11.51	MG	1	H	-1		
1960	6.10D-15	.47	K	1	SO4	1		
1995	1.85D-15	1.77	K	1	HA	1		
2000	1.17D-10	.57	NA	1	CO3	1		
2010	3.05D-09	.07	NA	1	SO4	1		
2060	1.17D-08	2.47	NA	1	HA	1		
2070	1.13D-16	2.31	FE3	1	SO4	1		
2080	1.08D-20	3.09	FE3	1	SO4	2		
2090	8.82D-18	.46	FE3	1	CL	1		
2100	9.38D-22	.53	FE3	1	CL	2		
2110	6.51D-27	-.59	FE3	1	CL	3		
2170	4.65D-14	17.87	FE3	1	PO4	1	H	1
2190	1.51D-13	21.93	FE3	1	SIO3	1	H	1
2666	1.09D-15	5.11	FE3	1	HA	1		
2670	1.60D-09	-2.33	FE3	1	H	-1		
2680	7.76D-06	-5.64	FE3	1	H	-2		
2690	3.09D-14	-21.04	FE3	1	H	-3		
2700	2.53D-08	-22.13	FE3	1	H	-4		
2710	5.82D-16	-2.30	FE3	2	H	-2		
3290	3.20D-16	10.84	CO3	1	MN2	1	H	1
3300	4.18D-17	1.04	SO4	1	MN2	1		
3310	6.29D-17	.47	CL	1	MN2	1		
3320	2.75D-21	.16	CL	2	MN2	1		
3330	7.86D-26	-.34	CL	3	MN2	1		
3360	4.31D-17	14.00	PO4	1	MN2	1	H	1
3900	9.06D-17	-10.41	MN2	1	H	-1		
3910	1.48D-26	-34.20	MN2	1	H	-3		
3920	1.83D-10	5.44	CU2	1	CO3	1		
3930	5.66D-14	8.64	CU2	1	CO3	2		
3932	7.29D-12	11.04	CU2	1	CO3	1	H	1
3940	6.02D-13	1.04	CU2	1	SO4	1		
3950	2.86D-13	-.03	CU2	1	CL	1		
3960	7.91D-18	-.54	CU2	1	CL	2		

MINE 1.2 1993 Feb 28 09:59

TSOLUM R at DUNCAN MAIN

--- Output Data ---

TYPE II: COMPLEXES (cont'd)

ID# w-B--	Equilibrium Concentration --- (MOLAR) ---	LogK	Species (Name:Stoichiometric Coeff)					
4010	1.56D-12	14.40	cu2	1	PO4	1	H	1
4813	4.59D-08	7.74	cu2	1	HA	1		
4840	2.07D-10	-8.21	cu2	1	H	-1		
4842	3.28D-09	-14.01	CU2	1	H	-2		
4844	5.37D-15	-26.80	cu2	1	H	-3		
4846	1.81D-20	-39.27	cu2	1	H	-4		
4850	2.79D-14	-10.61	cu2	2	H	-2		
4912	2.96D-11	2.74	BA	1	HA	1		
5060	1.68D-13	-13.11	BA	1	H	-1		
5070	1.51D-12	1.94	CD	1	co3	1		
5072	1.90D-10	11.04	CD	1	co3	1	H	1
5090	1.87D-10	1.37	CD	1	CL	1		
5100	4.11D-14	1.76	CD	1	CL	2		
5110	9.31D-19	1.16	CD	1	CL	3		
5270	1.67D-16	2.01	CD	1	PO4	1		
5930	4.28D-10	-9.31	CD	1	H	-1		
5940	3.40D-13	-19.41	CD	1	H	-2		
5950	3.51D-17	-30.40	CD	1	H	-3		
5954	4.20D-10	4.04	ZN	1	co3	1		
5956	4.20D-10	11.04	ZN	1	co3	1	H	1
5960	3.47D-11	1.04	ZN	1	so4	1		
5970	1.31D-12	-1.13	ZN	1	CL	1		
5980	1.81D-17	-1.94	ZN	1	CL	2		
5990	1.64D-20	-.94	ZN	1	CL	3		
6060	1.13D-11	13.50	ZN	1	PO4	1	H	1
6733	2.64D-10	3.74	ZN	1	HA	1		
6740	2.99D-10	-9.81	ZN	1	H	-1		
6745	7.51D-09	-15.41	ZN	1	H	-2		
6750	9.77D-14	-27.30	ZN	1	H	-3		
6760	4.15D-19	-39.67	ZN	1	H	-4		
6770	1.83D-09	1.04	NI	1	so4	1		
6780	6.91D-10	-.13	NI	1	CL	1		
7590	9.96D-08	-9.01	WI	1	H	-1		
9890	4.27D-33	3.01	CR	1	so4	1		
10000	3.03D-28	-3.93	CR	1	H	-1		
10010	4.64D-27	-9.74	CR	1	H	-2		
10020	9.57D-28	-24.43	CR	1	H	-4		
10030	7.32D-17	1.31	so4	1	AL	1		
10040	l.lOD-20	2.29	so4	2	AL	1		
10102	5.99D-26	5.17	PO4	1	AL	1	H	1
10104	1.24D-37	.49	PO4	1	AL	1	H	2
10340	1.64D-11	-5.13	AL	1	H	-	1	
10342	1.26D-09	-10.24	AL	1	H	-2		
10344	2.51D-08	-15.94	AL	1	H	-3		

MINE 1.2 1993 Feb 28 09:59

TSOLUM R at DUNCAN MAIN

--- Output Data ---

TYPE II: COMPLEXES (cont'd)

ID#	Equilibrium Concentration ---(MOLAR) ---	LogK	Species (Name:Stoichiometric Coeff)
10350	4.11D-09	-23.73	AL 1 H -4
10352	9.67D-20	-7.70	AL 2 H -2
10354	2.77D-24	-13.59	AL 3 H -4
12530	7.27D-05	9.57	co3 1 H 1
12540	7.04D-06	15.56	co3 1 H 2
12550	6.00D-11	1.57	so4 1 H 1
12600	6.61D-07	11.56	PO4 1 H 1
12610	3.91D-07	18.33	PO4 1 H 2
12620	1.89D-12	20.01	PO4 1 H 3
12710	1.55D-09	12.47	6103 1 H 1
12720	2.98D-07	21.76	SIO3 1 H 2
13595	2.06D-07	-13.69	H -1
13600	1.11D-11	******	CR 2 E -6 H -14
13610	1.62D-09	-66.20	CR 1 E -3 H -7
13620	1.91D-07	-71.13	CR 1 E -3 H -8

MINE 1.2 1993 Feb 28 09:59

TSOLUM R at DUNCAN MAIN

--- Output Data ---

TYPE III: FIXED SOLIDS

ID#	Equilibrium Concentration ---(MOLAR)---	LogK	Species (Name:Stoichiometric Coeff)
50	-5.22D-05	7.00	H 1
99	1.00D+00	13.00	E 1

TYPE IV: PRECIPITATED SOLIDS

ID# -a---	Equilibrium Concentration --- (MOLAR) ---	LogK --I-----	Species (Name:Stoichiometric Coeff)
21180	5.63D-06	-8.34	AL 1 H -3
21470	5.40D-07	-41.37	MN2 1 E -2 H -4

MINE 1.2 1993 Feb 28 09:59

TSOLUM R at DUNCAN MAIN

--- Output Data ---

TYPE'V: DISSOLVED SOLIDS

ID#	Equilibrium Concentration --- (MOLAR) ---	LogK w----B--	species (Name:Stoichiometric Coeff)							
20000	2.27D-04	7.04	CA	1	co3	1				
20010	4.71D-06	3.44	CA	1	so4	1				
20030	6.00D-08	37.87	CA	5	PO4	3	H	-1		
20040	1.48D-14	41.29	CA	4	PO4	3	H	1		
20050	2.44D-05	17.10	CA	1	PO4	1	H	1		
20070	1.53D-11	7.44	CA	1	6103	1				
20130	6.44D-13	-22.21	CA	1	H	-2				
20140	1.40D-07	4.14	MG	1	co3	1				
20160	2.23D-11	23.69	MG	3	PO4	2				
20200	9.96D-08	-16.71	MG	1	H	-2				
20280	5.85D-02	22.97	FE3	1	PO4	1				
20370	6.38D-11	9.14	co3	1	MN2	1				
20400	3.41D-18	9.44	6103	1	MN2	1				
20430	3.61D-14	-14.81	MN2	1	H	-2				
20438	1.56D-07	8.37	cu2	1	co3	1				
20440	6.01D-06	4.43	cu2	2	co3	1	H	-2		
20460	1.27D-14	32.99	CU2	3	PO4	2				
20500	1.64D-03	-8.31	cu2	1	H	-2				
20510	2.36D-05	8.74	BA	1	co3	1				
20520	3.09D-02	9.94	BA	1	so4	1				
20570	1.90D-04	10.04	CD	1	co3	1				
20582	1.77D-15	27.89	CD	3	PO4	2				
20620	1.07D-07	-13.91	CD	1	H	-2				
20630	1.33D-04	9.54	ZN	1	co3	1				
20650	2.41D-10	31.99	ZN	3	PO4	2				
20660	1.78D-04	17.24	SI03	1	ZN	1				
20700	9.45D-05	-11.31	ZN	1	H	-2				
20710	1.76D-05	6.94	NI	1	co3	1				
20750	3.96D-02	-10.41	HI	1	H	-2				
21140	7.36D-21	-10.54	CR	1	H	-3				
21150	1.89D-04	19.67	PO4	1	AL	1				
21160	1.12D-04	35.93	SI03	2	A L	2	H	-2		
21440	1.50D-04	24.46	SI03	1	H	2				
21480	2.60D-18	-61.70	MN2	3	E	-2	H	-8		
21490	4.69D-05	-25.70	MN2	1	E	-1	H	-3		
21510	8.51D-24	11.40	cu2	1	E	2				

MINE 1.2 1993 Feb 28 09:59

TSOLUM R at DUNCAN MAIN

--- Output Data ---

TYPE VI: SPECIES NOT CONSIDERED

ID#	Equilibrium Concentration ---(MOLAR)---	LogK	Species (Name:Stoichiometric Coeff)
20310	2.29D+03	-4.17	FE3 1 H -3
21460	2.95D+05	2.87	FE3 3E 1 H -8
25000	2.22D-04	17.06	co3 1 H 2

MINE 1.2 1993 Feb 28 09:59

TSOLUM R at DUNCAN MAIN

--- Output Data ---

DISTRIBUTION OF COMPONENTS

ID#	Component	Percent Bound in Species (%)	ID#	(Name:Stoichiometric Coeff)					
1	CA	99.9	1	CA	1				
2	MG	99.9	2	MG	1				
4	K	100.0	4	K	1				
5	NA	100.0	5	NA	1				
6	FE3	99.7	2680	FE3	1	H	-2		
8	MN2	100.0	21470	MN2	1	E	-2	H	-4
9	cu2	6.4	9	cu2	1				
		86.7	4813	cu2	1	HA	1		
		6.2	4842	cu2	1	H	-2		
10	BA	100.0	10	BA	1				
11	CD	99.1	11	CD	1				
12	ZN	95.6	12	ZN	1				
		3.7	6'745	ZN	1	H	-2		
13	NI	99.0	13	NI	1				
19	CR	99.1	13620	CR	1	E	-3	H	-8
20	AL	99.5	21180	AL	1	H	-3		
50	H	139.2	12530	co3	1	H	1		
		26.9	12540	co3	1	H	2		
		1.3	12600	PO4	1	H	1		
		1.5	12610	PO4	1	H	2		
		1.1	12720	SI03	1	H	2		

MINE 1.2 1993 Feb 28 09:59

TSOLUM R at DUNCAN MAIN

--- Output Data ---

DISTRIBUTION OF COMPONENTS

ID#	Component	Percent Bound in Species (%)	ID#	(Name:Stoichiometric Coeff)
99	E	34.5	13620	CR 1 E -3 H -8
		65.2	21470	MN2 1 E -2 H -4
101	co3	90.9	12530	co3 1 H 1
		8.8	12540	co3 1 H 2
102	so4	99.8	102	so4 1
103	CL	100.0	103	CL 1
109	PO4	62.8	12600	PO4 1 H 1
		37.1	12610	PO4 1 H 2
112	SI03	99.5	12720	SI03 1 H 2
157	NO3	100.0	157	NO3 1
160	HA	77.7	160	HA 1
		3.0	1200	CA 1 HA 1
		3.7	2060	NA 1 HA 1
		14.6	4813	cu2 1 HA 1

TSOLUM RIVER AT FARNHAM USING 1.61 MG/L

MINE 1.2 1993 Feb 27 17:12

Tsolum far Average

--- Output Data ---

FINAL CONDITIONS

Number of iterations = 59

pE = 13.0
pH = 7.0 Ionic Strength = 6.55E-04

ID#	Concentration (MOLAR) Equilibrium	Analytical	Remainder	Component
1	1.86D-05	1.87D-05	1.73D-14	CA
2	3.24D-05	3.27D-05	3.80D-14	MG
4	1.28D-10	1.28D-10	8.43D-21	K
5	1.61D-04	1.61D-04	4.22D-15	NA
6	2.58D-15	4.34D-06	5.54D-21	FE3
8	8.92D-13	6.48D-07	0.00D+00	MN2
9	3.36D-08	2.61D-07	3.13D-17	cu2
10	1.92D-07	2.19D-07	-5.93D-12	BA
11	7.66D-13	7.83D-13	1.76D-27	CD
12	2.53D-07	2.78D-07	2.36D-16	ZN
13	8.31D-07	8.52D-07	7.74D-16	NI
19	1.24D-27	3.853):07	2.07D-21	CR
20	2.98D-14	3.73D-05	0.00D+00	AL
50	1.00D-07	1.00D-09	0.00D+00	H
99	1.00D-13	0.00D+00	0.00D+00	E
101	4.75D-08	8.00D-05	5.27D-20	co3
102	4.14D-05	4.18D-05	0.00D+00	so4
103	5.45D-05	5.45D-05	6.80D-20	CL
109	1.22D-12	1.05D-06	3.00D-21	P04
112	7.09D-16	3.00D-07	-l.lOD-21	SI03
157	3.04D-06	3.04D-06	4.66D-21	N03
160	5.73D-09	1.61D-07	-7.10D-23	HA

MINE 1.2 1993 Feb 27 17 :12

Tsolum far Average

--- Output Data ---

DISTRIBUTION OF COMPONENTS

ID#	Component	Percent Bound in Species (%)	ID#	(Name:Stoichiometric Coeff)					
1	CA	99.2	1	CA	1				
2	MG	99.0	2	MG	1				
4	K	100.0	4	K	1				
5	NA	100.0	5	NA	1				
6	FE3	99.8	2680	FE3	1	H	-2		
8	MN2	100.0	21470	MN2	1	H	-4	E	-2
9	cu2	12.9	9	cu2	1				
		2.4	3920	cu2	1	co3	1		
		58.7	4813	CU2	1	HA	1		
		1.5	4840	CU2	1	H	-1		
		24.3	4842	CU2	1	H	-2		
10	BA	87.7	10	BA	1				
		12.3	20520	BA	1	so4	1		
11	CD	97.9	11	CD	1				
12	ZN	90.9	12	ZN	1				
		6.8	6745	ZN	1	H	-2		
13	NI	97.5	13	NI	1				
		1.8	7590	NI	1	H	-1		
19	CR	19.2	13610	CR	1	H	-7	E	-3
		80.8	13620	CR	1	H	-8	E	-3
20	AL	99.9	21180	H	-3	AL	1		
50	ii	1.6	13610	CR	1	H	-7	E	-3
		7 . 9	13620	CR	1	H	-8	E	-3
		27.4	2680	FE3	1	H	-2		
		8.2	21470	MN2	1	H	-4	E	-2
		354.0	21180	H	-3	AL	1		

MINE 1.2 1993 Feb 27 17:12

Tsolum far Average

--- Output Data ---

DISTRIBUTION OF COMPONENTS

ID#	Component	Percent Bound in Species (%)	ID#	(Name:Stoichiometric Coeff)					
99	E	9.0	13610	CR	1	H	-7	E	-3
		38.1	13620	CR	1	H	-8	E	-3
		52.9	21470	MN2	1	H	-4	E	-2
101	co3	84.0	12530	co3	1	H	1		
		15.8	12540	co3	1	H	2		
102	so4	98.9	102	so4	1				
103	CL	100.0	103	CL	1				
109	PO4	30.7	12600	PO4	1	H	1		
		68.9	12610	PO4	1	H	2		
112	SI03	99.7	12720	S103	1	H	2		
157	NO3	100.0	157	NO3	1				
160	HA	3.6	160	HA	1				
		95.0	4813	cu2	1	HA	1		

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Tsolum far Average

--- Output Data ---

TYPE I: COMPONENTS

ID#	Equilibrium Concentration ---(MOLAR)---	LogK	Species (Name:Stoichiometric Coeff)
2	3.24D-05	.00	MG 1
4	1.28D-10	.00	K 1
5	1.61D-04	.00	NA 1
6	2.58D-15	.00	FE3 1
8	8.92D-13	.00	MN2 1
9	3.36D-08	.00	Cu2 1
10	1.92D-07	.00	BA 1
11	7.66D-13	.00	CD 1
12	2.53D-07	.00	ZN 1
13	8.31D-07	.00	NI 1
19	1.24D-27	.00	CR 1
20	2.98D-14	.00	AL 1
101	4.75D-08	.00	co3 1
102	4.14D-05	.00	so4 1
103	5.45D-05	.00	CL 1
109	1.22D-12	.00	PO4 1
112	7.09D-16	.00	S103 1
157	3.04D-06	.00	NO3 1
160	5.73D-09	.00	HA 1

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Tsolum far Average

--- Output Data ---

TYPE II: COMPLEXES

ID#	Equilibrium Concentration ---(MOLAR)---	LogK	Species (Name:Stoichiometric Coeff)					
1	1.86D-05	.00	CA	1				
1000	7.02D-10	2.90	CA	1	co3	1		
1010	2.79D-08	11.50	CA	1	co3	1	H	1
1020	1.22D-07	2.20	CA	1	so4	1		
1080	6.02D-10	14.43	CA	1	PO4	1	H	1
1200	5.58D-10	3.72	CA	1	HA	1		
1350	1.11D-10	-12.22	CA	1	H	-1		
1360	1.94D-09	3.10	MG	1	co3	1		
1370	4.88D-08	11.50	MG	1	co3	1	H	1
1380	2.68D-07	2.30	MG	1	so4	1		
1440	3.32D-09	14.93	MG	1	PO4	1	H	1
1580	5.87D-10	3.50	MG	1	HA	1		
1740	1.93D-09	-11.22	MG	1	H	-1		
1960	5.94D-14	1.05	K	1	so4	1		
1995	1.64D-16	2.35	X	1	HA	1		
2000	1.08D-10	1.15	NA	1	co3	1		
2010	2.98D-08	.65	NA	1	so4	1		
2060	1.03D-09	3.05	NA	1	HA	1		
2070	1.20D-15	4.05	FE3	1	so4	1		
2080	1.11D-18	5.40	FE3	1	so4	2		
2090	2.98D-18	1.33	FE3	1	CL	1		
2100	7.26D-22	1.98	FE3	1	CL	2		
2110	5.92D-27	1.15	FE3	1	CL	3		
2170	9.39D-14	20.48	FE3	1	PO4	1	H	1
2190	4.34D-14	23.38	FE3	1	S103	1	H	1
2666	1.05D-16	6.85	FE3	1	HA	1		
2670	4.59D-10	-1.75	FE3	1	H	-1		
2680	4.33D-06	-4.77	FE3	1	H	-2		
2690	1.73D-14	-20.17	FE3	1	H	-3		
2700	7.27D-09	-21.55	FE3	1	H	-4		
2710	3.33D-18	-2.30	FE3	2	H	-2		
3290	4.25D-15	12.00	co3	1	MN2	1	H	1
3300	5.86D-15	2.20	MN2	1	so4	1		
3310	5.46D-16	1.05	CL	1	MN2	1		
3320	2.81D-20	1.03	CL	2	MN2	1		
3330	4.85D-25	.53	CL	3	MN2	1		
3360	1.15D-15	16.03	PO4	1	MN2	1	H	1
3900	6.69D-16	-10.12	MN2	1	H	-1		
3910	5.63D-26	-34.20	MN2	1	H	-3		
3920	6.37D-09	6.60	cu2	1	co3	1		
3930	4.80D-13	9.80	cu2	1	co3	2		
3932	2.53D-10	12.20	CU2	1	co3	1	H	1
3940	2.21D-10	2.20	cu2	1	so4.	1		
3950	6.50D-12	.55	cu2	1	CL	1		

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Tsolum far Average

--- Output Data ---

TXPE II: COMPLEXES (cont'd)

ID#	Equilibrium Concentration ---(MOLAR)---	LogK	Species (Name:Stoichiometric Coeff)
3960	2.11D-16	.33	cu2 1 CL 2
4010	1.09D-10	16.43	cu2 1 PO4 1 H 1
4813	1.53D-07	8.90	cu2 1 HA 1
4840	3.99D-09	-7.92	cu2 1 H -1
4842	6.33D-08	-13.72	cu2 1 H -2
4844	5.32D-14	-26.80	cu2 1 H -3
4846	4.74D-20	-39.85	cu2 1 H -4
4850	5.34D-12	-10.32	cu2 2 H -2
4912	8.73D-12	3.90	BA 1 HA 1
5060	2.87D-13	-12.82	BA 1 H -1
5070	4.59D-17	3.10	CD 1 co3 1
5072	5.78D-15	12.20	CD 1 co3 1 H 1
5090	3.73D-15	1.95	CD 1 CL 1
5100	9.62D-19	2.63	CD 1 CL 2
5110	1.32D-23	2.03	CD 1 CL 3
5270	5.25D-21	3.75	CD 1 PO4 1
5930	7.24D-15	-9.02	CD 1 H -1
5940	5.75D-18	-19.12	CD 1 H -2
5950	3.05D-22	-30.40	CD 1 H -3
5954	1.91D-09	5.20	ZN 1 co3 1
5956	1.91D-09	12.20	ZN 1 co3 1 H 1
5960	1.66D-09	2.20	ZN 1 so4 1
5970	3.89D-12	-.55	ZN 1 CL 1
5980	6.33D-17	-1.07	ZN 1 CL 2
5990	3.45D-20	-.07	ZN 1 CL 3
6060	1.03D-10	15.53	ZN 1 PO4 1 H 1
6733	1.15D-10	4.90	ZN 1 HA 1
6740	7.55D-10	-9.52	ZN 1 H -1
6745	1.90D-08	-15.12	ZN 1 H -2
6750	1.27D-13	-27.30	ZN 1 H -3
6760	1.42D-19	-40.25	ZN 1 H -4
6770	5.46D-09	2.20	NI 1 so4 1
6780	1.28D-10	.45	NI 1 CL 1
7590	1.57D-08	-8.72	NI 1 H -1
9890	2.90D-27	4.75	CR 1 so4 1
10000	5.56D-24	-3.35	CR 1 H -1
10010	1.66D-22	-8.87	CR 1 H -2
10020	1.76D-23	-23.85	CR 1' H -4
10030	1.39D-15	3.05	AL 1 so4 1
10040	2.04D-18	4.60	AL 1 so4 2
10102	2.17D-25	7.78	PO4 1 H 1 AL 1
10104	2.29D-37	2.80	PO4 1 H 2 A L 1
10340	8.41D-12	-4.55	H -1 AL 1
10342	1.26D-09	-9.37	H -2 AL 1

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Tsolum far Average

--- Output Data ---

TYPE II: COMPLEXES (cont'd)

ID#	Equilibrium Concentration ---(MOLAR)---	LogK	Species (Name:Stoichiometric Coeff)					
10344	2.51D-08	-15.07	H	-3	AL	1		
10350	2.11D-09	-23.15	H	-4	AL	1		
10352	1.77D-21	-7.70	H	-2	AL	2		
10354	3.53D-27	-13.88	H	-4	AL	3		
12530	6.72D-05	10.15	co3	1	H	1		
12540	1.27D-05	16.43	co3	1	H	2		
12550	5.85D-10	2.15	H	1	so4	1		
12600	3.24D-07	12.43	PO4	1	H	1		
12610	7.25D-07	19.78	PO4	1	ii	2		
12620	6.85D-12	21.75	PO4	1	H	3		
12710	7.96D-10	13.05	SI03	1	H	1		
12720	2.99D-07	22.63	SI03	1	H	2		
13595	1.06D-07	-13.98	H	-1				
13600	5.42D-13	******	CR	2	H	-14	E	-6
13610	7.38D-08	-68.23	CR	1	H	-7	E	-3
13620	3.11D-07	-74.60	CR	1	H	-8	E	-3

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Tsolum far Average

--- Output Data ---

TYPE III: FIXED SOLIDS

ID#	Equilibrium Concentration ---(MOLAR)---	LogK	Species (Name:Stoichiometric Coeff)
50	3.16D-05	7.00	H 1
99	2.45D-06	13.00	E 1

TYPE IV: PRECIPITATED SOLIDS

ID#	Equilibrium Concentration ---(MOLAR)---	LogK	Species (Name:Stoichiometric Coeff)
20520	2.68D-08	11.10	BA 1 so4 1
21180	3.73D-05	-7.47	H -3 AL 1
21470	6.48D-07	-41.95	MN2 1 H -4 E -2

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Tsolum far Average

--- Output Data ---

TYPE V: DISSOLVED SOLIDS

ID#	Equilibrium Concentration --- (MOLAR) ---	LogK	Species (Name:Stoichiometric Coeff)						
20000	1.40D-04	8.20	CA	1	co3	1			
20010	3.06D-05	4.60	CA	1	so4	1			
20030	1.33D-08	44.53	CA	5	PO4	3	H	-1	
20040	9.59D-15	47.65	CA	4	PO4	3	H	1	
20050	3.02D-05	19.13	CA	1	PO4	1	H	1	
20070	5.24D-12	8.60	CA	1	SI03	1			
20130	2.21D-13	-21.92	CA	1	H	-2			
20140	3.08D-07	5.30	MG	1	co3	1			
20160	5.35D-10	28.03	MG	3	PO4	2			
20200	1.22D-07	-16.42	MG	1	H	-2			
20280	1.18D-01	25.58	FE3	1	PO4	1			
20370	8.47D-10	10.30	co3	1	MN2	1			
20400	2.52D-17	10.60	SI03	1	MN2	1			
20430	2.66D-13	-14.52	MN2	1	H	-2			
20438	5.42D-06	9.53	cu2	1	co3	1			
20440	4.03D-03	5.88	cu2	2	co3	1	H	-2	
20460	1.19D-09	37.33	CU2	3	PO4	2			
20500	3.17D-02	-8.02	cu2	1	H	-2			
20510	7.25D-05	9.90	BA	1	co3	1			
20570	5.78D-09	11.20	CD	1	co3	1			
20582	1.12D-28	32.23	CD	3	PO4	2			
20620	1.82D-12	-13.62	CD	1	H	-2			
20630	6.03D-04	10.70	ZN	1	co3	1			
20650	5.06D-08	36.33	ZN	3	PO4	2			
20660	4.51D-04	18.40	SI03	1	ZN	1			
20700	2.39D-04	-11.02	ZN	1	H	-2			
20710	4.98D-06	8.10	NI	1	co3	1			
20750	6.23D-03	-10.12	NI	1	H	-2			
21140	2.63D-16	-9.67	CR	1	H	-3			
21150	6.85D-04	22.28	PO4	1	AL	1			
21160	1.13D-04	39.40	SI03	2	H	-2	AL	2	
21440	1.50D-04	25.33	S103	1	H	2			
21480	1.42D-16	-61.70	MN2	3	H	-8	E	-2	
21490	1.78D-04	-25.70	MN2	1	H	-3	E	-1	
21510	8.44D-23	11.40	cu2	1	E	2			

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Tsolum far Average

--- Output Data ---

TYPE VI: SPECIES NOT CONSIDERED

ID#	Equilibrium Concentration --- (MOLAR) ---	LogK	Species (Name:Stoichiometric Coeff)
20310	1.28D+03	-3.30	FE3 1 H -3
21460	5.14D+04	5.48	FE3 3 H -8 E 1
25000	4.00D-04	17.93	co3 1 H 2

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Tsolum far Average

--- Output Data ---

FINAL CONDITIONS

Number of iterations = 59

pE = 13.0
pH = 7.0 Ionic Strength = 6.55E-04

ID#	Concentration (MOLAR) Equilibrium	Analytical	Remainder	Component
1	1.86D-05	1.87D-05	1.73D-14	CA
2	3.24D-05	3.27D-05	3.80D-14	MG
4	1.28D-10	1.28D-10	8.43D-21	K
5	1.61D-04	1.61D-04	4.22D-15	NA
6	2.58D-15	4.34D-06	5.54D-21	FE3
8	8.92D-13	6.48D-07	0.00D+00	MB2
9	3.36D-08	2.61D-07	3.13D-17	cu2
10	1.92D-07	2.19D-07	-5.93D-12	BA
11	7.66D-13	7.83D-13	1.76D-27	CD
12	2.53D-07	2.78D-07	2.36D-16	ZN
13	8.31D-07	8.52D-07	7.74D-16	NI
19	1.24D-27	3.85D-07	2.07D-21	CR
20	2.98D-14	3.73D-05	0.00D+00	AL
50	1.00D-07	1.00D-09	0.00D+00	H
99	1.00D-13	0.00D+00	0.00D+00	E
101	4.75D-08	8.00D-05	5.27D-20	co3
102	4.14D-05	4.18D-05	0.00D+00	so4
103	5.45D-05	5.45D-05	6.80D-20	CL
109	1.22D-12	1.05D-06	3.00D-21	PO4
112	7.09D-16	3.00D-07	-1.10D-21	SI03
157	3.04D-06	3.04D-06	4.66D-21	NO3
160	5.73D-09	1.61D-07	-7.10D-23	HA

APPENDIX III

MODEL CALCULATION OF CHEMICAL SPECIATION AT ROSSITER

MINE 1.2 1993 Feb 28 10:01

TSOLUM R at ROSSITER

--- Output Data ---

FINAL CONDITIONS

Number of iterations = 73

pE = 13.0
pH = 7.0 Ionic Strength = 5.01E-01

ID#	Concentration (MOLAR) Equilibrium	Analytical	Remainder	Component
1	6.71D-05	6.71D-05	7.06D-20	CA
2	2.07D-05	2.07D-05	-1.41D-20	MG
4	1.28D-10	1.28D-10	-4.00D-25	K
5	1.61D-04	1.61D-04	-1.65D-19	NA
6	7.14D-14	1.63D-05	-1.69D-21	FE3
8	2.35D-13	2.55D-06	0.00D+00	MN2
9	3.12D-07	7.87D-07	-9.82D-22	cu2
10	2.18D-07	2.19D-07	1.03D-22	BA
11	8.83D-08	8.90D-08	7.71D-23	CD
12	4.44D-07	4.64D-07	2.70D-22	ZN
13	1.01D-06	1.02D-06	-6.19D-22	WI
19	8.98D-31	6.73D-07	1.29D-12	CR
20	2.20D-13	5.60D-06	4.23D-22	AL
50	1.00D-07	1.00D-09	-8.47D-22	H
99	1.00D-13	1.00D+00	0.00D+00	E
101	1.95D-07	8.00D-05	-5.940-20	co3
102	3.59D-05	3.59D-05	-2.98D-14	so4
103	4.42D-05	4.42D-05	-9.06D-21	CL
109	1.83D-11	1.05D-06	6.31D-22	PO4
112	5.22D-15	3.00D-07	2.36D-22	S103
157	3.04D-06	3.04D-06	-1.69D-21	NO3
160	7.91D-09	1.45D-07	-2.94D-22	HA

MINE 1.2 1993 Feb 28 10:01

TSOLUM R at ROSSITER

--- Output Data ---

TYPE I: COMPONENTS

ID#	Equilibrium Concentration --- (MOLAR) ---	LogK	Species (Name:Stoichiometric Coeff)
1	6.71D-05	.00	CA 1
2	2.07D-05	.00	MG 1
4	1.28D-10	.00	K 1
5	1.61D-04	.00	NA 1
6	7.14D-14	.00	FE3 1
8	2.35D-13	.00	MN2 1
9	3.12D-07	.00	CU2 1
10	2.18D-07	.00	BA 1
11	8.83D-08	.00	CD 1
12	4.44D-07	.00	ZN 1
13	l.OlD-06	.00	NI 1
19	8.98D-31	.00	CR 1
20	2.20D-13	.00	AL 1
101	1.95D-07	.00	co3 1
102	3.59D-05	.00	so4 1
103	4.42D-05	.00	CL 1
109	1.83D-11	.00	P04 1
112	5.22D-15	.00	S103 1
157	3.04D-06	.00	N03 1
160	7.91D-09	.00	HA 1

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TSOLUM R at ROSSITER

--- Output Data ---

TYPE II: COMPLEXES

ID#	Equilibrium Concentration ---(MOLAR)---	LogK	Species (Name:Stoichiometric Coeff)					
1000	7.24D-10	1.74	CA	1	CO3	1		
1010	2.88D-08	10.34	CA	1	CO3	1	H	1
1020	2.66D-08	1.04	CA	1	SO4	1		
1080	3.09D-10	12.40	CA	1	PO4	1	H	1
1200	1.94D-10	2.56	CA	1	HA	1		
1350	2.05D-10	-12.51	CA	1	H	-1		
1360	3.54D-10	1.94	MG	1	CO3	1		
1370	8.88D-09	10.34	MG	1	CO3	1	H	1
1380	1.03D-08	1.14	MG	1	SO4	1		
1440	3.01D-10	12.90	MG	1	PO4	1	H	1
1580	3.60D-11	2.34	MG	1	HA	1		
1740	6.33D-10	-11.51	MG	1	H	-1		
1960	1.36D-14	.47	K	1	SO4	1		
1995	5.98D-17	1.77	K	1	HA	1		
2000	1.17D-10	.57	NA	1	CO3	1		
2010	6.81D-09	.07	NA	1	SO4	1		
2060	3.77D-10	2.47	NA	1	HA	1		
2070	5.29D-16	2.31	FE3	1	SO4	1		
2080	1.12D-19	3.09	FE3	1	SO4	2		
2090	9.05D-18	.46	FE3	1	CL	1		
2100	4.71D-22	.53	FE3	1	CL	2		
2110	1.60D-27	-.59	FE3	1	CL	3		
2170	9.75D-14	17.87	FE3	1	PO4	1	H	1
2190	3.16D-13	21.93	FE3	1	S103	1	H	1
2666	7.35D-17	5.11	FE3	1	HA	1		
2670	3.35D-09	-2.33	FE3	1	H	-1		
2680	1.63D-05	-5.64	FE3	1	H	-2		
2690	6.47D-14	-21.04	FE3	1	H	-3		
2700	5.31D-08	-22.13	FE3	1	H	-4		
2710	2.56D-15	-2.30	FE3	2	H	-2		
3290	3.20D-16	10.84	CO3	1	MN2	1	H	1
3300	9.32D-17	1.04	SO4	1	MN2	1		
3310	3.08D-17	.47	CL	1	MN2	1		
3320	6.60D-22	.16	CL	2	MN2	1		
3330	9.22D-27	-.34	CL	3	MN2	1		
3360	4.32D-17	14.00	PO4	1	MN2	1	H	1
3900	9.06D-17	-10.41	MN2	1	H	-1		
3910	1.48D-26	-34.20	MN2	1	H	-3		
3920	1.69D-08	5.44	CU2	1	CO3	1		
3930	5.21D-12	8.64	CU2	1	CO3	2		
3932	6.71D-10	11.04	CU2	1	CO3	1	H	1
3940	1.24D-10	1.04	CU2	1	SO4	1		
3950	1.29D-11	-.03	CU2	1	CL	1		
3960	1.75D-16	-.54	CU2	1	CL	2		

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TSOLUM R at ROSSITER

--- Output Data ---

TYPE II: COMPLEXES (cont'd)

ID#	Equilibrium Concentration ---(MOLAR)---	LogK	Species (Name:Stoichiometric Coeff)					
a----								
4010	1.44D-10	14.40	cu2	1	PO4	1	H	1
4813	1.36D-07	7.74	cu2	1	HA	1		
4840	1.90D-08	-8.21	cu2	1	H	-1		
4842	3.02D-07	-14.01	cu2	1	H	-2		
4844	4.94D-13	-26.80	cu2	1	H	-3		
4846	1.67D-18	-39.27	CU2	1	H	-4		
4850	2.36D-10	-10.61	cu2	2	H	-2		
4912	9.56D-13	2.74	BA	1	HA	1		
5060	1.68D-13	-13.11	BA	1	H	-1		
5070	1.51D-12	1.94	CD	1	co3	1		
5072	1.90D-10	11.04	CD	1	co3	1	H	1
5090	9.17D-11	1.37	CD	1	a	1		
5100	9.86D-15	1.76	CD	1	CL	2		
5110	1.09D-19	1.16	CD	1	a	3		
5270	1.67D-16	2.01	CD	1	PO4	1		
5930	4.28D-10	-9.31	CD	1	H	-1		
5940	3.40D-13	-19.41	CD	1	H	-2		
5950	3.51D-17	-30.40	CD	1	H	-3		
5954	9.56D-10	4.04	ZN	1	co3	1		
5956	9.56D-10	11.04	ZN	1	co3	1	H	1
5960	1.76D-10	1.04	ZN	1	so4	1		
5970	1.46D-12	-1.13	ZN	1	a	1		
5980	9.89D-18	-1.94	ZN	1	a	2		
5990	4.37D-21	-.94	ZN	1	CL	3		
6060	2.58D-11	13.50	ZN	1	PO4	1	H	1
6733	1.940-U	3.74	ZN	1	HA	1		
6740	6.81D-10	-9.81	ZN	1	H	-1		
6745	1.71D-08	-15.41	ZN	1	H	-2		
6750	2.23D-13	-27.30	ZN	1	H	-3		
6760	9.46D-19	-39.67	ZN	1	H	-4		
6770	4.01D-10	1.04	WI	1	so4	1		
6780	3.33D-11	-.13	NI	1	a	1		
7590	9.79D-09	-9.01	NI	1	H	-1		
9890	3.33D-32	3.01	CR	1	so4	1		
10000	1.06D-27	-3.93	CR	1	H	-1		
10010	1.62D-26	-9.74	CR	1	H	-2		
10020	3.35D-27	-24.43	CR	1	H	-4		
10030	1.63D-16	1.31	so4	1	AL	1		
10040	5.48D-20	2.29	so4	2	AL	1		
10102	5.99D-26	5.17	PO4	1	AL	1	H	1
10104	1.24D-37	.49	PO4	1	AL	1	H	2
10340	1.64D-11	-5.13	AL	1	H	-1		
10342	1.26D-09	-10.24	AL	1	H	-2		
10344	2.51D-08	-15.94	AL	1	H	-3		

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TSOLUM R at ROSSITER

--- **Output** Data ---

TYPE II: COMPLEXES (cont'd)

ID#	Equilibrium Concentration ---(MOLAR) ---	LogK	Species (Name:Stoichiometric Coeff)
10350	4.11D-09	-23.73	AL 1 H -4
10352	9.67D-20	-7.70	AL 2 H -2
10354	2.77D-24	-13.59	AL 3 H -4
12530	7.27D-05	9.57	co3 1 H 1
12540	7.04D-06	15.56	co3 1 H 2
12550	1.34D-10	1.57	so4 1 H 1
12600	6.61D-07	11.56	PO4 1 H 1
12610	3.91D-07	18.33	PO4 1 H 2
12620	1.90D-12	20.01	PO4 1 H 3
12710	1.55D-09	12.47	6103 1 H 1
12720	2.98D-07	21.76	6103 1 H 2
13595	2.06D-07	-13.69	H -1
13600	1.36D-10	******	CR 2 E -6 H -14
13610	5.66D-09	-66.20	CR 1 E -3 H -7
13620	6.67D-07	-71.13	CR 1 E -3 H -8

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TSOLUM R at ROSSITER

--- Output Data ---

TYPE III: FIXED SOLIDS

ID#	Equilibrium Concentration --- (MOLAR) ---	LogK 1-11-m-B	Species (Name:Stoichiometric Coeff)
SO	-2.29D-05	7.00	E 1
99	1.00D+00	13.00	E 1

TYPE IV: PRECIPITATED SOLIDS

ID#	Equilibrium Concentration ---(MOLAR)---	LogK ---B-e--	Species (Name:Stoichiometric Coeff)
21180	5.57D-06	-8.34	AL 1 H -3
21470	2.55D-06	-41.37	MN2 1 E -2 H -4

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TSOLUM R at ROSSITER

--- Output Data ---

TYPE V: DISSOLVED SOLIDS

ID#	Equilibrium Concentration --- (MOLAR) ---	LogK I--I----	Species (Name:Stoichiometric Coeff)					
20000	1.44D-04	7.04	CA	1	co3	1		
20010	6.68D-06	3.44	CA	1	so4	1		
20030	6.23D-09	37.87	CA	5	PO4	3	H	-1
20040	2.41D-15	41.29	CA	4	PO4	3	H	1
20050	1.55D-05	17.10	CA	1	PO4	1	H	1
20070	9.71D-12	7.44	CA	1	SI03	1		
20130	4.10D-13	-22.21	CA	1	H	-2		
20140	5.60D-08	4.14	MG	1	co3	1		
20160	1.44D-12	23.69	MG	3	PO4	2		
20200	3.99D-08	-16.71	MG	1	H	-2		
20280	1.23D-01	22.97	FE3	1	PO4	1		
20370	6.38D-11	9.14	co3	1	MN2	1		
20400	3.41D-18	9.44	SIO3	1	MN2	1		
20430	3.61D-14	-14.81	MN2	1	H	-2		
20438	1.44D-05	8.37	cu2	1	co3	1		
20440	5.09D-02	4.43	cu2	2	co3	1	H	-2
20460	9.87D-09	32.99	cu2	3	PO4	2		
20500	1.51D-01	-8.31	cu2	1	H	-2		
20510	2.36D-05	8.74	BA	1	co3	1		
20520	6.88D-02	9.94	BA	1	so4	1		
20570	1.90D-04	10.04	CD	1	co3	1		
20582	1.78D-15	27.89	CD	3	PO4	2		
20620	1.08D-07	-13.91	CD	1	H	-2		
20630	3.02D-04	9.54	ZN	1	co3	1		
20650	2.85D-09	31.99	ZN	3	PO4	2		
20660	4.06D-04	17.24	SI03	1	ZN	1		
20700	2.15D-04	-11.31	ZN	1	H	-2		
20710	1.73D-06	6.94	WI	1	co3	1		
20750	3.90D-03	-10.41	NI	1	H	-2		
21140	2.57D-20	-10.54	CR	1	H	-	3	
21150	1.90D-04	19.67	PO4	1	AL	1		
21160	1.12D-04	35.93	SIO3	2	AL	2	H	-2
21440	1.50D-04	24.46	SI03	1	H	2		
21480	2.60D-18	-61.70	MN2	3	E	-2	H	-8
21490	4.69D-05	-25.70	MN2	1	E	-1	H	-3
21510	7.83D-22	11.40	cu2	1	E	2		

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TSOLUM R at ROSSITER
--------------W-W--

--- Output Data ---

TXPE VI: SPECIES NOT CONSIDERED

ID#	Equilibrium Concentration ---(MOLAR)---	LogK	Species (Name:Stoichiometric Coeff)
20310	4.80D+03	-4.17	FE3 1 H -3
21460	2.71D+06	2.87	FE3 3 E 1 H .-8
25000	2.23D-04	17.06	co3 1 H 2

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TSOLUM R at ROSSITER

--- Output Data ---

DISTRIBUTION OF COMPONENTS

ID#	Component	Percent Bound in Species (%)	ID#	(Name:Stoichiometric Coeff)					
1	CA	99.9	1	CA	1				
2	MG	99.9	2	MG	1				
4	K	100.0	4	K	1				
5	NA	100.0	5	NA	1				
6	FE3	99.7	2680	FE3	1	H	-2		
8	MN2	100.0	21470	MN2	1	E	-2	H	-4
9	cu2	39.6	9	cu2	1				
		2.1	3920	cu2	1	co3	1		
		17.3	4813	cu2	1	HA	1		
		2.4	4840	cu2	1	H	-1		
		38.3	4842	cu2	1	H	-2		
10	BA	100.0	10	BA	1				
11	CD	99.2	11	CD	1				
12	ZN	95.7	12	ZN	1				
		3.7	6745	ZN	1	H	-2		
13	NI	99.0	13	NI	1				
19	CR	99.1	13620	CR	1	E	-3	H	-8
20	AL	99.5	21180	AL	1	H	-3		
50	H	318.0	12530	co3	1	H	1		
		61.6	12540	co3	1	H	2		
		2.9	12600	PO4	1	H	1		
		3.4	12610	PO4	1	H	2		
		2.6	12720	SI03	1	H	2		

TSOLUM R at ROSSITER

--- Output Data ---

DISTRIBUTION OF COMPONENTS

ID#	Component	Percent Bound in Species (%)	ID#	(Name:Stoichiometric Coeff)					
99	E	28.1	13620	CR	1	E	-3	H	-8
		71.6	21470	MN2	1	E	-2	H	-4
101	co3	90.9	12530	co3	1	H	1		
		8.8	12540	co3	1	H	2		
102	so4	99.9	102	so4	1				
103	CL	100.0	103	CL	1				
109	PO4	62.8	12600	PO4	1	H	1		
		37.1	12610	PO4	1	H	2		
112	SI03	99.5	12720	SI03	1	H	2		
157	NO3	100.0	157	NO3	1				
160	HA	5.5	160	HA	1				
		94.1	4813	cu2	1	HA	1		

II OPERATIONS MANUAL

TABLE OF CONTENTS

1.0 INSTALLATION

MINE has been developed to run on a simple IBM compatible computer. However, it is strongly recommended that the program be run on a unit fitted with a math coprocessor. While not required, such a configuration will significantly reduce the time taken for each operation.

MINE is- composed of several data files and is menu driven. The MINE disk can easily be copied to a hard drive if available and, again, operation on a hard drive will improve the speed of operation.

The ANSI driver supplied with the MS-DOS System must be resident in the host computer system in order for the MINE package to function properly. To do this:

- Edit the **CONFIG.SYS** file on the booting disk's main directly using any text file editor (the line editor, EDLIN, is supplied with MD-DOS). If CONFIG.SYS does not exist, create it.

- Add the line **"DEVICE=<path>ANSI.SYS"** where <path> designates the pathtothe directory containing the MS-DOS file ANSI.SYS.

- Save the updated CONFIG.SYS file and reboot the system.

As an alternative method, if CONFIG.SYS does not exist:

- Type "COPY CON **CONFIG.SYS"** and press <ENTER>,

or if CONFIG.SYS does exist, then type

- "COPY CONFIG.SYS+CON **CONFIG.SYS"** and press <ENTER>

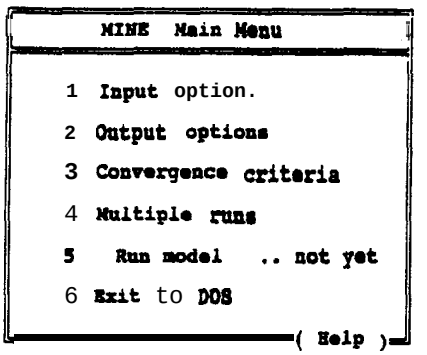
followed by,

- type "DEVICE=<path>ANSI.SYS" and press <ENTER>
- press "Z" while holding down the <Ctrl> key.

Use the DOS TYPE command to verify the contents (or modifications) of the file CONFIG.SYS, then reboot the system.

2.1 MAIN MENU

Operation of MINE 1.2 is controlled by a series of menus. Each menu has a help function which can be accessed by pressing H. In order to run MINE 1.2 each of the menu items 1 to 4 must be addressed before the model can be run.



ENTER option >

MINeral Equilibrium Model

* * * Welcome to MINE * * *

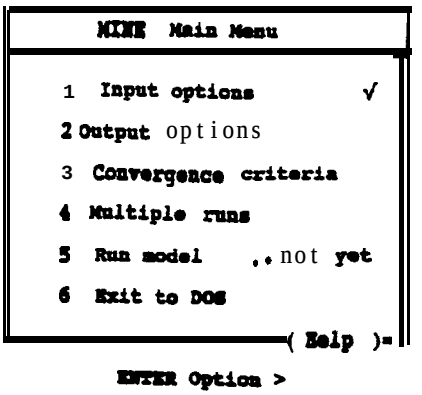
MINE is an ion interaction model used am an aid in evaluating speciation in the environment. The Main Menu consists of 6 options - Options 1 to 4 must be completed before the actual model (Option 5) may be run; Option 6 returns the user to the DOS environment.

Input Options	- ♦ □□⍟⌘↗⍓ problem
Output Options	- report destination
Convergence Criteria	- set limits for solving thm problem
Multiple Runs	- set ranges of pH and Eh
Run Model	- ♦ ⊠○⍟♦♦□ MINE
Exit to DOS	- finished

NOTE: Because of the extent of calculations involved, a math co-processor is highly recommended!

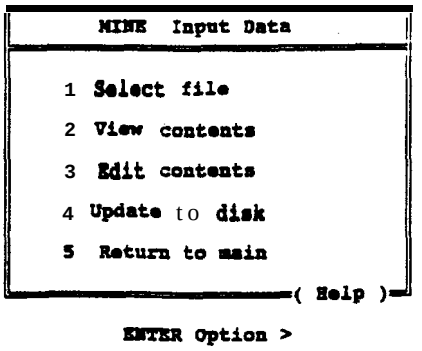
Press ENTER to continue..

After each operation is complete and you return to the main menu, a tick will appear on the main menu to show completion of the task.



2.2 INPUT OPTIONS

Input options can be selected by either typing 1 or I and enter. Once in this file, five options are available as shown.



Input data file: DEFAULT.DAT

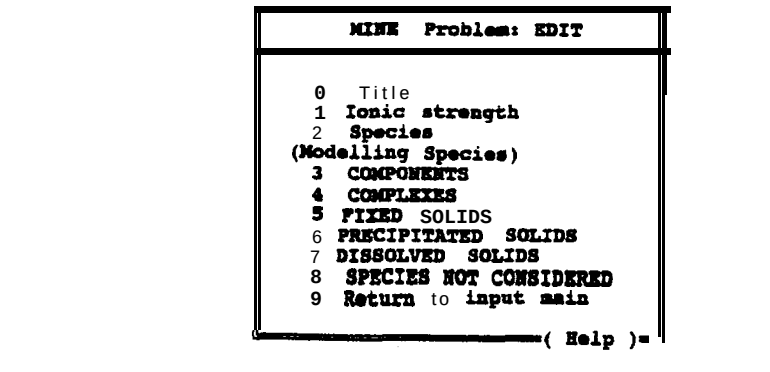
MINeral Equilibrium Model

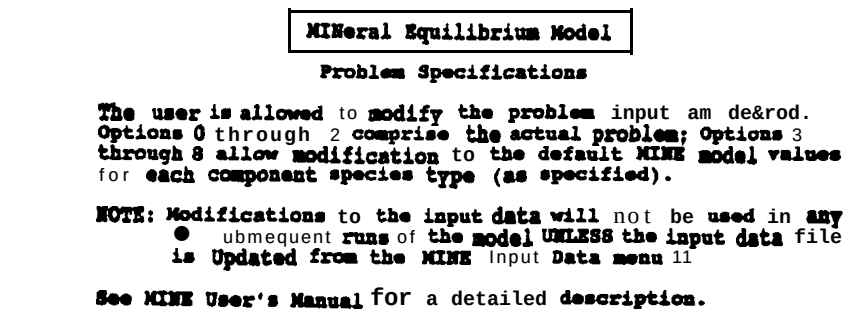
Input Specifications

The input data which defines a problem for MINE is defined in several groups. The first group contains the information for the components which arm to be included in the computation. This is followed by several groups of data in which the TYPE specification of a species may be modified. The default data sot (DEFAULT.DAT) has been compiled from average numbers for British Columbia. These numbers may be modified for specific locations using the Edit option.

See MINE User's Manual for a detailed description.

The EDIT Menu is shown below. By typing the appropriate number or letter each of the three components may be edited. Ionic strength is calculated and usually should not be changed. 'Provided you do not violate the phase rule it is probable that you will only need to edit the title and the species. Other types of associations may be changed if required but generally require a solid understanding of the phase equilibrium and redox conditions.





Problems of phase rule violations can be solved in two ways. If the species concerned are redox influenced reactions and of little consequence to the speciation of the metals of interest, the precipitating reactions can be classified as type 8 species. However, it is often better to put precipitated solutions in type 6 species.

There are a number of terms which have particular significance with regard to the classification of various forms.

1. Components

In a mathematical sense this is the independent base set from which every species can be defined and upon which the mass balance equations are based. In a chemical sense, the components are a set of chemical entities such that every species can be represented as the product of a reaction involving only these components,. and no component can be represented as the product of a reaction involving only the other components. The particular set of components for a given problem is certainly not unique, but once a set of components has been chosen, every species has a unique representation in terms of this set. There has been a tendency-to consider only neutral entities for the set of components; however, there is no reason for the exclusion of ionic entities from this set, and in this discussion ionic entities will be included as components.

2. Species

Mathematically, a species represents a log linear combination of the components; chemically, a species is the product of a chemical reaction involving the components as reactants. The species include every chemical entity to be considered in a chemical equilibrium problem. Species are of two kinds: soluble species and solids.

3. Soluble Species

Soluble species include every species in the aqueous phase. They can be simple ions: Ca^{2+}, H^{+}, OH'; ion pairs: $CaCO_3$ (aq); chelates Ca EDTA; etc. Soluble species can be both the soluble components and complexes (products of reactions involving components). The concentration (activity) of every soluble species is variable, being a function of the concentration of the components of which the species is composed.

4. **Solids**

Solids are species of a fixed activity (for normal solid phases such as $CaCO_3$ (s), $Ca(OH)_2(s)$, this fixed activity is equal to one). However, gases at a fixed partial pressure are also solids according to this definition. Solids may be in two states, dissolved or precipitated.

5. Dissolved Solids

Dissolved solids pay no direct role in a chemical equilibrium computation. The fact that a dissolved solid exists indicates simply that the solubility data for the solid are present, and after an -equilibrium computation has been made, the solubility of this solid phase may be checked. If the solubility product is exceeded, the solid may be precipitated and become directly involved in the computation.

6. Precipitated Solids

Precipitated solids are those solid phases which are present at a fixed activity. This implies a certain fixed relationship among the components with the result that the chemical equilibrium problem loses one degree of freedom. This is equivalent to transforming the set of components to include the solid phase, which is then set at fixed activity. If, after a chemical equilibrium computation has been made with a given phase, the amount of that solid phase is calculated to be negative, the solid may be dissolved, i.e., removed from the computation and the fixed relationship among the constituents disestablished.

These six definitions are applicable to chemical equilibrium in general. For the-purpose of presenting the program, these definitions will further be used to define six types of species which have significance within the program.

Type I Species: are the soluble species which correspond to the component.

Type II Species: are the complexes (all soluble species which are not components).

Type III Species: are precipitated solids which are not allowed to dissolve, even if the amount of these solids becomes negative. Examples are gases at a fixed partial pressure, or simply a solid phase which is specified to be present.

In addition, if the concentration (activity) of any soluble species is to be fixed, i.e., set to a certain value (for example, fixed pH), this fixed soluble species is included as a Type III species.

Type IV Species: are precipitated solids which are subject to dissolution if the amount present becomes less than zero.

Type V Species: are dissolved solids which are subject to precipitation if the solubility product is exceeded.

Type VI Species: are species which are not to be considered at all (e.g., dissolved solids which are not subject to precipitation, or the electron which does not exist in solution).

Edit Function

Ions can be added by: 1) typing in a new reference number that is not currently being used; 2) using an existing reference number and typing a new species ID number and new concentration data; or 3) a line may be deleted by typing "D" prior to an existing reference number.

Input COMPONENT SPECIES

Ref#	SpecID	Chemical Name	Electr Charge	Analytical Concentration — Molar —	— mg/l —	Guess for Free Comp Log10Conc
1	2	Mg	+2	.1728E-03	4.199	-4.0
2	4	K	+1	.1279E-09	.5001E-05	-10.
3	5	Na	+1	.1609E-03	3.699	-4.0
4	6	Pa	+3	.5380E-05	.3002	-5.0
5	8	Mn	+2	.2190E-05	.1202	-6.0
6	9	cu	+2	.7874E-07	.5000E-02	-7.0
7	10	Ba	+2	.2185E-06	.3001E-01	-7.0
8	12	Zn	+2	.6118E-07	.4000E-02	-7.0
9	SO	H	+1	.1000E-08	.1000E-05	-9.0
10	99	e	-1	1.000	1000.	.00
11	101	co3	-2	.8000E-04	4.800	-5.0
12	102	so4	-2	.3123E-03	30.00	4.0
13	103	cl	-1	.2820E-07	.9997E-03	-8.0
14	109	PO4	-3	.1053E-05	.1000	-6.0
15	112	$iO2(OH)2	-2	.3000E-06	.2823E-01	-7.0
16	157	NO3	-1	.3043E-05	.1400	-6.0

More↓ (NextPage BottomOfList)

ENTER Ref# >
(Help Exit)

MINeral Equilibrium Model

Edit Control

Enter the reference number (Ref#) of the component desired to edit. To ADD a component, choose a Ref# larger than the last shown in the current set (999 Will always work!). To DELETE a component, enter a "D" (for Delete) immediately preceding the reference number. Deleted components • UJU an asterisk. after the Ref# on the list. To retain a deleted component, component, simply update the Species ID (which is changed to zero when flagged for deletion).

Analytical concentrations are input in mg/l UNLESS preceded by the letter "M" (for Molar concentration). Concentrations for Fulvic(SpecID#159) and Humic(SpecID#160) acids may be entered from Dissolved Organic Carbon (in mg/l) by preceding the concentration with a "D" (for DOG).

See MINE User's Manual for a detailed description.

Type I - COMPONENTS

Ref#	SpecID	Log10 of Comp FormationConst	Stoichiometric Pain ComponentID:StoichiometricCoefficient ┌Pair1┐	┌Pair2┐	┌Pair3┐	┌Pair4┐

(none found)

ENTER Ref# >
(Help Exit)

MINeral Equilibrium Model

Edit Control

Enter the reference number (Ref#) of the component desired to edit. To ADD a component, choose a Ref# larger than the last shown in the current sot (999 will always work:). To DELETE a component, enter a "D" (for Delete) immediately preceding the reference number. Deleted components Shw an • sterimk . after the Ref# on the list. To retain a deleted component, component, simply update the Species ID (which is changed to zero when flagged for deletion).

See MINE User's Manual for a detailed description.

In the model, humic and fulvic acid have been added as potential metal binding ligands. It is possible to make very rough approximations of humic and fulvic concentrations if DOC data is available. In this case the concentrates should be preceded by a "D" for DOC. The proportion of DOC expected in either humic or fulvic acids will then be calculated.

The screen also shows the (free comp/Log10Conc). This is the log of the concentration data and is the number used by the program for the first iteration. These numbers are refined with each iteration of the model to provide the final output.

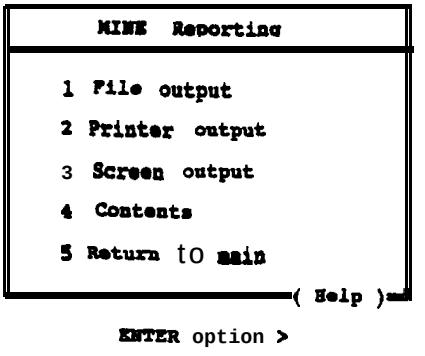
NB: Once you have edited a file you must update the data file on disc before running MINE 1.0.

Each ion included in the model has an identification number (see Table 2.1). Once the line number has been chosen the ion of choice is then selected using its identification number and its concentration in mg/L is input.

In order to calculate ionic interactions, molar concentrations are used. If data are already in molar concentrations then "M" must be typed prior to exiting the concentration. Other edit functions are explained in the Help screen shown.

2.3 OUTPUT OPTIONS

Once you have entered your input data and are satisfied that you have made the required modifications you are nearly ready to run MINE 1.0. You must first select the MINE Options. The first of these are the Output Option 5, Return to Main Menu and Select Output Options.



Report Contents: SELECTED

Table 2.1 List of Components and Identification Numbers in THRM DATA

I.D. NUMBER	COMPONENT	I.D. NUMBER	COMPONENT	I.D. NUMBER	COMPONENT
1	Ca^{2+}	22	Li+	106	I-
2	Mg^{2+}	23	Be^{2+}	107	NH_3
3	Sr^{2+}	24	Sc^{3+}	108	S^{2-}
4	K^{+}	25	TiO^{2+}	109	PO_4^{3-}
5	Na^{+}	26	Sn^{2+}	110	$P_2O_4^{4-}$
6	Fe^{3+}	27	Sn^{4+}	111	P_3O^{-}
7	Fe^{2+}	28	La^{3+}	112	$SiO_2(OH)_2^{2-}$
8	Mn^{2+}	29	Ce^{3+}	113	S_2O_{32-}
9	Cu^{2+}	30	Au+	114	CN^{-}
10	Ba^{2+}	31	Th^{4+}	115	AC- *
11	Cd^{2+}	32	UO_2^{2+}	148	$B(OH)_4^{-}$
12	Zn^{2+}	33	Cu^{2+}	149	SO_3^{2-}
13	Ni^{2+}	34	U^{4+}	150	SCN^{-}
14	Hg^{2+}	35	Ra^{2+}	151	NH_2OH
15	Pb^{2+}	50	H^{+}	154	AsO_4^{3-}
16	Co^{2+}	99	e^{-}	155	HVO_4^{2-}
17	Co^{3+}	101	CO_3^{2-}	156	SeO_3^{2-}
18	Ag^{+}	102	SO_4^{2-}	157	NO_3^{-}
19	Cr^{3+}	103	Cl'	158	TRIS
20	Al^{3+}	104	F^{-}	159	FA^{2-} **
21	cs+	105	Br^{-}	160	HA^{2-} ***

* 1125 AC = Acetic acid
** 159 FA = Fulvic acid
*** 160 HA = Humic acid

MINeral Equilibrium Model

Output Specifications

The reports generated by MINE may be directed to on. of three destinations, ☺○ ● pociffed by the user.

File - report sent to a file; thm name is specified by the user and must consist of a (optional) DOS path and a DOS filename, both valid
eg. A:\REPORT\RUN.DMP , A:\REPORT is the path RUN.DMP is the filename
Printer - report sent to the default printing device (PRN or LPT1:)
Screen - report sent to the video display (CON)
Contents- selection of report contents

The output can be directed to one of the three locations as shown in menu. The Help menu gives details on each option.

MINE Report Contents

(Problem Input)
1 Components √
2 Species √

(Model Output)
3 Components √
√
5 Distribution √

6 Concentration8 . . MOLAR

7 Return to report main

(Help)

ENTER Option >

MINeral Equilibrium Model

Report Specifications

The user may choose general report contents. One or more of the MINE model output options MUST be selected before continuing. Toggle ON or OFF.

PROBLEM INPUT: Parameters ● ntormd by the user for input to the MINE model. Divided into 2 categories - Components and Species.

MODEL OUTPUT: The MINE model results based on the problem input. Divided into Components, Species and Percent Distribution of Components. Component concentrations are MOLAR or MG/L.

See MINE User's Manual for a detailed description.

Press ENTER to continue..

By use of a toggle switch, each report option can be selected. For example, if it is wished to print the **import** components, then press 1, a ✓ will be put by this input parameter. If a ✓ is already there and it is not a requirement to print this, then a **repeat** press of 1 will **remove** toggle.

The concentrations in the report can be displayed in either molar concentrations or **mg/L.** Again change from one to the other is accessed via the depression of the number 6.

2.4 CONVERGENCE OPTIONS

After returning to **MAIN** Menu the convergence screen must next be selected.

```
        MINE  Convergence

    1  Select file
    2  Edit  contents
    3  Update  to  disk
    4  Bell  is  ON
    5  Return to main

                          ( Help )

          ENTER Option >

Maximum Iterations:        75
Convergence Limit:      .10E-03
Detection Threshold:    .10E-01
Convergence critmria  in file: CONVERGE.DAT
```

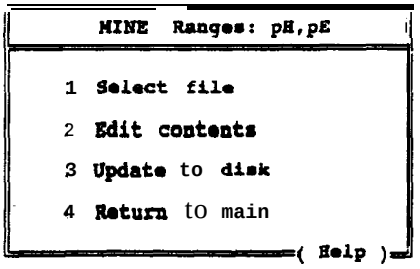
```
I MINeral Equilibrium Model

Convergence Specifications

Convergence criteria determine if a solution will be found to
the problem at hand.  The critmria supplied  (default) should
be sot ficient for most purposes. However, if MINE should not
converge, changing t h m criteria i s recommended.

Maximum Iterations  - maximum number o f iterations allowed
                      for a problem (default 40)
Convergence Limit   - tolerance in the convergence tmmt
                      (default .0001)
Dmtmctfoa Threshold - the threshold for percentage
                      distribution output (default .01 or 1%)

The BELL sounded at  acb iteration may be toggled ON or OFF.

NOTE: To reduce computing time, raise thm Convergence Limit.

          Press ENTER t o continue..
```

The menu gives you the option to change the conditions for convergence.. It is not normally required to change these criteria. Before changing these criteria the operator is asked first to check the error messages. The most common event that prevents convergence is a phase rule violation.

The value for the convergence limit is the level at which the program allows a solution. If only approximate values are required then this limit can be raised. It is usually not a parameter that needs to be changed. However, if the number of iterations (40) is exceeded, increasing the convergence limit may allow a solution within 40 iterations. It is recommended that when convergence limit is to be changed that orders of magnitude are used.

2.5 pH AND Eh RANGES

On returning to the MAIN menu the ranges after which the model is to run may be scheduled. Due to the time it takes to run each model, **if** the operator has not had much experience with the model it is recommended that runs be performed one at a time to avoid ineffective runs.



	Minimum	Maximum	Increment
pE:	7.00	7.00	1.00
pE:	13.00	13.00	1.00

pH,pE Ranges in file: RANGE.DAT

MINeral Equilibrium Model

Ranges Specifications

Major speciation changes occur under varying conditions of pE and pH. In order to ● raluatm thr probla over ● xpoctmd pE and pH criteria, MINE may be run at a series of these values.

pH Min/Max/Inc - MINE will execute overthe pH range, from the MINimum to the MAXimum value (inclusive) by the INCrement
eg. if Min=4, Max=5, Inc=.5
then pH=4(Run1), 4.5(Run2), etc..

pE Min/Max/Inc - the MINimum, MAXimum and INCrement values of pE, applied similar to pH (above)

NOTE: Specified pE ranges are executed first.

Convergence criteria determine if a solution will be found to the problem at hand. The criteria supplied (default) should be sufficient for most purposes. However, if MINE should not converge, changing the criteria is recommended.

The output for MINE 1.0 has been broken down into three sections:

1. Input data
2. Solution for all components showing concentrations and specific associations
3. Percentage distribution of components

An example is given in the appendices.

The printing of the input data file is included for verification. Changes to specific components may be considered in hard copy before a new one is made.

The data showing concentration of each class of compound allows the operator to consider all species of a given ion. This section is also most informative when considering ERROR messages.

The percentage contribution of each cation shows only those species that represent more than 1% of a given cation's forms.

3.1 ERROR MESSAGES

There are several problems which cause an error message to be printed and execution to be terminated. The error messages, the subroutine from which they are called, the probable cause and corrective response are given below.

1. "COMPONENTS > NXDIM", SUBROUTINE INPUT:

The number of components in the problem is greater than the dimension of the arrays allocated for their storage. Response: Either remove non-essential components from the computation or increase the dimension of the arrays (See Section I, "Storage").

2. "SPECIES > NYDIM,", SUBROUTINE INPUT:

The number of species in the problem is greater than the dimension of the arrays allocated for their storage. Response: Either remove non-essential components from, the computation or increase the dimension for the arrays (See Section I, "Storage").

3. "ID NOT FOUND: INPUT", SUBROUTINE INPUT:

The species identification number used to re-specify an existing species type was not found, and the stoichiometry was not valid for generating a new species. Response: Check (a) input format; (b) whether the indicated species was included in the computation.

4. "ID NOT FOUND: LADY" FUNCTION LADY

A species identification number was not found. Response: Verify that the identification number is valid., and that the species is included in the computation.

5. "ID NOT FOUND: IADX" FUNCTION LADY

A component identification number was not found. Response: Verify that the identification number is valid, and that the component is included in the computation.

6. "PHASE RULE VIOLATION" SUBROUTINE SOLID

More solid phases have been specified than there are allowed by the Phase Rule. Response: Restart computation with an alternate set of Type III and/or Type IV solids.

7. "ITERATIONS > ITMAX" SUBROUTINE SOLVE

The number of iterations allowed in subroutine SOLVE has been exceeded. The number of allowable iterations is set at 40 and should be sufficient for most calculations. If this error message is given it is probable that the initial concentration data have been poorly chosen. It is also possible that the

model would converge if some species types are re-examined. To do this the user requires some knowledge of **redox** reactions and is advised to seek the help of a chemist if they do not feel they can make appropriate changes.

8. "SINGULAR Z MATRIX" SUBROUTINE **SIMQ**

The Jacobian has been found to be singular. Response: Check for an input error; the Jacobian is very largely singular if the problem has been correctly specified.

The most common errors involve 6 and 7 and stem from the inclusion of **redox** reaction in the computations. In order to do this it is necessary to include the electron in the input data (Identification **#99).**

In order to run the program both H+ and E^- must be included as fixed solids **type** III species. The appropriate **E** concentrations must be included in the input data.

Phase rule violations may occur if species are allowed to precipitate and dissolve with successive iterations. Again fixing some **redox** control precipitates as solids will alleviate this problem and reduce the number of iterations.

Example of Input and Output Data

SPECIES IDENTIFICATION

It should be noted that compound identification is performed using only capital letters.

In addition, OH- and H^+ are represented as H^- and H^+ respectively.

MINE 1.2

1992 Nay 20 16:09

BC. RECEIVING HATER 1

--- Input Data ---

INITIAL CONDITIONS

pE = 13.0
pa = 7.0

Ionic Strength = 5.01E-01

ID#	Analytical Concentration ---(MG/L)---	Component
2	4.20D+00	MG
4	5.00D-06	K
5	3.70D+00	NA
6	3.00D-01	FE3
8	1.20D-01	MN2
9	5.00D-03	Cu2
10	3.00D-02	BA
12	4.00D-03	ZN
50	1.00D-06	H

ID#	Analytical Concentration ---(MG/L)---	Component
99	1.00D+03	E
101	4.80D+00	co3
102	3.00D+01	so4
103	1.00D-03	CL
109	1.00D-01	P04
112	2.82D-02	SI03
157	1.40D-01	N03
159	5.00D-02	FA
160	5.00D-02	HA

MINE 1.2 1992 May 20 16:09

BC. RECEIVING WATER 1

--- Output Data ---

FINAL CONDITIONS

Number of iterations = 7

pE = 13.0
pa = 7.0 Ionic Strength = 5.01E-01

ID#	Concentration (MG/L) Equilibrium	Analytical	Remainder	Component
2	4.18D+00	4.20D+00	l.llD-17	MG
4	5.00D-06	5.00D-06	-1.16D-20	K
5	3.70D+00	3.70D+00	-3.15D-16	NA
6	1.31D-09	3.00D-01	2.59D-15	FE3
8	1.29D-08	1.20D-01	0.00D+00	MN2
9	2.29D-03	5.00D-03	3.89D-18	cu2
10	3.00D-02	3.00D-02	-2.69D-17	BA
12	3.82D-03	4.00D-03	2.33D-18	ZN
50	1.00D-04	l.00D-06	0.00D+00	H
99	l.00D-10	1.00D+03	0.00D+00	E
101	1.17D-02	4.80D+00	-3.88D-16	co3
102	2.99D+01	3.00D+01	-5.83D-16	so4
103	l.00D-03	l.00D-03	-1.44D-18	CL
109	1.74D-06	l.00D-01	2.46D-16	PO4
112	4.91D-10	2.82D-02	4.37D-15	SI03
157	1.40D-01	1.40D-01	-7.79D-17	NO3
159	4.90D-02	5.00D-02	3.58D-17	FA
160	1.62D-02	5.00D-02	-1.64D-17	HA

MINE 1.2

1992 May 20 16:09

BC. RECEIVING HATER 1

--- Output Data ---

DISTRIBUTION OF COMPONENTS

ID#	Component	Percent Bound in Species (%)	ID#	(Name:Stoichiometric Coeff)					
2	MG	99.5	2	MG	1				
4	K	99.9	4	K	1				
5	NA	100.0	5	NA	1				
6	FE3	99.7	2680	FE3	1	H	-2		
a	MN2	100.0	21470	H	-4	E	-2	MN2	1
9	cu2	45.8	9	Cu2	1				
		2.5	3920	co3	1	CD2	1		
		4.1	4813	Cu2	1	HA	1		
		2.8	4840	cu2	1	H	-1		
		44.4	4842	cu2	1	H	-2		
10	BA	100.0	10	BA	1				
12	ZN	95.4	12	ZN	1				
		3.7	6745	ZN	1	H	-2		
50	H	105.3	12530	co3	1	H	1		
		20.4	12540	co3	1	H	2		
		1.1	12610	PO4	1	H	2		

MINE 1.2 1992 May 20 16:09

BC. RECEIVING WATER 1

--- Output Data ---

DISTRIBUTION OF COMPONENTS

ID# --a--	Component	(%)	ID#	Percent Bound in Species (Name:Stoichiometric Coeff)					
99	E	100.0	21470	H	-4	E	-2	MN2	1
101	co3	90.9	12530	co3	1	H	1		
		8.8	12540	co3	1	H	2		
102	so4	99.7	102	so4	1				
103	CL	100.0	103	CL	1				
109	PO4	62.7	12600	PO4	1	H	1		
		37.1	12610	PO4	1	H	2		
112	SIO3	99.5	12720	SIO3	1	H	2		
157	NO3	100.0	157	NO3	1				
159	FA	97.9	159	FA	1				
160	HA	32.4	160	HA	1				
		1.2	1580	HA	1	MG	1		
		1.5	2060	HA	1	NA	1		
		64.8	4813	CU2	1	HA	1		