SOFTWARE RELEASE NOTICE

1. SRN Number: GHGC-SRN-262

2. Project Title: Radionuclide Transport Key Technical Issue | Project No. 20.01402.871

3. SRN Title: MINTEQA2/PRODEFA2, Version 4.02

4. Originator/Requestor: David R. Turner | Date: 02/20/2002

5. Summary of Actions

- X Release of new software
- ☐ Change of access software
- ☐ Release of modified software:
- ☐ Software Retirement
  - ☐ Enhancements made
  - ☐ Corrections made

6. Validation Status

- ☐ Validated
- ☐ Limited Validation
- X Not Validated — Explain: Validation Plan Approved, to be implemented

7. Persons Authorized Access

Name	Read Only/Read-Write	Addition/Change/Delete
David R. Turner	Read-Write	
F. Paul Bertetti	Read-Write	

8. Element Manager Approval: F. C. Bertetti Date: 2/22/02

9. Remarks:

NOTE: This acquired code was developed by the U.S. Environmental Protection Agency and supersedes/replaces MINTEQA2/PRODEFA2, Version 3.11/3.12 currently under configuration management.

CNWRA Form TOP-6 (09/01)

SOFTWARE SUMMARY FORM

01. Summary Date: 02/20/2002	02. Summary prepared by (Name and phone) David R. Turner (CNWRA): (201) 522-2139	03. Summary Action: REPLACEMENT (Replaces MINTEQA2, Version 3.11/3.12)
04. Software Date: 06/2000	05. Short Title:MINTEQA2/PRODEFA2, Version 4.02	
06. Software Title: MINTEQA2/PRODEFA2, Version 4.02: A Geochemical Assessment Model for Environmental Systems		07. Internal Software ID: None

08. Software Type: ☐ Automated Data System X Computer Program ☐ Subroutine/Module	09. Processing Mode: ☐ Interactive ☐ Batch X Combination	10. Application Area a. General: X Scientific/Engineering ☐ Auxiliary Analyses ☐ Total System PA ☐ Subsystem PA ☐ Other b. Specific: Acquired Geochemical Equilibrium Speciation Code. Developed by U.S. EPA.
11. Submitting Organization and Address: CNWRA/SwRI 6220 Culebra Road San Antonio, TX 78228		12. Technical Contact(s) and Phone: David R. Turner (210) 522-2139

13. Software Application: MINTEQA2, Version 4.02 is a DOS-based geochemical equilibrium speciation model for dilute aqueous species. MINTEQA2, Version 4.02 uses a thermodynamic database with formatted chemical reactions, equilibrium constants, and enthalpies of reaction to solve mass action and mass balance constraints in geochemical systems. The code is used to investigate geochemical processes such as aqueous speciation, precipitation/dissolution, gas partial pressures, redox behavior, sorption, and ion exchange. PRODEFA2 is an interactive pre-processor that uses menus to build the formatted input files for MINTEQA2.

14. Computer Platform PC/Pentium II	15. Computer Operating System: Windows NT, Version 4.00	16. Programming Language(s): Fortran 90	17. Number of Source Program Statements: Unknown
18. Computer Memory Requirements: 640 K RAM/1.4 Mb storage	19. Tape Drives: N/A	20. Disk Units: N/A	21. Graphics: N/A

22. Other Operational Requirements
ANSI.SYS device driver for PRODEFA2 menus

23. Software Availability: X Available ☐ Limited ☐ In-House ONLY	24. Documentation Availability: X Available ☐ Preliminary ☐ In-House ONLY

25. Acquired Code developed by U.S. Environmental Protection Agency

Software Developer: David R. Turner Date: 02/20/2002

CNWRA Form TOP-4-1 (05/98)

```
Directory PATH listing for volume 020313_1509
Volume serial number is 0012FC9[redacted]B9:8389
F:\
+---MINTEQA2_Configuration
    +---DOCUMENT
    |       SUPPLE1.PDF
    |       SUPPLE2.PDF
    |       USERMANU.PDF
    |
    +---Download File
    |       INSTALMT.EXE
    |
    +---README
    |       ABSTRACT.TXT
    |       READ.ME
    |       RELEASE.TXT
    |       RESPONSE.TXT
    |       UPDATE.TXT
    |       YEAR2000.TXT
    |
    +---Source
    |   +---FRMTCODE
    |   |       DUMMY.FOR
    |   |       ENQUIRE.FOR
    |   |       FRMT.FOR
    |   |       MAKEFILE.FRM
    |   |       MAKEFILE.UFM
    |   |       UNFRMT.FOR
    |   |
    |   +---INC_CODE
    |   |       CONST.INC
    |   |       MINTEQA2.INC
    |   |       PRODEFA2.INC
    |   |
    |   +---MINTCODE
    |   |       ACTIVH2O.FOR
    |   |       ACTVTY.FOR
    |   |       ACT_COEF.FOR
    |   |       ADSORB.FOR
    |   |       ALKCOR.FOR
    |   |       CLIGZ.FOR
    |   |       CLM_ACT.FOR
    |   |       CLRSCR.FOR
    |   |       COMPOSIT.FOR
    |   |       DBASE.FOR
    |   |       DELAY.FOR
    |   |       DISPLAY.FOR
    |   |       DISSOLV2.FOR
    |   |       DISSOLVE.FOR
    |   |       DOMPREP.FOR
    |   |       DUMMY.FOR
    |   |       DUMMYCMP.FOR
    |   |       DUPCMP.FOR
    |   |       ENQUIRE.FOR
    |   |       ERROR.FOR
    |   |       EXCLUDE.FOR
    |   |       EXCOL.FOR
    |   |       EXROW.FOR
    |   |       GUESS.FOR
    |   |       GUESS1.FOR
    |   |       IADX.FOR
    |   |       IADY.FOR
    |   |       IAP.FOR
    |   |       INFILE.FOR
    |   |       INIT.FOR
    |   |       INPUT.FOR
    |   |       ION_STR.FOR
    |   |       KCORR.FOR
    |   |       MAIND.FOR
    |   |       MAKEFILE
    |   |       MINTEQA2.FOR
    |   |       MINVAL.FOR
    |   |       NEWX.FOR
    |   |       NXTPRB.FOR
    |   |       OUFILE.FOR
    |   |       OUTPUT.FOR
    |   |       PHASECHK.FOR
    |   |       POINTER.FOR
    |   |       PRECIPIT.FOR
    |   |       PREP.FOR
    |   |       PREP2.FOR
    |   |       SATUR.FOR
    |   |       SIMQ.FOR
    |   |       SOLID.FOR
    |   |       SOLIDX.FOR
    |   |       SOLVE.FOR
    |   |       SWITCH.FOR
    |   |       TSTAMP.FOR
    |   |       VHOFF.FOR
    |   |
    |   +---PRODCODE
    |           ADDSPE.FOR
    |           ADSFILIN.FOR
    |           ADSINIT.FOR
    |           ADSORB.FOR
    |           ADSREACT.FOR
    |           CACALC.FOR
    |           CATCID.FOR
    |           CLRSCR.FOR
    |           COMINC.FOR
    |           CPRINT.FOR
    |           CWRITE.FOR
    |           DISPLAY.FOR
    |           DLTCOMP.FOR
    |           DOMMENU.FOR
    |           DOMSTAT.FOR
    |           DUMMY.FOR
    |           EDITL1.FOR
    |           EDITL[redacted]R
    |           EDITL[redacted]R
    |           EDITL4.FOR
    |           ENQUIRE.FOR
    |           EXCLUDEE.FOR
    |           FGUESS.FOR
    |           FINI.FOR
    |           FIXORDER.FOR
    |           GETFILES.FOR
    |           IDADSO.FOR
    |           IDCOMP.FOR
    |           IDGASG.FOR
    |           IDMINE.FOR
    |           IDREDX.FOR
    |           IDSPEC.FOR
    |           INCR.FOR
    |           INFILE.FOR
    |           INIT.FOR
    |           MAKEFILE
    |           MPORT123.FOR
    |           NAMESP.FOR
    |           OUFILE.FOR
    |           PECALC.FOR
    |           PHCALC.FOR
    |           PRINTP.FOR
    |           PRODEFA2.FOR
    |           READP.FOR
    |           SEARCH.FOR
    |           SITCOUNT.FOR
    |           SITE.FOR
    |           SPEADD.FOR
    |           SURFACE.FOR
    |           SWEEPR.FOR
    |           SWPSTAT.FOR
    |           THCONST.FOR
    |           WRITEP.FOR
    |
    +---TestProb
    |   +---Output_As_Received
    |   |       TEST1A.OUT
    |   |       TEST1B.OUT
    |   |       TEST2A.OUT
    |   |       TEST2B.OUT
    |   |       TEST2C.OUT
    |   |       TEST3.OUT
    |   |       TEST30.OUT
    |   |       TEST4.OUT
    |   |       TEST5A.OUT
    |   |       TEST5B.OUT
    |   |       TEST5C.OUT
    |   |       TEST6.OUT
    |   |
    |   +---Output_CNWRA
    |   |       TEST1A.OUT
    |   |       TEST1B.OUT
    |   |       TEST2A.OUT
    |   |       TEST2B.OUT
    |   |       TEST2C.OUT
    |   |       TEST2C.PRN
    |   |       TEST3.OUT
    |   |       TEST30.OUT
    |   |       TEST4.OUT
    |   |       TEST5A.OUT
    |   |       TEST5B.OUT
    |   |       TEST5C.OUT
    |   |       TEST6.OUT
    |   |
    |   +---Test_Input
    |           TEST1A.INP
    |           TEST1B.INP
    |           TEST2A.INP
    |           TEST2B.INP
    |           TEST2C.INP
    |           TEST3.INP
    |           TEST30.INP
    |           TEST4.INP
    |           TEST5A.INP
    |           TEST5B.INP
    |           TEST5C.INP
    |           TEST6.INP
    |
    +---ThermoData
        +---Data_As_Received
        |       ALK.DBS
        +---Data_As_Received
        |       ALK.DBS
        |       ANALYT.DBS
        |       COMP.DBS
        |       ERROR.DBS
        |       FEO-DLM.DBS
        |       GASES.DBS
        |       GAUSSIAN.DBS
        |       REDOX.DBS
        |       THERMO.DBS
        |       THERMO.UNF
        |       TYPE6.DBS
        |       TYPE6.UNF
        |
        +---Data_CNWRA_NEA
                Comp4_rad.dbs
                RADREFS.DAT
                Redox4_nea.dbs
                Therm4rad_nea.dbs
                Thermo4_nea.dbs
                Type64_nea.dbs
```

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
FOR
→ *ACQUIRED SOFTWARE NOT TO BE MODIFIED* ←

Software Title/Name: MINTEQA/PRODEFA2

Version: 4.02

Demonstration workstation: Pentium II IBM Workstation in Room A218

Operating System: Windows NT Version 4.00

User: David R. Turner

NOTE: Acquired software may or may not meet all requirements and will be evaluated on a case-by-case basis.

Installation Testing [TOP-018, Section 5.6]

Has *installation testing* been conducted for each intended computer platform and operating system? IBM Workstation, Pentium II Yes: ☑ No: ☐ N/A: ☐

Computer Platforms: Room A218 Operating Systems: Windows NT Version 4.0

Location of Acceptance Test Results: QA Records Room

Comments:. Installation testing complete for IBM Workstation, Windows NT 4.0

Software Output [TOP-018, Section 5.5.4]

Is software designed so that individual runs are uniquely identified by date, time, name of software and version? Yes: ☑ No: ☐ N/A: ☐

Date and Time Displayed: Yes

Name/Version Displayed: Yes

Comments:

NOTE: Output identification content and format is typically taken as is.

Medium Documentation [TOP-018, Section 5.5.6]

The physical labeling of software medium (tapes, disks, etc.) contains: Program Name, Module/Name/Title, Module Revision, File type (ASCII, OBJ, EXE), Recording Date, and Operating System(s)? Yes: ☑ No: ☐ N/A: ☐

Comments:

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
FOR
→*ACQUIRED SOFTWARE NOT TO BE MODIFIED*←

User Documentation [TOP-018, Section 5.5.7]

Is there a Users' Manual for the software and is it up-to-date? Yes: ☑ No: ☐ N/A: ☐

User's Manual Version and Date: Version 3.0, dated 1991

Comments: Updates to version 4.0 dated (Revised) Septembles 1999

Are there basic instructions for the *installation* and *use* of the software? Yes: ☑ No: ☐ N/A: ☐

Location of Instructions: Users Manual / Readme files on the installation CD.

Comments:

Configuration Control [TOP-018, Section 5.7, 5.9.3]

Is the Software Summary Form (Form TOP-4-1) completed and signed? Yes: ☑ No: ☐ N/A: ☐

Date of Approval: 2/20/2002

Is the list of files attached to the Software Summary Form complete and accurate? Yes: ☑ No: ☐ N/A: ☐

Comments:

Is the source code available or, is the executable code available in the case of (acquired/commercial codes)? Yes: ☑ No: ☐ N/A: ☐

Location of Source Code: located on the CD.

Comments: located in the Mintcode and Prodcode files.

Have all the script/make files and executable files been submitted to the Software Custodian?

Only the executable files are being submitted. Yes: ☑ No: ☐ N/A: ☐

Location of executable files: QA Records Room

Comments:

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
FOR
→ *ACQUIRED SOFTWARE NOT TO BE MODIFIED* ←

Software Release [TOP-018, Section 5.9]

Upon acceptance of the software as verified above, has a Software Release Notice (SRN), Form TOP-6 been issued and does the version number of the software match the documentation?

Yes: ☑ No: ☐ N/A: ☐

SRN Number: 262

Comments:

Software Validation [TOP-018, Section 5.10]

Has a Software Validation Test Plan (SVTP) been prepared for the ***range of application*** of the software?

Yes: ☑ No: ☐ N/A: ☐

Version and Date of SVTP: Version 4.02, SVTP dated 11/08/2001

Date Reviewed and Approved via QAP-002: 12/13/2001

Comments:

Has a Software Validation Test Report (SVTR) been prepared that documents the results of the validation cases, interpretation of the results, and determination if the software has been validated?

Yes: ☐ No: ☑ N/A: ☐

Version and Date of SVTR: ____

Date Reviewed and Approved via QAP-002: ____

Comments.: SVTR scheduled for May/June 2002

Additional Comments:

David R Lamm 03/07/2002
Software Evaluator/User/Date

Bruce Mabrito 3/7/2002
~~David R Lamm 03/07/2002~~
Software Custodian/Date

Test1a.out
MINTEQA2, ver 4.02
w/ original database
As distributed by EPA

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 5-JUN-2000 TIME: 14: 6:27

TEST1A - Compute total H+ of a solution of known pH.
This together with TEST1B illustrate a two run set to compute pH.

Component file (COMP.DBS):	comp.dbs	COMP v4.00 09/30/1999
Thermodynamic file (THERMO.UNF):	thermo.unf	THERMO V4.00 09/30/1999
Gaussian DOM file (GAUSSIAN.DBS):	gaussian.dbs	GAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF):	type6.unf	TYPE6 V4.00 09/30/1999

Temperature (Celsius): 25.00
Units of concentration: MOLAL
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed only for those solids specified as ALLOWED
in the input file (if any).
Maximum iterations: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

330	0.000E+00	-2.50
732	1.580E-03	-2.80
410	7.700E-05	-4.11
140	0.000E+00	-16.00

H2O has been inserted as a COMPONENT

3	2	
3301403	21.6600	-0.5300
330	2.5000	0.0000

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	3.162E-03	-2.500	0.000E+00
732	SO4-2	1.585E-03	-2.800	1.580E-03
410	K+1	7.762E-05	-4.110	7.700E-05
140	CO3-2	1.000E-16	-16.000	0.000E+00
2	H2O	1.000E+00	0.000	0.000E+00

Charge Balance: UNSPECIATED

Sum of CATIONS= 7.700E-05 Sum of ANIONS = 3.160E-03

PERCENT DIFFERENCE = 9.524E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:

SO4-2	Log activity guess:	-2.92
CO3-2	Log activity guess:	-16.66

CONSTRAINTS ON COMPONENT ACTIVITIES

As specified, this chemical system is OPEN with respect to the following components:

H2O H+1 CO3-2

Activities of the following components are constrained by the species shown:

COMPONENT	SPECIES	TYPE
CO3-2	CO2 (g)	3
H+1	H+1	3
H2O	H2O	3

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL mol/L	DIFF FXN	LOG ACTVTY	RESIDUAL
0	SO4-2	1.580E-03	6.594E-07	-2.91757	5.014E-07
1	SO4-2	1.580E-03	4.193E-04	-2.91775	4.192E-04
2	SO4-2	1.580E-03	8.125E-06	-3.01997	7.967E-06
3	SO4-2	1.580E-03	1.693E-07	-3.02220	1.135E-08

ID No	Name	Total Conc(M)	Conc (M)	log Activity	Diff fxn
410	K+1	7.700E-05	7.649E-05	-4.14759	5.093E-11
732	SO4-2	1.580E-03	1.266E-03	-3.02224	3.557E-09
2	H2O	0.000E+00	-1.049E-05	-0.00004	0.000E+00
330	H+1	0.000E+00	3.398E-03	-2.50000	0.000E+00
140	CO3-2	0.000E+00	2.916E-17	-16.66004	0.000E+00

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
330	H+1	3.398E-03	-2.50000	1.00	0.93070	0.031
732	SO4-2	1.266E-03	-3.02224	-2.00	0.75031	0.125
410	K+1	7.649E-05	-4.14759	1.00	0.93070	0.031
140	CO3-2	2.916E-17	-16.66004	-2.00	0.75031	0.125

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
3301400	HCO3-	1.588E-09	-8.83038	-1.00	0.93070	10.361
3301401	H2CO3 (aq)	1.048E-05	-4.97904	0.00	1.00102	16.681
3300020	OH-	3.421E-12	-11.49704	-1.00	0.93070	-13.966
3307320	HSO4-	3.132E-04	-3.53530	-1.00	0.93070	2.018
4107320	KSO4-	5.106E-07	-6.32310	-1.00	0.93070	0.878

Type III - SPECIES WITH FIXED ACTIVITY

ID No	Name	Conc (M)	New logK	Enthalpy
2	H2O	-1.049E-05	0.000	0.000
330	H+1	-3.711E-03	2.500	0.000
3301403	CO2 (g)	-1.049E-05	21.660	-0.530

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

K+1				
	99.3	Percent bound in species #	410	K+1
SO4-2				
	80.1	Percent bound in species #	732	SO4-2
	19.8	Percent bound in species #	3307320	HSO4-
H2O				
	100.0	Percent bound in species #	3300020	OH-
H+1				
	91.0	Percent bound in species #	330	H+1
	8.4	Percent bound in species #	3307320	HSO4-
CO3-2				
	100.0	Percent bound in species #	3301401	H2CO3 (aq)

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
410	K+1	7.700E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	1.580E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	3.421E-12	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	3.732E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	1.049E-05	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 3.474E-03 Sum of ANIONS 2.846E-03

PERCENT DIFFERENCE = 9.936E+00 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 4.426E-03

EQUILIBRIUM pH = 2.500

DATE ID NUMBER: 20000605
TIME ID NUMBER: 14062757

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components

Test1b.out
MINTEQA2 ver. 4.02
w/ original database
As distributed by EPA

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 5-JUN-2000 TIME: 14: 6:30

TEST1B - Compute equilibrium pH when 0.001 moles gibbsite is added
to the aqueous system of problem TEST1A.

Component file (COMP.DBS):	comp.dbs	COMP v4.00 09/30/1999
Thermodynamic file (THERMO.UNF):	thermo.unf	THERMO V4.00 09/30/1999
Gaussian DOM file (GAUSSIAN.DBS):	gaussian.dbs	GAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF):	type6.unf	TYPE6 V4.00 09/30/1999

Temperature (Celsius): 25.00
Units of concentration: MOLAL
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
Maximum iterations: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

330	3.732E-03	-7.00
732	1.580E-03	-2.80
410	7.700E-05	-4.11
140	0.000E+00	-16.00
30	0.000E+00	-16.00

H2O has been inserted as a COMPONENT

```
  3   1
3301403    21.6600    -0.5300
  4   1
2003003    -8.7700    22.8000   1.000E-03
```

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	1.000E-07	-7.000	3.732E-03
732	SO4-2	1.585E-03	-2.800	1.580E-03
410	K+1	7.762E-05	-4.110	7.700E-05
140	CO3-2	1.000E-16	-16.000	0.000E+00
30	Al+3	1.000E-16	-16.000	0.000E+00
2	H2O	1.000E+00	0.000	0.000E+00

Charge Balance: UNSPECIATED

Sum of CATIONS= 3.809E-03 Sum of ANIONS = 3.160E-03

PERCENT DIFFERENCE = 9.313E+00 (ANIONS - CATIONS)/(ANIONS + CATIONS)

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:
SO4-2 Log activity guess: -2.80
CO3-2 Log activity guess: -7.66

The following TYPE 4 solids have been pre-dissolved:
GIBBSITE

CONSTRAINTS ON COMPONENT ACTIVITIES

As specified, this chemical system is OPEN with respect to the following components:

H2O

Activities of the following components are constrained by the species shown:

COMPONENT	SPECIES	TYPE
CO3-2	CO2 (g)	3
H2O	H2O	3

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL mol/L	DIFF FXN	LOG ACTVTY	RESIDUAL
0	Al+3	1.000E-03	-1.000E-03	-16.00000	9.999E-04
1	Al+3	1.000E-03	-9.999E-04	-8.36062	9.998E-04
2	Al+3	1.000E-03	-6.494E-04	-4.23434	6.493E-04
3	Al+3	1.000E-03	1.245E-04	-3.80217	1.244E-04
4	Al+3	1.000E-03	2.100E-06	-3.83981	2.000E-06
5	Al+3	1.000E-03	-1.655E-07	-3.84058	6.555E-08

ID No	Name	Total Conc(M)	Conc (M)	log Activity	Diff fxn
330	H+1	7.320E-04	6.937E-04	-3.18698	-3.707E-09
732	SO4-2	1.580E-03	7.951E-04	-3.21211	-2.032E-08
410	K+1	7.700E-05	7.667E-05	-4.14351	-3.947E-10
30	Al+3	1.000E-03	2.586E-04	-3.84053	-1.577E-08
2	H2O	3.000E-03	2.987E-03	-0.00003	0.000E+00
140	CO3-2	0.000E+00	6.706E-16	-15.28606	0.000E+00

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
330	H+1	6.937E-04	-3.18698	1.00	0.93729	0.028
732	SO4-2	7.951E-04	-3.21211	-2.00	0.77178	0.113
410	K+1	7.667E-05	-4.14351	1.00	0.93729	0.028
140	CO3-2	6.706E-16	-15.28606	-2.00	0.77178	0.113
30	Al+3	2.586E-04	-3.84053	3.00	0.55828	0.253

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
3301401	H2CO3 (aq)	1.049E-05	-4.97903	0.00	1.00081	16.681
3300020	OH-	1.652E-11	-10.81004	-1.00	0.93729	-13.969
303300	AlOH+2	2.897E-06	-5.65057	2.00	0.77178	-4.884
303301	Al(OH)2+	2.934E-08	-7.56062	1.00	0.93729	-10.066
303303	Al(OH)3 (aq)	8.492E-12	-11.07066	0.00	1.00081	-16.791
303302	Al(OH)4-	1.768E-14	-13.78070	-1.00	0.93729	-22.660
3307320	HSO4-	4.130E-05	-4.41215	-1.00	0.93729	2.015
307320	AlSO4+	7.336E-04	-3.16264	1.00	0.93729	3.918
307321	Al(SO4)2-	4.824E-06	-5.34475	-1.00	0.93729	4.948
4107320	KSO4-	3.306E-07	-6.50888	-1.00	0.93729	0.875
3301400	HCO3-	7.669E-09	-8.14339	-1.00	0.93729	10.358

Type III - SPECIES WITH FIXED ACTIVITY

ID No	Name	Conc (M)	New logK	Enthalpy
2	H2O	2.987E-03	0.000	0.000
3301403	CO2 (g)	-1.049E-05	21.660	-0.530

Type V - UNDERSATURATED SOLIDS (not present at equilibrium)

ID No	Name	Conc (M)	New logK	Enthalpy
2003003	GIBBSITE	8.920E-04	-8.770	22.800
2003002	DIASPORE	7.037E-02	-6.873	103.052
2003001	BOEHMITE	1.388E-03	-8.578	117.696
3003000	Al2O3	6.143E-09	-19.652	258.590
6003000	AlOHSO4	2.314E-01	3.230	0.000
6003001	Al4(OH)10SO4	3.939E-10	-22.700	0.000
6041000	K-ALUM	5.773E-10	5.170	-30.209
6041001	ALUNITE	2.044E-21	1.400	210.000
2003000	Al(OH)3 (am)	8.324E-06	-10.800	111.000

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

H+1				
	92.1	Percent bound in species #	330	H+1
	2.8	Percent bound in species #	3301401	H2CO3 (aq)
	5.5	Percent bound in species #	3307320	HSO4-
SO4-2				
	50.3	Percent bound in species #	732	SO4-2
	2.6	Percent bound in species #	3307320	HSO4-
	46.4	Percent bound in species #	307320	AlSO4+
K+1				
	99.6	Percent bound in species #	410	K+1
Al+3				
	25.9	Percent bound in species #	30	Al+3
	73.4	Percent bound in species #	307320	AlSO4+
H2O				
	98.0	Percent bound in species #	303300	AlOH+2
	2.0	Percent bound in species #	303301	Al(OH)2+
CO3-2				
	99.9	Percent bound in species #	3301401	H2CO3 (aq)

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
330	H+1	7.530E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	1.580E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.700E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
30	Al+3	1.000E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	2.956E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	1.049E-05	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 2.286E-03 Sum of ANIONS 1.637E-03

PERCENT DIFFERENCE = 1.655E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 3.535E-03

EQUILIBRIUM pH = 3.187

DATE ID NUMBER: 20000605
TIME ID NUMBER: 14063130

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
2003000	Al(OH)3 (am)	-5.080	[1.000] 30 [3.000] 2 [-3.000]330
2003001	BOEHMITE	-2.858	[-3.000]330 [1.000] 30 [2.000] 2
2003002	DIASPORE	-1.153	[-3.000]330 [1.000] 30 [2.000] 2
2003003	GIBBSITE	-2.571	[1.000] 30 [3.000] 2 [-3.000]330
3003000	Al2O3	-8.212	[2.000] 30 [3.000] 2 [-6.000]330
6003000	AlOHSO4	-0.636	[-1.000]330 [1.000] 30 [1.000]732 [1.000] 2
6003001	Al4(OH)10SO4	-9.405	[-10.000]330 [4.000] 30 [1.000]732 [10.000] 2
6041000	K-ALUM	-9.239	[1.000]410 [1.000] 30 [2.000]732 [12.000] 2
6041001	ALUNITE	-20.689	[1.000]410 [3.000] 30 [2.000]732 [6.000] 2

Test2a.out
MINTEQA2 ver 4.02
w/original database
As distributed by EPA

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 5-JUN-2000 TIME: 14: 6:34

TEST2A - Typical groundwater with Ag+ added as a contaminant.
Solve for speciation at pH 7.0 and pe -3.21

Component file (COMP.DBS):	comp.dbs	COMP v4.00 09/30/1999
Thermodynamic file (THERMO.UNF):	thermo.unf	THERMO V4.00 09/30/1999
Gaussian DOM file (GAUSSIAN.DBS):	gaussian.dbs	GAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF):	type6.unf	TYPE6 V4.00 09/30/1999

Temperature (Celsius): 14.00
Units of concentration: mg/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
Maximum iterations: 500 and use convergence assist measure
The method used to compute activity coefficients is: Davies equation
Intermediate output file

330	0.000E+00	-7.00
1	0.000E+00	3.21
20	2.230E+00	-4.68
30	2.000E-01	-5.13
150	4.800E+01	-2.92
280	1.000E-01	-5.75
281	1.000E-01	-5.75
460	1.400E+02	-2.24
470	4.000E-03	-7.14
471	3.600E-02	-6.18
410	2.900E+00	-4.13
500	2.200E+01	-3.02
140	1.870E+02	-2.51
130	3.000E-01	-5.43
180	1.500E+01	-3.37
492	1.000E+00	-4.79
580	9.000E-02	-6.02
730	2.060E-01	-5.21
732	2.500E+01	-3.58
992	4.320E+02	-2.14
967	1.370E+02	-3.14
963	1.370E+02	-2.64

H2O has been inserted as a COMPONENT

3	5	
2802810	0.0000	0.0000
4704710	0.0000	0.0000
7307320	0.0000	0.0000
1	-3.2100	0.0000
330	7.0000	0.0000
6	1	
3028100	4.0080	30.8450

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	1.000E-07	-7.000	0.000E+00
1	E-1	1.622E+03	3.210	0.000E+00
20	Ag+1	2.089E-05	-4.680	2.230E+00
30	Al+3	7.413E-06	-5.130	2.000E-01
150	Ca+2	1.202E-03	-2.920	4.800E+01
280	Fe+2	1.778E-06	-5.750	1.000E-01
281	Fe+3	1.778E-06	-5.750	1.000E-01
460	Mg+2	5.754E-03	-2.240	1.400E+02

470	Mn+2	7.244E-08	-7.140	4.000E-03
471	Mn+3	6.607E-07	-6.180	3.600E-02
410	K+1	7.413E-05	-4.130	2.900E+00
500	Na+1	9.550E-04	-3.020	2.200E+01
140	CO3-2	3.090E-03	-2.510	1.870E+02
130	Br-1	3.715E-06	-5.430	3.000E-01
180	Cl-1	4.266E-04	-3.370	1.500E+01
492	NO3-1	1.622E-05	-4.790	1.000E+00
580	PO4-3	9.550E-07	-6.020	9.000E-02
730	HS-1	6.166E-06	-5.210	2.060E-01
732	SO4-2	2.630E-04	-3.580	2.500E+01
992	Acetate	7.244E-03	-2.140	4.320E+02
967	Citrate	7.244E-04	-3.140	1.370E+02
963	EtDiAm	2.291E-03	-2.640	1.370E+02
2	H2O	1.000E+00	0.000	0.000E+00

Charge Balance: UNSPECIATED

Sum of CATIONS= 1.502E-02 Sum of ANIONS = 1.671E-02

PERCENT DIFFERENCE = 5.345E+00 (ANIONS - CATIONS)/(ANIONS + CATIONS)

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:

Al+3	Log activity guess:	-9.71
Fe+2	Log activity guess:	-5.45
Fe+3	Log activity guess:	-21.97
Mn+2	Log activity guess:	-6.14
Mn+3	Log activity guess:	-35.42
CO3-2	Log activity guess:	-6.04
PO4-3	Log activity guess:	-11.92
HS-1	Log activity guess:	-6.83
SO4-2	Log activity guess:	-3.57

CONSTRAINTS ON COMPONENT ACTIVITIES

As specified, this chemical system is OPEN with respect to the following components:

H2O H+1 E-1

Activities of the following components are constrained by the species shown:

COMPONENT	SPECIES	TYPE
HS-1	HS-/SO4-2	3
Mn+2	Mn+2/Mn+3	3
Fe+2	Fe+2/Fe+3	3
E-1	E-1	3
H+1	H+1	3
H2O	H2O	3

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL mol/L	DIFF FXN	LOG ACTVTY	RESIDUAL
0	PO4-3	9.487E-07	1.401E-06	-11.92218	1.401E-06
1	PO4-3	9.487E-07	-4.418E-07	-12.23448	4.417E-07
2	PO4-3	9.487E-07	4.295E-07	-12.52920	4.294E-07
3	PO4-3	9.487E-07	-2.794E-07	-12.41112	2.793E-07
4	PO4-3	9.487E-07	-3.103E-08	-12.24860	3.094E-08
5	PO4-3	9.487E-07	-6.764E-10	-12.24089	5.815E-10
6	PO4-3	9.487E-07	2.732E-10	-12.24028	1.783E-10
7	PO4-3	9.487E-07	1.950E-10	-12.23991	1.001E-10
8	PO4-3	9.487E-07	1.117E-10	-12.23977	1.682E-11
9	Ag+1	2.070E-05	-1.869E-05	-12.27957	1.869E-05

ITERATIONS= 10: SOLID ACANTHITE PRECIPITATES

ITERATIONS= 10: SOLID DIASPORE PRECIPITATES

CONSTRAINTS ON COMPONENT ACTIVITIES

As specified, this chemical system is OPEN with respect to the following components:

H2O H+1 E-1

Activities of the following components are constrained by the species shown:

COMPONENT	SPECIES	TYPE
Al+3	DIASPORE	4
HS-1	ACANTHITE	4
SO4-2	HS-/SO4-2	3
Mn+2	Mn+2/Mn+3	3
Fe+3	Fe+2/Fe+3	3
E-1	E-1	3
H+1	H+1	3
H2O	H2O	3

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL mol/L	DIFF FXN	LOG ACTVTY	RESIDUAL
10	Cl-1	4.236E-04	-5.532E-05	-3.43384	5.528E-05
11	Cl-1	4.236E-04	3.154E-04	-3.19082	3.153E-04
12	Cl-1	4.236E-04	1.989E-04	-3.26661	1.988E-04
13	Cl-1	4.236E-04	8.196E-05	-3.35700	8.191E-05
14	Cl-1	4.236E-04	2.480E-06	-3.43090	2.438E-06
15	Cl-1	4.236E-04	-4.881E-08	-3.43343	6.448E-09
16	Na+1	9.580E-04	-5.601E-07	-3.08100	4.643E-07
17	Cl-1	4.236E-04	4.380E-08	-3.43338	1.435E-09
18	Cl-1	4.236E-04	4.145E-06	-3.43342	4.103E-06
19	Cl-1	4.236E-04	-1.931E-06	-3.43765	1.888E-06
20	Cl-1	4.236E-04	-1.109E-06	-3.43567	1.066E-06
21	Cl-1	4.236E-04	-4.608E-07	-3.43453	4.185E-07
22	Cl-1	4.236E-04	-1.715E-07	-3.43406	1.291E-07
***	Temporarily holding ionic strength constant				
23	Mn+3	7.289E-07	-2.155E-10	-35.73196	1.426E-10
***	Releasing temporary hold on ionic strength				

ITERATIONS= 25: SOLID PYRITE PRECIPITATES

CONSTRAINTS ON COMPONENT ACTIVITIES

As specified, this chemical system is OPEN with respect to the following components:

H2O H+1 E-1

Activities of the following components are constrained by the species shown:

COMPONENT	SPECIES	TYPE
Fe+2	PYRITE	4
Al+3	DIASPORE	4
HS-1	ACANTHITE	4
SO4-2	HS-/SO4-2	3
Mn+2	Mn+2/Mn+3	3
Fe+3	Fe+2/Fe+3	3
E-1	E-1	3
H+1	H+1	3
H2O	H2O	3

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL mol/L	DIFF FXN	LOG ACTVTY	RESIDUAL
25	Br-1	3.759E-06	-4.909E-07	-5.48573	4.905E-07
26	Br-1	3.759E-06	5.500E-07	-5.42495	5.495E-07
27	Br-1	3.759E-06	1.267E-08	-5.48425	1.229E-08
28	Mn+3	7.289E-07	-7.560E-11	-35.73170	2.709E-12

ID No	Name	Total Conc(M)	Conc (M)	log Activity	Diff fxn
180	Cl-1	4.236E-04	4.236E-04	-3.43382	-2.316E-10
992	Acetate	7.325E-03	6.887E-03	-2.22273	-3.984E-09
20	Ag+1	2.070E-05	2.000E-19	-18.75968	-3.617E-09
492	NO3-1	1.615E-05	1.612E-05	-4.85352	-8.830E-12
150	Ca+2	1.199E-03	9.758E-04	-3.25366	-2.133E-09
967	Citrate	7.253E-04	9.452E-06	-5.57133	-3.625E-10
580	PO4-3	9.487E-07	2.030E-12	-12.23939	-8.472E-13
460	Mg+2	5.767E-03	4.727E-03	-2.56842	-1.039E-08
963	EtDiAm	2.282E-03	3.406E-07	-6.46563	-3.810E-09
471	Mn+3	6.560E-07	6.534E-36	-35.73169	-1.363E-12
410	K+1	7.426E-05	7.398E-05	-4.19165	-4.007E-11
500	Na+1	9.580E-04	9.535E-04	-3.08143	-5.169E-10
140	CO3-2	3.120E-03	1.373E-06	-6.10537	-1.385E-09
130	Br-1	3.759E-06	3.759E-06	-5.48571	-2.056E-12
2	H2O	4.913E-20	3.079E-05	-0.00016	0.000E+00
330	H+1	-7.115E-20	1.150E-07	-7.00000	0.000E+00
1	E-1	1.855E-19	-8.668E-05	3.21000	0.000E+00
281	Fe+3	1.793E-06	1.106E-28	-28.50299	0.000E+00
470	Mn+2	7.289E-08	6.235E-07	-6.44818	0.000E+00
732	SO4-2	2.605E-04	1.882E-04	-3.96845	0.000E+00
730	HS-1	6.236E-06	6.864E-08	-7.22416	0.000E+00
30	Al+3	7.421E-06	1.294E-13	-13.43503	0.000E+00
280	Fe+2	1.793E-06	1.856E-12	-11.97440	0.000E+00

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
330	H+1	1.150E-07	-7.00000	1.00	0.86944	0.061
963	EtDiAm	3.406E-07	-6.46563	0.00	1.00493	-0.002
20	Ag+1	2.000E-19	-18.75968	1.00	0.86944	0.061
30	Al+3	1.294E-13	-13.43503	3.00	0.28390	0.547
150	Ca+2	9.758E-04	-3.25366	2.00	0.57143	0.243
280	Fe+2	1.856E-12	-11.97440	2.00	0.57143	0.243
281	Fe+3	1.106E-28	-28.50299	3.00	0.28390	0.547
460	Mg+2	4.727E-03	-2.56842	2.00	0.57143	0.243
470	Mn+2	6.235E-07	-6.44818	2.00	0.57143	0.243
471	Mn+3	6.534E-36	-35.73169	3.00	0.28390	0.547
410	K+1	7.398E-05	-4.19165	1.00	0.86944	0.061
500	Na+1	9.535E-04	-3.08143	1.00	0.86944	0.061
140	CO3-2	1.373E-06	-6.10537	-2.00	0.57143	0.243
130	Br-1	3.759E-06	-5.48571	-1.00	0.86944	0.061
180	Cl-1	4.236E-04	-3.43382	-1.00	0.86944	0.061
492	NO3-1	1.612E-05	-4.85352	-1.00	0.86944	0.061
580	PO4-3	2.030E-12	-12.23939	-3.00	0.28390	0.547
730	HS-1	6.864E-08	-7.22416	-1.00	0.86944	0.061
732	SO4-2	1.882E-04	-3.96845	-2.00	0.57143	0.243
992	Acetate	6.887E-03	-2.22273	-1.00	0.86944	0.061
967	Citrate	9.452E-06	-5.57133	-3.00	0.28390	0.547

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
1509920	Ca[Acetate]	5.464E-05	-4.32324	1.00	0.86944	1.214
5009920	Na[Acetate]	2.711E-06	-5.56470	0.00	1.00493	-0.263
4109921	K[Acetate]	2.290E-07	-6.63796	0.00	1.00493	-0.226
3307301	S-2	2.440E-18	-17.85572	-2.00	0.57143	-17.389
3300020	OH-	4.887E-08	-7.37174	-1.00	0.86944	-14.311
303300	AlOH+2	3.090E-12	-11.75308	2.00	0.57143	-5.075
303301	Al(OH)2+	3.399E-10	-9.52936	1.00	0.86944	-10.033
303303	Al(OH)3 (aq)	5.907E-10	-9.22653	0.00	1.00493	-16.793
303302	Al(OH)4-	5.948E-10	-9.28640	-1.00	0.86944	-23.790
203300	AgOH (aq)	1.742E-24	-23.75684	0.00	1.00493	-11.999
203301	Ag(OH)2-	1.980E-29	-28.76401	-1.00	0.86944	-23.943
2803300	FeOH+	2.064E-15	-14.74614	1.00	0.86944	-9.711
2803302	Fe(OH)2 (aq)	5.325E-20	-19.27157	0.00	1.00493	-21.299
2803301	Fe(OH)3-	1.763E-21	-20.81444	-1.00	0.86944	-29.779
2813300	FeOH+2	1.872E-24	-23.97076	2.00	0.57143	-2.225
2813301	Fe(OH)2+	9.193E-20	-19.09731	1.00	0.86944	-4.533
2813302	Fe(OH)3 (aq)	1.729E-21	-20.76014	0.00	1.00493	-13.259
2813303	Fe(OH)4-	9.314E-23	-22.09164	-1.00	0.86944	-21.527
2813304	Fe2(OH)2+4	5.310E-46	-46.24702	4.00	0.10662	-2.269
2813305	Fe3(OH)4+5	1.921E-63	-64.23547	5.00	0.03027	-5.207
4703300	MnOH+	4.374E-11	-10.41992	1.00	0.86944	-10.911
4703301	Mn(OH)3-	6.488E-21	-20.24867	-1.00	0.86944	-34.739
4703302	Mn(OH)4-2	3.208E-27	-26.73684	-2.00	0.57143	-48.045
4700020	MnO4-	1.762-100	-99.81473	-1.00	0.86944	-133.255
4700021	MnO4-2	5.755E-87	-86.48302	-2.00	0.57143	-122.951
4603300	MgOH+	1.890E-08	-7.78430	1.00	0.86944	-12.155
1503300	CaOH+	4.783E-10	-9.38110	1.00	0.86944	-13.067
201800	AgCl (aq)	1.566E-19	-18.80296	0.00	1.00493	3.388
201801	AgCl2-	6.178E-21	-20.26994	-1.00	0.86944	5.418
201802	AgCl3-2	2.409E-24	-23.86115	-2.00	0.57143	5.443
201803	AgCl4-3	3.646E-27	-26.98497	-3.00	0.28390	6.057
2811800	FeCl+2	4.284E-31	-30.61117	2.00	0.57143	1.569
2811801	FeCl2+	6.609E-34	-33.24063	1.00	0.86944	2.191
2811802	FeCl3 (aq)	2.106E-38	-37.67445	0.00	1.00493	1.128
4701800	MnCl+	1.900E-10	-9.78200	1.00	0.86944	0.161
4701801	MnCl2 (aq)	8.552E-14	-13.06582	0.00	1.00493	0.248
4701802	MnCl3-	1.003E-17	-17.05965	-1.00	0.86944	-0.249
201300	AgBr (aq)	2.252E-20	-19.64539	0.00	1.00493	4.598
201301	AgBr2-	6.756E-23	-22.23109	-1.00	0.86944	7.561
201302	AgBr3-2	1.337E-27	-27.11680	-2.00	0.57143	8.343
3307300	H2S (aq)	7.485E-08	-7.12365	0.00	1.00493	7.098
207300	AgHS (aq)	6.738E-13	-12.16934	0.00	1.00493	13.812
207301	Ag(HS)2-	5.851E-16	-15.29351	-1.00	0.86944	17.975
2807300	Fe(HS)2 (aq)	3.351E-18	-17.47273	0.00	1.00493	8.948
2807301	Fe(HS)3-	2.517E-23	-22.65990	-1.00	0.86944	11.048
3307320	HSO4-	8.894E-10	-9.11167	-1.00	0.86944	1.918
307320	AlSO4+	2.287E-14	-13.70141	1.00	0.86944	3.763
307321	Al(SO4)2-	3.380E-17	-16.53181	-1.00	0.86944	4.901
207320	AgSO4-	3.900E-22	-21.46974	-1.00	0.86944	1.319
2807320	FeSO4 (aq)	2.462E-14	-13.60655	0.00	1.00493	2.334
2817320	FeSO4+	2.962E-29	-28.58923	1.00	0.86944	3.943
2817321	Fe(SO4)2-	7.447E-32	-31.18875	-1.00	0.86944	5.312
4707320	MnSO4 (aq)	5.927E-09	-8.22502	0.00	1.00493	2.189
4607320	MgSO4 (aq)	4.809E-05	-4.31580	0.00	1.00493	2.219
1507320	CaSO4 (aq)	1.225E-05	-4.90976	0.00	1.00493	2.310
5007320	NaSO4-	5.422E-07	-6.32659	-1.00	0.86944	0.784
4107320	KSO4-	4.580E-08	-7.39992	-1.00	0.86944	0.821
204920	AgNO3 (aq)	1.358E-24	-23.86488	0.00	1.00493	-0.254
2814921	FeNO3+2	1.364E-32	-32.10818	2.00	0.57143	1.491
4704921	MnNO3+	9.100E-12	-11.10170	1.00	0.86944	0.261
4704920	Mn(NO3)2 (aq)	2.843E-16	-15.54410	0.00	1.00493	0.609
1504921	CaNO3+	3.089E-08	-7.57093	1.00	0.86944	0.597
3305800	HPO4-2	3.015E-07	-6.76371	-2.00	0.57143	12.719
3305801	H2PO4-	3.275E-07	-6.54558	-1.00	0.86944	19.755
3305802	H3PO4	3.526E-12	-11.45060	0.00	1.00493	21.787
2805800	FeH2PO4+	1.318E-16	-15.94079	1.00	0.86944	22.334
2805801	FeHPO4 (aq)	5.742E-16	-15.23879	0.00	1.00493	15.973
2815801	FeH2PO4+2	2.250E-31	-30.89087	2.00	0.57143	24.095
2815800	FeHPO4+	6.537E-26	-25.24538	1.00	0.86944	22.558
4605800	MgPO4-	6.606E-11	-10.24085	-1.00	0.86944	4.628
4605801	MgH2PO4+	3.471E-08	-7.52025	1.00	0.86944	21.348

4605802	MgHPO4 (aq)	2.428E-07	-6.61267	0.00	1.00493	15.193
1505800	CaHPO4 (aq)	3.630E-08	-7.43791	0.00	1.00493	15.053
1505801	CaPO4-	8.723E-10	-9.12010	-1.00	0.86944	6.434
1505802	CaH2PO4+	3.396E-09	-8.52977	1.00	0.86944	21.024
5005800	NaHPO4-	1.531E-09	-8.87581	-1.00	0.86944	13.506
4105800	KHPO4-	7.669E-11	-10.17604	-1.00	0.86944	13.316
3301400	HCO3-	2.490E-03	-2.66450	-1.00	0.86944	10.502
3301401	H2CO3 (aq)	5.407E-04	-3.26491	0.00	1.00493	16.838
2801400	FeHCO3+	2.570E-14	-13.65077	1.00	0.86944	11.490
4701400	MnHCO3+	1.612E-08	-7.85341	1.00	0.86944	11.761
4601400	MgCO3 (aq)	1.700E-06	-5.76750	0.00	1.00493	2.904
4601401	MgHCO3+	7.363E-05	-4.19373	1.00	0.86944	11.541
1501400	CaHCO3+	1.027E-05	-5.04906	1.00	0.86944	11.371
1501401	CaCO3 (aq)	5.036E-07	-6.29581	0.00	1.00493	3.061
5001400	NaCO3-	1.908E-08	-7.78022	-1.00	0.86944	1.467
5001401	NaHCO3 (aq)	1.203E-06	-5.91766	0.00	1.00493	10.267
3309631	H[Ethylenediamine]	7.199E-04	-3.20347	1.00	0.86944	10.323
3309632	H2[Ethylenediamine]	1.562E-03	-3.04938	2.00	0.57143	17.659
209631	Ag[Ethylenediamine]	5.808E-21	-20.29676	1.00	0.86944	4.989
209632	Ag[Ethylenediamine]2	1.663E-24	-23.83993	1.00	0.86944	7.912
209633	AgH[Ethylenediamine]	3.260E-20	-19.72985	2.00	0.57143	12.738
209634	Ag2[Ethylenediamine]	5.729E-38	-37.48499	2.00	0.57143	6.743
209635	Ag2[Ethylenediamine]2	1.393E-37	-37.09914	2.00	0.57143	13.595
209636	Ag[HEthylenediamine]2	7.311E-21	-20.68283	3.00	0.28390	25.555
209637	AgH[Ethylenediamine]2	1.872E-30	-29.97082	2.00	0.57143	8.963
2809631	Fe[Ethylenediamine]	1.156E-14	-14.18003	2.00	0.57143	4.503
2809632	Fe[Ethylenediamine]2	1.168E-17	-17.17567	2.00	0.57143	7.973
2809633	Fe[Ethylenediamine]3	1.101E-21	-21.20130	2.00	0.57143	10.413
4709631	Mn[Ethylenediamine]	1.406E-10	-10.09518	2.00	0.57143	3.062
4709632	Mn[Ethylenediamine]2	6.793E-15	-14.41096	2.00	0.57143	5.212
4609631	Mg[Ethylenediamine]	3.793E-09	-8.66405	2.00	0.57143	0.613
1509631	Ca[Ethylenediamine]	4.303E-10	-9.60929	2.00	0.57143	0.353
3309671	H[Citrate]	1.110E-06	-6.19780	-2.00	0.57143	6.617
3309672	H2[Citrate]	4.342E-09	-8.42304	-1.00	0.86944	11.209
3309673	H3[Citrate]	5.371E-13	-12.26780	0.00	1.00493	14.301
309671	Al[Citrate]	9.152E-10	-9.03637	0.00	1.00493	9.968
309672	Al[Citrate]2	5.877E-10	-9.77770	-3.00	0.28390	15.347
309673	AlH[Citrate]	8.024E-14	-13.15637	1.00	0.86944	12.911
2809671	Fe[Citrate]	4.121E-12	-11.44573	-1.00	0.86944	6.161
2809672	FeH[Citrate]	4.489E-15	-14.34573	0.00	1.00493	10.198
2819671	Fe[Citrate]	1.056E-21	-20.97432	0.00	1.00493	13.098
2819672	FeH[Citrate]	2.435E-27	-26.67432	1.00	0.86944	14.461
4709671	Mn[Citrate]	2.095E-08	-7.73951	-1.00	0.86944	4.341
4709672	MnH[Citrate]	3.788E-10	-9.41951	0.00	1.00493	9.598
1509671	Ca[Citrate]	1.452E-04	-3.89883	-1.00	0.86944	4.987
1509672	CaH[Citrate]	2.745E-07	-6.55938	0.00	1.00493	9.263
1509673	CaH2[Citrate]	3.110E-11	-10.56799	1.00	0.86944	12.318
4609671	Mg[Citrate]	5.687E-04	-3.30591	-1.00	0.86944	4.895
4609672	MgH[Citrate]	5.567E-07	-6.25221	0.00	1.00493	8.885
4609673	MgH2[Citrate]	1.321E-10	-9.93975	1.00	0.86944	12.261
5009671	Na[Citrate]	4.356E-08	-7.60395	-2.00	0.57143	1.292
5009672	Na2[Citrate]	7.258E-11	-10.19993	-1.00	0.86944	1.595
5009673	NaH[Citrate]	7.623E-10	-9.17861	-1.00	0.86944	6.535
4109671	K[Citrate]	3.496E-09	-8.69949	-2.00	0.57143	1.307
3309921	H[Acetate]	3.384E-05	-4.46848	0.00	1.00493	4.752
209921	Ag[Acetate]	5.313E-21	-20.27255	0.00	1.00493	0.708
209922	Ag[Acetate]2	2.989E-23	-22.58528	-1.00	0.86944	0.681
2809920	Fe[Acetate]	1.835E-13	-12.79713	1.00	0.86944	1.461
2819920	Fe[Acetate]	3.473E-27	-26.70232	2.00	0.57143	4.266
2819921	Fe[Acetate]2	4.837E-26	-25.37615	1.00	0.86944	7.633
2819922	Fe[Acetate]3	2.591E-26	-25.58448	0.00	1.00493	9.585
4709920	Mn[Acetate]	6.164E-08	-7.27091	1.00	0.86944	1.461
4609920	Mg[Acetate]	3.464E-04	-3.52115	1.00	0.86944	1.331

Type III - SPECIES WITH FIXED ACTIVITY

ID No	Name	Conc (M)	New logK	Enthalpy
2	H2O	3.079E-05	0.000	0.000
330	H+1	-7.601E-03	7.000	0.000
1	E-1	-8.668E-05	-3.210	0.000

2802810	Fe+2/Fe+3	1.793E-06	13.319	-42.700
4704710	Mn+2/Mn+3	6.560E-07	26.074	-107.800
7307320	HS-/SO4-2	1.143E-05	34.064	-60.140

Type IV - FINITE SOLIDS (present at equilibrium)

ID No	Name	Conc (M)	New logK	Enthalpy
1002000	ACANTHITE	1.035E-05	37.744	-227.000
2003002	DIASPORE	7.418E-06	-7.565	103.052
1028003	PYRITE	3.585E-06	18.843	-49.844

Type V - UNDERSATURATED SOLIDS (not present at equilibrium)

ID No	Name	Conc (M)	New logK	Enthalpy
1028002	MACKINAWITE	2.520E-09	3.600	0.000
1047000	MnS (grn)	8.768E-08	-0.385	32.000
1047001	MnS (pnk)	9.720E-11	-3.340	0.000
2003000	Al(OH)3 (am)	1.046E-04	-11.545	111.000
2003001	BOEHMITE	1.573E-02	-9.368	117.696
1028001	GREIGITE	1.439E-25	45.035	0.000
2003003	GIBBSITE	4.298E-02	-8.931	95.395
2002000	Ag2O	3.984E-37	-12.880	45.620
2028000	WUSTITE	1.882E-10	-12.385	103.938
2028001	Fe(OH)2	2.892E-12	-13.564	0.000
2028100	FERRIHYDRITE	6.502E-12	-3.683	73.374
2028101	Fe3(OH)8	6.256E-34	-20.222	0.000
2028102	GOETHITE	3.973E-09	-0.898	60.584
2047000	PYROLUSITE	8.432E-29	-43.206	272.000
2047001	BIRNESSITE	9.268E-30	-18.091	0.000
2047002	NSUTITE	3.581E-29	-17.504	0.000
2047003	PYROCHROITE	5.086E-09	-15.845	97.010
2047100	MANGANITE	1.003E-14	-25.340	0.000
2046000	BRUCITE	6.640E-07	-17.609	113.996
2046001	PERICLASE	6.797E-12	-22.599	151.230
2046002	Mg(OH)2 (active)	4.338E-08	-18.794	0.000
2015000	LIME	5.565E-24	-34.001	193.910
2015001	PORTLANDITE	1.199E-13	-23.667	128.620
3003000	Al2O3	5.514E-07	-21.388	258.590
3028000	MAGNETITE	1.647E-18	-4.802	208.526
3028001	HERCYNITE	1.429E-08	-25.000	313.920
1028000	FeS (ppt)	4.760E-10	2.876	11.000
3028101	MAGHEMITE	4.051E-22	-6.386	0.000
3028102	LEPIDOCROCITE	1.336E-09	-1.371	0.000
3047000	HAUSMANNITE	2.395E-34	-63.856	421.000
3047100	BIXBYITE	2.214E-30	-0.191	124.490
3046000	SPINEL	1.286E-13	-39.452	388.012
3046001	MAGNESIOFERRITE	4.935E-23	-18.732	278.920
3050000	NATRON	3.043E-11	1.753	-65.877
4102000	CERARGYRITE	9.865E-13	10.188	-65.200
4128100	Fe(OH)2.7Cl.3	2.549E-08	3.040	0.000
4147000	MnCl2:4H2O	7.866E-17	-2.788	10.830
4150000	HALITE	8.074E-09	-1.578	-3.700
4002000	BROMYRITE	4.185E-12	12.867	-84.500
5002000	Ag2CO3	5.600E-33	11.373	-42.150
5028000	SIDERITE	1.129E-08	10.133	16.000
5047000	RHODOCHROSITE	1.032E-02	10.567	1.880
5046000	ARTINITE	2.238E-08	-10.407	120.257
5046001	HYDROMAGNESITE	1.085E-16	7.300	218.447
5046002	MAGNESITE	8.326E-02	7.594	-20.000
5046003	NESQUEHONITE	6.810E-05	4.507	24.221
5015000	ARAGONITE	7.634E-02	8.242	12.000
5015001	CALCITE	1.149E-01	8.419	8.000
5015002	DOLOMITE (ordered)	6.195E-02	16.825	39.500
5015004	DOLOMITE (disordered)	1.570E-02	16.229	46.400
5015003	HUNTITE	7.315E-07	29.245	107.780
5050001	THERMONATRITE	1.057E-13	-0.707	10.480
6003000	AlOHSO4	6.704E-08	3.230	0.000
6003001	Al4(OH)10SO4	3.888E-11	-22.700	0.000

6002000	Ag2SO4	2.794E-37	4.934	-17.000
6028000	MELANTERITE	2.527E-14	2.347	-20.500
6028100	Fe2(SO4)3	0.000E+00	2.110	242.028
6028101	H-JAROSITE	0.000E+00	10.551	230.748
6050000	Na-JAROSITE	0.000E+00	10.184	151.377
6041002	K-JAROSITE	0.000E+00	13.922	130.875
6047000	MnSO4	3.674E-14	-3.018	64.840
6047100	Mn2(SO4)3	0.000E+00	4.614	163.427
6046000	EPSOMITE	4.635E-05	2.204	-11.560
6015000	ANHYDRITE	1.229E-03	4.312	7.200
6015001	GYPSUM	2.479E-03	4.617	-1.000
6050001	MIRABILITE	3.268E-09	1.647	-79.442
6050002	THENARDITE	3.060E-11	-0.383	9.121
6041000	K-ALUM	6.415E-21	5.373	-30.209
6041001	ALUNITE	0.000E+00	-0.009	210.000
7002000	Ag3PO4	0.000E+00	17.590	0.000
7028001	VIVIANITE	3.951E-25	36.000	0.000
7028100	STRENGITE	3.931E-15	26.337	9.360
7047000	Mn3(PO4)2	1.157E-20	23.887	-8.870
7047001	MnHPO4	5.157E-01	25.400	0.000
7046002	Mg3(PO4)2	1.247E-09	23.280	0.000
7046001	MgHPO4:3H2O	2.327E-04	18.175	0.000
7015003	HYDROXYLAPATITE	2.220E-02	44.333	0.000
7015004	CaHPO4:2H2O	4.529E-04	19.149	-23.000
7015005	CaHPO4	9.773E-04	19.483	-31.000
7015006	Ca3(PO4)2 (beta)	1.103E-05	29.282	-54.000
7015007	Ca4H(PO4)3:3H2O	2.222E-10	47.080	0.000
73100	Sulfur	2.462E-05	2.036	16.300
2000	Ag metal	4.643E-02	14.217	-105.790

Type VI - EXCLUDED SPECIES (not included in mole balance)

ID No	Name	Conc (M)	New logK	Enthalpy
3028100	HEMATITE	6.230E-12	3.801	30.845
3300021	O2 (g)	0.000E+00	-86.926	571.660
3301404	CH4 (g)	2.219E-08	42.771	-257.133
3301403	CO2 (g)	1.172E-02	18.174	-4.060
3307302	H2S (g)	6.107E-07	8.010	0.000

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

Cl-1				
	100.0	Percent bound in species #	180	Cl-1
Acetate				
	94.0	Percent bound in species #	992	Acetate
	4.7	Percent bound in species #	4609920	Mg[Acetate]
Ag+1				
	99.9	Percent bound in species #	207300	AgHS (aq)
NO3-1				
	99.8	Percent bound in species #	492	NO3-1
Ca+2				
	81.4	Percent bound in species #	150	Ca+2
	4.6	Percent bound in species #	1509920	Ca[Acetate]
	1.0	Percent bound in species #	1507320	CaSO4 (aq)
	12.1	Percent bound in species #	1509671	Ca[Citrate]
Citrate				
	1.3	Percent bound in species #	967	Citrate
	20.0	Percent bound in species #	1509671	Ca[Citrate]
	78.4	Percent bound in species #	4609671	Mg[Citrate]
PO4-3				
	31.8	Percent bound in species #	3305800	HPO4-2
	34.5	Percent bound in species #	3305801	H2PO4-
	3.7	Percent bound in species #	4605801	MgH2PO4+
	25.6	Percent bound in species #	4605802	MgHPO4 (aq)
	3.8	Percent bound in species #	1505800	CaHPO4 (aq)
Mg+2				
	82.0	Percent bound in species #	460	Mg+2
	1.3	Percent bound in species #	4601401	MgHCO3+
	9.9	Percent bound in species #	4609671	Mg[Citrate]
	6.0	Percent bound in species #	4609920	Mg[Acetate]
EtDiAm				
	31.5	Percent bound in species #	3309631	H[Ethylenediamine]

	68.4	Percent bound in species #3309632	H2[Ethylenediamine]
Mn+3			
	100.0	Percent bound in species # 471	Mn+3
K+1			
	99.6	Percent bound in species # 410	K+1
Na+1			
	99.5	Percent bound in species # 500	Na+1
CO3-2			
	79.8	Percent bound in species #3301400	HCO3-
	17.3	Percent bound in species #3301401	H2CO3 (aq)
	2.4	Percent bound in species #4601401	MgHCO3+
Br-1			
	100.0	Percent bound in species # 130	Br-1
H2O			
	66.8	Percent bound in species #3300020	OH-
	2.4	Percent bound in species # 303303	Al(OH)3 (aq)
	3.3	Percent bound in species # 303302	Al(OH)4-
	25.8	Percent bound in species #4603300	MgOH+
H+1			
	33.0	Percent bound in species #3301400	HCO3-
	14.3	Percent bound in species #3301401	H2CO3 (aq)
	9.6	Percent bound in species #3309631	H[Ethylenediamine]
	41.4	Percent bound in species #3309632	H2[Ethylenediamine]
E-1			
	100.0	Percent bound in species #4700021	MnO4-2
Fe+3			
	97.0	Percent bound in species #2813301	Fe(OH)2+
	1.8	Percent bound in species #2813302	Fe(OH)3 (aq)
	1.1	Percent bound in species #2819671	Fe[Citrate]
Mn+2			
	85.5	Percent bound in species # 470	Mn+2
	2.2	Percent bound in species #4701400	MnHCO3+
	2.9	Percent bound in species #4709671	Mn[Citrate]
	8.5	Percent bound in species #4709920	Mn[Acetate]
SO4-2			
	75.5	Percent bound in species # 732	SO4-2

	19.3	Percent bound in species #4607320	MgSO4 (aq)
	4.9	Percent bound in species #1507320	CaSO4 (aq)
HS-1			
	47.8	Percent bound in species # 730	HS-1
	52.2	Percent bound in species #3307300	H2S (aq)
Al+3			
	11.2	Percent bound in species # 303301	Al(OH)2+
	19.5	Percent bound in species # 303303	Al(OH)3 (aq)
	19.6	Percent bound in species # 303302	Al(OH)4-
	30.2	Percent bound in species # 309671	Al[Citrate]
	19.4	Percent bound in species # 309672	Al[Citrate]2
Fe+2			
	29.8	Percent bound in species # 280	Fe+2
	66.1	Percent bound in species #2809671	Fe[Citrate]
	2.9	Percent bound in species #2809920	Fe[Acetate]

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
180	Cl-1	4.236E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
992	Acetate	7.325E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
20	Ag+1	6.744E-13	0.0	0.000E+00	0.0	2.069E-05	100.0
492	NO3-1	1.615E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
150	Ca+2	1.199E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
967	Citrate	7.253E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	9.487E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	5.767E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
963	EtDiAm	2.282E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
471	Mn+3	6.534E-36	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.426E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
500	Na+1	9.580E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	3.120E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
130	Br-1	3.759E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	7.312E-08	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	7.538E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
1	E-1	-2.302E-86	100.0	0.000E+00	0.0	0.000E+00	0.0
281	Fe+3	9.481E-20	100.0	0.000E+00	0.0	0.000E+00	0.0
470	Mn+2	7.289E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	2.491E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
730	HS-1	1.435E-07	0.8	0.000E+00	0.0	1.752E-05	99.2
30	Al+3	3.032E-09	0.0	0.000E+00	0.0	7.418E-06	100.0
280	Fe+2	6.230E-12	0.0	0.000E+00	0.0	3.585E-06	100.0

Charge Balance: SPECIATED

Sum of CATIONS = 1.676E-02 Sum of ANIONS 1.095E-02

PERCENT DIFFERENCE = 2.100E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 2.134E-02

EQUILIBRIUM pH = 7.000

EQUILIBRIUM pe = -3.210 or Eh = -182.88 mv

DATE ID NUMBER: 20000605
TIME ID NUMBER: 14063526

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
73100	Sulfur	-4.609	[1.000]730 [-1.000]330 [-2.000] 1
2000	Ag metal	-1.333	[1.000] 20 [1.000] 1
1002000	ACANTHITE	0.000	[2.000] 20 [-1.000]330 [1.000]730
1028000	FeS (ppt)	-9.322	[1.000]280 [1.000]730 [-1.000]330
1028001	GREIGITE	-24.842	[-4.000]330 [2.000]281 [1.000]280 [4.000]730
1028002	MACKINAWITE	-8.599	[1.000]280 [1.000]730 [-1.000]330
1028003	PYRITE	0.000	[-2.000]330 [-2.000] 1 [1.000]280 [2.000]730
1047000	MnS (grn)	-7.057	[1.000]470 [1.000]730 [-1.000]330
1047001	MnS (pnk)	-10.012	[1.000]470 [1.000]730 [-1.000]330
2003000	Al(OH)3 (am)	-3.981	[1.000] 30 [3.000] 2 [-3.000]330
2003001	BOEHMITE	-1.803	[-3.000]330 [1.000] 30 [2.000] 2
2003002	DIASPORE	0.000	[-3.000]330 [1.000] 30 [2.000] 2
2003003	GIBBSITE	-1.367	[1.000] 30 [3.000] 2 [-3.000]330
2002000	Ag2O	-36.400	[2.000] 20 [1.000] 2 [-2.000]330
2028000	WUSTITE	-9.725	[-2.000]330 [0.947]280 [1.000] 2
2028001	Fe(OH)2	-11.539	[1.000]280 [2.000] 2 [-2.000]330
2028100	FERRIHYDRITE	-11.187	[1.000]281 [3.000] 2 [-3.000]330
2028101	Fe3(OH)8	-33.204	[-8.000]330 [2.000]281 [1.000]280 [8.000] 2
2028102	GOETHITE	-8.401	[1.000]281 [2.000] 2 [-3.000]330
2047000	PYROLUSITE	-28.074	[1.000]470 [2.000] 2 [-4.000]330 [-2.000] 1
2047001	BIRNESSITE	-29.033	[-4.000]330 [-1.000] 1 [1.000]471 [2.000] 2
2047002	NSUTITE	-28.446	[-4.000]330 [-1.000] 1 [1.000]471 [2.000] 2
2047003	PYROCHROITE	-8.294	[1.000]470 [2.000] 2 [-2.000]330
2047100	MANGANITE	-13.999	[1.000]470 [2.000] 2 [-3.000]330 [-1.000] 1
2046000	BRUCITE	-6.178	[1.000]460 [2.000] 2 [-2.000]330
2046001	PERICLASE	-11.168	[-2.000]330 [1.000]460 [1.000] 2
2046002	Mg(OH)2 (active)	-7.363	[1.000]460 [2.000] 2 [-2.000]330
2015000	LIME	-23.255	[-2.000]330 [1.000]150 [1.000] 2
2015001	PORTLANDITE	-12.921	[1.000]150 [2.000] 2 [-2.000]330
3003000	Al2O3	-6.259	[2.000] 30 [3.000] 2 [-6.000]330
3028000	MAGNETITE	-17.783	[-8.000]330 [2.000]281 [1.000]280 [4.000] 2
3028001	HERCYNITE	-7.845	[-8.000]330 [1.000]280 [2.000] 30 [4.000] 2
3028100	HEMATITE	-14.454	[2.000]281 [3.000] 2 [-6.000]330
3028101	MAGHEMITE	-21.392	[-6.000]330 [2.000]281 [3.000] 2

ID No	Name	SI	Composition by stoich. of components
3028102	LEPIDOCROCITE	-8.874	[-3.000]330 [1.000]281 [2.000] 2
3047000	HAUSMANNITE	-33.621	[3.000]470 [4.000] 2 [-8.000]330 [-2.000] 1
3047100	BIXBYITE	-29.655	[-6.000]330 [2.000]471 [3.000] 2
3046000	SPINEL	-12.891	[-8.000]330 [1.000]460 [2.000] 30 [4.000] 2
3046001	MAGNESIOFERRITE	-22.307	[-8.000]330 [1.000]460 [2.000]281 [4.000] 2
3050000	NATRON	-10.517	[2.000]500 [1.000]140 [10.000] 2
4102000	CERARGYRITE	-12.006	[1.000] 20 [1.000]180
4128100	Fe(OH)2.7Cl.3	-7.594	[-2.700]330 [1.000]281 [2.700] 2 [0.300]180
4147000	MnCl2:4H2O	-16.104	[1.000]470 [2.000]180 [4.000] 2
4150000	HALITE	-8.093	[1.000]500 [1.000]180
4002000	BROMYRITE	-11.378	[1.000] 20 [1.000]130
5002000	Ag2CO3	-32.252	[2.000] 20 [1.000]140
5028000	SIDERITE	-7.947	[1.000]280 [1.000]140
5047000	RHODOCHROSITE	-1.986	[1.000]470 [1.000]140
5046000	ARTINITE	-7.650	[-2.000]330 [2.000]460 [1.000]140 [5.000] 2
5046001	HYDROMAGNESITE	-15.965	[5.000]460 [4.000]140 [-2.000]330 [6.000] 2
5046002	MAGNESITE	-1.080	[1.000]460 [1.000]140
5046003	NESQUEHONITE	-4.167	[1.000]460 [1.000]140 [3.000] 2
5015000	ARAGONITE	-1.117	[1.000]150 [1.000]140
5015001	CALCITE	-0.940	[1.000]150 [1.000]140
5015002	DOLOMITE (ordered)	-1.208	[1.000]150 [1.000]460 [2.000]140
5015004	DOLOMITE (disordered)	-1.804	[1.000]150 [1.000]460 [2.000]140
5015003	HUNTITE	-6.136	[3.000]460 [1.000]150 [4.000]140
5050001	THERMONATRITE	-12.976	[2.000]500 [1.000]140 [1.000] 2
6003000	AlOHSO4	-7.174	[-1.000]330 [1.000] 30 [1.000]732 [1.000] 2
6003001	Al4(OH)10SO4	-10.410	[-10.000]330 [4.000] 30 [1.000]732 [10.000] 2
6002000	Ag2SO4	-36.554	[2.000] 20 [1.000]732
6028000	MELANTERITE	-13.597	[1.000]280 [1.000]732 [7.000] 2
6028100	Fe2(SO4)3	-66.801	[2.000]281 [3.000]732
6028101	H-JAROSITE	-47.896	[-5.000]330 [3.000]281 [2.000]732 [7.000] 2
6050000	Na-JAROSITE	-44.344	[-6.000]330 [1.000]500 [3.000]281 [2.000]732 [6.000] 2
6041002	K-JAROSITE	-41.717	[-6.000]330 [1.000]410 [3.000]281 [2.000]732 [6.000] 2
6047000	MnSO4	-13.435	[1.000]470 [1.000]732
6047100	Mn2(SO4)3	-78.755	[2.000]471 [3.000]732
6046000	EPSOMITE	-4.334	[1.000]460 [1.000]732 [7.000] 2
6015000	ANHYDRITE	-2.910	[1.000]150 [1.000]732
6015001	GYPSUM	-2.606	[1.000]150 [1.000]732 [2.000] 2
6050001	MIRABILITE	-8.486	[2.000]500 [1.000]732 [10.000] 2
6050002	THENARDITE	-10.514	[2.000]500 [1.000]732
6041000	K-ALUM	-20.193	[1.000]410 [1.000] 30 [2.000]732 [12.000] 2

ID No	Name	SI	Composition by stoich. of components
6041001	ALUNITE	-52.444	[1.000]410 [3.000] 30 [2.000]732 [6.000] 2
7002000	Ag3PO4	-50.928	[3.000] 20 [1.000]580
7028001	VIVIANITE	-24.403	[3.000]280 [2.000]580 [8.000] 2
7028100	STRENGITE	-14.406	[1.000]281 [1.000]580 [2.000] 2
7047000	Mn3(PO4)2	-19.937	[3.000]470 [2.000]580
7047001	MnHPO4	-0.288	[1.000]470 [1.000]580 [1.000]330
7046002	Mg3(PO4)2	-8.904	[3.000]460 [2.000]580
7046001	MgHPO4:3H2O	-3.633	[1.000]460 [1.000]330 [1.000]580 [3.000] 2
7015003	HYDROXYLAPATITE	-1.654	[5.000]150 [3.000]580 [1.000] 2 [-1.000]330
7015004	CaHPO4:2H2O	-3.344	[1.000]150 [1.000]330 [1.000]580 [2.000] 2
7015005	CaHPO4	-3.010	[1.000]150 [1.000]330 [1.000]580
7015006	Ca3(PO4)2 (beta)	-4.957	[3.000]150 [2.000]580
7015007	Ca4H(PO4)3:3H2O	-9.653	[4.000]150 [1.000]330 [3.000]580 [3.000] 2

Test3.out
MINTEQA2, v4.02
Original database
As distributed by EPA

PART 1 of OUTPUT FILE
MINTEQA2 v4.02 DATE OF CALCULATIONS: 5-JUN-2000 TIME: 14: 6:46

TEST3 - Metal activities controlled by solid phases.
Illustrates the defining of species not in the database.
Component file (COMP.DBS): comp.dbs COMP v4.00 09/30/1999
Thermodynamic file (THERMO.UNF): thermo.unf THERMO V4.00 09/30/1999
Gaussian DOM file (GAUSSIAN.DBS): gaussian.dbsGAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF): type6.unf TYPE6 V4.00 09/30/1999

Temperature (Celsius): 25.00
Units of concentration: MOLAL
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed only for those solids specified as ALLOWED
in the input file (if any).
Maximum iterations: 200
The method used to compute activity coefficients is: Davies equation
Full output file

```
    330  1.585E-08   -7.80
      1  6.310E-06   -5.20
    460  1.260E-03   -2.90
    500  1.000E-03   -3.00
    410  1.000E-03   -3.00
    180  1.590E-03   -2.80
    732  1.260E-03   -2.90
    492  1.000E-03   -3.00
    140  0.000E+00   -6.00
    280  0.000E+00  -12.00
    470  0.000E+00  -12.00
    230  0.000E+00   -9.00
    281  0.000E+00  -16.00
    471  0.000E+00  -16.00
    231  0.000E+00   -7.00
     30  0.000E+00  -16.00
    770  0.000E+00   -7.00
    150  0.000E+00   -6.00
    950  0.000E+00  -10.00
    580  0.000E+00  -12.00

 H2O has been inserted as a COMPONENT
  3  11
3301403    21.6600    -0.5300
2802810     0.0000     0.0000
4704710     0.0000     0.0000
2302310     0.0000     0.0000
8603001    -5.7260    35.2800
2077002     4.0060    -6.2200
2028100    -4.8910     0.0000
5015001     8.4750     2.5850
2095000   -12.4500     0.0000
      1     5.2000     0.0000
    330     7.8000     0.0000
  3   3
9947101 MnPO4,1.5H2O     0.0000   34.7800   0.000   0.000 0.00 0.00 0.00 176.9320
0.00 3   1.000 580   1.000 471   1.500   2   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
9915002 b-Ca3(PO4)2      0.0000   28.9260   0.000   0.000 0.00 0.00 0.00 310.1830
0.00 2   2.000 580   3.000 150   0.000   0   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
9923103 Cu(OH)2          0.0000   -2.8000   0.000   0.000 0.00 0.00 0.00  97.5320
0.00 3   2.000   2   1.000 231  -2.000 330   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
```

0.000 0 0.000 0 0.000 0

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	1.585E-08	-7.800	1.585E-08
1	E-1	6.310E-06	-5.200	6.310E-06
460	Mg+2	1.259E-03	-2.900	1.260E-03
500	Na+1	1.000E-03	-3.000	1.000E-03
410	K+1	1.000E-03	-3.000	1.000E-03
180	Cl-1	1.585E-03	-2.800	1.590E-03
732	SO4-2	1.259E-03	-2.900	1.260E-03
492	NO3-1	1.000E-03	-3.000	1.000E-03
140	CO3-2	1.000E-06	-6.000	0.000E+00
280	Fe+2	1.000E-12	-12.000	0.000E+00
470	Mn+2	1.000E-12	-12.000	0.000E+00
230	Cu+1	1.000E-09	-9.000	0.000E+00
281	Fe+3	1.000E-16	-16.000	0.000E+00
471	Mn+3	1.000E-16	-16.000	0.000E+00
231	Cu+2	1.000E-07	-7.000	0.000E+00
30	Al+3	1.000E-16	-16.000	0.000E+00
770	H4SiO4	1.000E-07	-7.000	0.000E+00
150	Ca+2	1.000E-06	-6.000	0.000E+00
950	Zn+2	1.000E-10	-10.000	0.000E+00
580	PO4-3	1.000E-12	-12.000	0.000E+00
2	H2O	1.000E+00	0.000	0.000E+00

ALL SPECIES CONSIDERED IN THIS PROBLEM

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID No	Name	Enthalpy	logK	Min logK	Max logK	Charge	DHa	DHb	gfw
330	H+1	0.0000	0.0000	0.000	0.000	1.00	9.00	0.00	1.0079
	Source of log K:								
580	PO4-3	0.0000	0.0000	0.000	0.000	-3.00	5.00	0.00	94.9714
	Source of log K:								
460	Mg+2	0.0000	0.0000	0.000	0.000	2.00	6.50	0.20	24.3050
	Source of log K:								
500	Na+1	0.0000	0.0000	0.000	0.000	1.00	4.00	0.08	22.9898
	Source of log K:								
410	K+1	0.0000	0.0000	0.000	0.000	1.00	3.00	0.01	39.0983
	Source of log K:								
180	Cl-1	0.0000	0.0000	0.000	0.000	-1.00	3.00	0.01	35.4530
	Source of log K:								
732	SO4-2	0.0000	0.0000	0.000	0.000	-2.00	4.00	-0.04	96.0630
	Source of log K:								
492	NO3-1	0.0000	0.0000	0.000	0.000	-1.00	3.00	0.00	62.0049
	Source of log K:								
140	CO3-2	0.0000	0.0000	0.000	0.000	-2.00	5.40	0.00	60.0094
	Source of log K:								
280	Fe+2	0.0000	0.0000	0.000	0.000	2.00	6.00	0.00	55.8470
	Source of log K:								
470	Mn+2	0.0000	0.0000	0.000	0.000	2.00	6.00	0.00	54.9380
	Source of log K:								
230	Cu+1	0.0000	0.0000	0.000	0.000	1.00	2.50	0.00	63.5460
	Source of log K:								
281	Fe+3	0.0000	0.0000	0.000	0.000	3.00	9.00	0.00	55.8470
	Source of log K:								
471	Mn+3	0.0000	0.0000	0.000	0.000	3.00	9.00	0.00	54.9380
	Source of log K:								
231	Cu+2	0.0000	0.0000	0.000	0.000	2.00	6.00	0.00	63.5460
	Source of log K:								
30	Al+3	0.0000	0.0000	0.000	0.000	3.00	9.00	0.00	26.9815
	Source of log K:								
770	H4SiO4	0.0000	0.0000	0.000	0.000	0.00	0.00	0.00	96.1149
	Source of log K:								
150	Ca+2	0.0000	0.0000	0.000	0.000	2.00	6.00	0.17	40.0780
	Source of log K:								
950	Zn+2	0.0000	0.0000	0.000	0.000	2.00	6.00	0.00	65.3900
	Source of log K:								

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID No	Name	Enthalpy	logK	Min logK	Max logK	Charge	DHa	DHb	gfw
5001401	NaHCO3 (aq)	-28.3301	10.0790	0.000	0.000	0.00	0.00	0.00	84.0069
Source of log K: NIST46.3			NIST2.1.1						
3307701	H2SiO4-2	61.0000	-23.0400	0.000	0.000	-2.00	5.40	0.00	94.0991
Source of log K: NIST46.4			NIST46.4						
3307700	H3SiO4-	20.0000	-9.8400	0.000	0.000	-1.00	4.00	0.00	95.1070
Source of log K: NIST46.4			NIST46.4						
3300020	OH-	55.8100	-13.9970	0.000	0.000	-1.00	3.50	0.00	17.0074
Source of log K: NIST46.4			NIST46.4						
303300	AlOH+2	47.8100	-4.9970	0.000	0.000	2.00	5.40	0.00	43.9889
Source of log K: NIST46.3			NIST46.3						
303301	Al(OH)2+	0.0000	-10.0940	0.000	0.000	1.00	5.40	0.00	60.9963
Source of log K: NIST46.3			MTQ3.11						
303303	Al(OH)3 (aq)	0.0000	-16.7910	0.000	0.000	0.00	0.00	0.00	78.0037
Source of log K: NIST46.3			MTQ3.11						
303302	Al(OH)4-	173.2400	-22.6880	0.000	0.000	-1.00	4.50	0.00	95.0111
Source of log K: NIST46.3			NIST46.3						
9503300	ZnOH+	55.8100	-8.9970	0.000	0.000	1.00	0.00	0.00	82.3974
Source of log K: NIST46.3			NIST46.3						
9503301	Zn(OH)2 (aq)	0.0000	-17.7940	0.000	0.000	0.00	0.00	0.00	99.4048
Source of log K: NIST46.3			MTQ3.11						
9503302	Zn(OH)3-	0.0000	-28.0910	0.000	0.000	-1.00	0.00	0.00	116.4122
Source of log K: NIST46.3			MTQ3.11						
9503303	Zn(OH)4-2	0.0000	-40.4880	0.000	0.000	-2.00	0.00	0.00	133.4196
Source of log K: NIST46.3			MTQ3.11						
2313300	CuOH+	35.8100	-7.4970	0.000	0.000	1.00	4.00	0.00	80.5534
Source of log K: NIST46.3			NIST46.3						
2313301	Cu(OH)2 (aq)	0.0000	-16.1940	0.000	0.000	0.00	0.00	0.00	97.5608
Source of log K: NIST46.3			MTQ3.11						
2313302	Cu(OH)3-	0.0000	-26.8790	0.000	0.000	-1.00	0.00	0.00	114.5682
Source of log K: NIST46.3			MTQ3.11						
2313303	Cu(OH)4-2	0.0000	-39.9800	0.000	0.000	-2.00	0.00	0.00	131.5756
Source of log K: NIST46.3			MTQ3.11						
2313304	Cu2(OH)2+2	76.6200	-10.5940	0.000	0.000	2.00	0.00	0.00	161.1068
Source of log K: NIST46.3			NIST46.3						
2803300	FeOH+	55.8100	-9.3970	0.000	0.000	1.00	5.00	0.00	72.8544
Source of log K: NIST46.3			NIST46.3						
2803302	Fe(OH)2 (aq)	119.6200	-20.4940	0.000	0.000	0.00	0.00	0.00	89.8618
Source of log K: NIST46.3			NIST46.3						
2803301	Fe(OH)3-	126.4300	-28.9910	0.000	0.000	-1.00	5.00	0.00	106.8692
Source of log K: NIST46.3			NIST46.3						
2813300	FeOH+2	41.8100	-2.1870	0.000	0.000	2.00	5.00	0.00	72.8544
Source of log K: NIST46.3			NIST46.3						
2813301	Fe(OH)2+	0.0000	-4.5940	0.000	0.000	1.00	5.40	0.00	89.8618
Source of log K: NIST46.3			MTQ3.11						
2813302	Fe(OH)3 (aq)	103.8000	-12.5600	0.000	0.000	0.00	0.00	0.00	106.8692
Source of log K: Nord90			Nord90						
2813303	Fe(OH)4-	0.0000	-21.5880	0.000	0.000	-1.00	5.40	0.00	123.8766
Source of log K: NIST46.3			MTQ3.11						
2813304	Fe2(OH)2+4	57.6200	-2.8540	0.000	0.000	4.00	0.00	0.00	145.7088

```
Source of log K: NIST46.3                                NIST46.3
2813305 Fe3(OH)4+5                  65.2400    -6.2880     0.000     0.000     5.00   0.00
0.00  235.5706
Source of log K: NIST46.3                                NIST46.3
4703300 MnOH+                       55.8100   -10.5970     0.000     0.000     1.00   5.00
0.00   71.9454
Source of log K: NIST46.3                                NIST46.3
4703301 Mn(OH)3-                     0.0000   -34.8000     0.000     0.000    -1.00   5.00
0.00  105.9602
Source of log K: MTQ3.11                                 MTQ3.11
4703302 Mn(OH)4-2                    0.0000   -48.2880     0.000     0.000    -2.00   5.00
0.00  122.9676
Source of log K: NIST46.4                                MTQ3.11
4700020 MnO4-                      822.6699  -127.7945     0.000     0.000    -1.00   3.00
0.00  118.9360
Source of log K: NIST2.1.1                               NIST2.1.1
4700021 MnO4-2                     711.0699  -118.4218     0.000     0.000    -2.00   5.00
0.00  118.9360
Source of log K: NIST2.1.1                               NIST2.1.1
4603300 MgOH+                       67.8100   -11.3970     0.000     0.000     1.00   6.50
0.00   41.3124
Source of log K: NIST46.3                                NIST46.3
1503300 CaOH+                       64.1100   -12.6970     0.000     0.000     1.00   6.00
0.00   57.0854
Source of log K: NIST46.3                                NIST46.3
9501800 ZnCl+                        5.4000     0.4000     0.000     0.000     1.00   4.00
0.00  100.8430
Source of log K: NIST46.3                                NIST46.3
9501801 ZnCl2 (aq)                  37.0000     0.6000     0.000     0.000     0.00   0.00
0.00  136.2960
Source of log K: NIST46.3                                NIST46.3
9501802 ZnCl3-                      39.9990     0.5000     0.000     0.000    -1.00   4.00
0.00  171.7490
Source of log K: MTQ3.11                                 MTQ3.11
9501803 ZnCl4-2                     45.8566     0.1990     0.000     0.000    -2.00   5.00
0.00  207.2020
Source of log K: MTQ3.11                                 MTQ3.11
9501804 ZnOHCl (aq)                  0.0000    -7.4800     0.000     0.000     0.00   0.00
0.00  117.8504
Source of log K: MTQ3.11                                 MTQ3.11
2311800 CuCl+                        8.3000     0.2000     0.000     0.000     1.00   4.00
0.00   98.9990
Source of log K: NIST46.3                                NIST46.3
2311801 CuCl2 (aq)                  44.1830    -0.2600     0.000     0.000     0.00   0.00
0.00  134.4520
Source of log K: SCD3.02 (1989 IPa)                      MTQ3.11
2311802 CuCl3-                      57.2790    -2.2900     0.000     0.000    -1.00   4.00
0.00  169.9050
Source of log K: MTQ3.11                                 MTQ3.11
2311803 CuCl4-2    1                32.5515    -4.5900     0.000     0.000    -2.00   5.00
0.00  205.3580
Source of log K: MTQ3.11                                 MTQ3.11
2301800 CuCl2-                      -1.7573     5.4200     0.000     0.000    -1.00   4.00
0.00  134.4520
Source of log K: NIST46.3                                MTQ3.11
2301801 CuCl3-2                      1.0878     4.7500     0.000     0.000    -2.00   5.00
0.00  169.9050
Source of log K: NIST46.3                                MTQ3.11
2301802 CuCl (aq)                    0.0000     3.1000     0.000     0.000     0.00   0.00
0.00   98.9990
Source of log K: NIST46.4                                MTQ3.11
2811800 FeCl+2                      23.0000     1.4800     0.000     0.000     2.00   5.00
0.00   91.3000
Source of log K: NIST46.3                                NIST46.3
2811801 FeCl2+                       0.0000     2.1300     0.000     0.000     1.00   5.00
0.00  126.7530
Source of log K: NIST46.3                                MTQ3.11
2811802 FeCl3 (aq)                   0.0000     1.1300     0.000     0.000     0.00   0.00
0.00  162.2060
Source of log K: Nord90                                  MTQ3.11
4701800 MnCl+                        0.0000     0.1000     0.000     0.000     1.00   5.00
0.00   90.3910
Source of log K: NIST46.3                                MTQ3.11
4701801 MnCl2 (aq)                   0.0000     0.2500     0.000     0.000     0.00   0.00
0.00  125.8440
Source of log K: Nord90                                  MTQ3.11
```

4701802 MnCl3-	0.0000	-0.3100	0.000	0.000	-1.00	5.00
0.00 161.2970						
Source of log K: Nord90		MTQ3.11				
3307320 HSO4-	22.0000	1.9900	0.000	0.000	-1.00	4.50
0.00 97.0709						
Source of log K: NIST46.3		NIST46.3				
307320 AlSO4+	28.0000	3.8900	0.000	0.000	1.00	4.50
0.00 123.0445						
Source of log K: NIST46.3		NIST46.3				
307321 Al(SO4)2-	11.9000	4.9200	0.000	0.000	-1.00	4.50
0.00 219.1075						
Source of log K: Nord90		Nord90				
9507320 ZnSO4 (aq)	6.2000	2.3400	0.000	0.000	0.00	0.00
0.00 161.4530						
Source of log K: NIST46.3		NIST46.3				
9507321 Zn(SO4)2-2	0.0000	3.2800	0.000	0.000	-2.00	0.00
0.00 257.5160						
Source of log K: MTQ3.11		MTQ3.11				
2317320 CuSO4 (aq)	8.7000	2.3600	0.000	0.000	0.00	0.00
0.00 159.6090						
Source of log K: NIST46.3		NIST46.3				
2807320 FeSO4 (aq)	8.0000	2.3900	0.000	0.000	0.00	0.00
0.00 151.9100						
Source of log K: NIST46.3		NIST46.3				
2817320 FeSO4+	25.0000	4.0500	0.000	0.000	1.00	5.00
0.00 151.9100						
Source of log K: NIST46.3		NIST46.3				
2817321 Fe(SO4)2-	19.2000	5.3800	0.000	0.000	-1.00	0.00
0.00 247.9730						
Source of log K: Nord90		Nord90				
4707320 MnSO4 (aq)	8.7000	2.2500	0.000	0.000	0.00	0.00
0.00 151.0010						
Source of log K: NIST46.3		NIST46.3				
4607320 MgSO4 (aq)	5.8000	2.2600	0.000	0.000	0.00	0.00
0.00 120.3680						
Source of log K: NIST46.3		NIST46.3				
1507320 CaSO4 (aq)	7.1000	2.3600	0.000	0.000	0.00	0.00
0.00 136.1410						
Source of log K: NIST46.3		NIST46.3				
5007320 NaSO4-	1.0000	0.7300	0.000	0.000	-1.00	5.40
0.00 119.0528						
Source of log K: NIST46.3		NIST46.3				
4107320 KSO4-	4.1000	0.8500	0.000	0.000	-1.00	5.40
0.00 135.1613						
Source of log K: NIST46.3		NIST46.3				
2314921 CuNO3+	-4.1000	0.5000	0.000	0.000	1.00	0.00
0.00 125.5509						
Source of log K: NIST46.4		NIST46.4				
2314922 Cu(NO3)2 (aq)	0.0000	-0.4000	0.000	0.000	0.00	0.00
0.00 187.5558						
Source of log K: NIST46.4		MTQ3.11				
9504921 ZnNO3+	-4.6000	0.4000	0.000	0.000	1.00	0.00
0.00 127.3949						
Source of log K: NIST46.4		NIST46.4				
9504922 Zn(NO3)2 (aq)	0.0000	-0.3000	0.000	0.000	0.00	0.00
0.00 189.3998						
Source of log K: NIST46.4		MTQ3.11				
2814921 FeNO3+2	-37.0000	1.0000	0.000	0.000	2.00	0.00
0.00 117.8519						
Source of log K: NIST46.4		NIST46.4				
4704921 MnNO3+	0.0000	0.2000	0.000	0.000	1.00	0.00
0.00 116.9429						
Source of log K: NIST46.4		MTQ3.11				
4704920 Mn(NO3)2 (aq)	-1.6569	0.6000	0.000	0.000	0.00	0.00
0.00 178.9478						
Source of log K: NIST46.3		MTQ3.11				
1504921 CaNO3+	-5.4000	0.5000	0.000	0.000	1.00	0.00
0.00 102.0829						
Source of log K: NIST46.4		NIST46.4				
3305800 HPO4-2	-15.0000	12.3750	0.000	0.000	-2.00	5.00
0.00 95.9793						
Source of log K: NIST46.3		NIST46.3				
3305801 H2PO4-	-18.0000	19.5730	0.000	0.000	-1.00	5.40
0.00 96.9872						
Source of log K: NIST46.3		NIST46.3				
3305802 H3PO4	-10.1000	21.7210	0.000	0.000	0.00	0.00

```
0.00   97.9951
Source of log K: NIST46.3                                NIST46.3
2805800 FeH2PO4+                  0.0000    22.2730    0.000     0.000    1.00  5.40
0.00  152.8342
Source of log K: NIST46.3                                MTQ3.11
2805801 FeHPO4 (aq)               0.0000    15.9750    0.000     0.000    0.00  0.00
0.00  151.8263
Source of log K: NIST46.3                                MTQ3.11
2815801 FeH2PO4+2                 0.0000    23.8515    0.000     0.000    2.00  5.40
0.00  152.8342
Source of log K: NIST46.3                                MTQ3.11
2815800 FeHPO4+                 -30.5432    22.2920    0.000     0.000    1.00  5.40
0.00  151.8263
Source of log K: NIST46.3                                MTQ3.11
4605800 MgPO4-                   12.9704     4.6540    0.000     0.000   -1.00  5.40
0.00  119.2764
Source of log K: SCD3.02 (1993 GMa)                      MTQ3.11
4605801 MgH2PO4+                 -4.6861    21.2561    0.000     0.000    1.00  5.40
0.00  121.2922
Source of log K: NIST46.3                                MTQ3.11
4605802 MgHPO4 (aq)              -3.0000    15.1750    0.000     0.000    0.00  0.00
0.00  120.2843
Source of log K: NIST46.3                                NIST46.3
1505800 CaHPO4 (aq)              -3.0000    15.0350    0.000     0.000    0.00  0.00
0.00  136.0573
Source of log K: NIST46.3                                NIST46.3
1505801 CaPO4-                   12.9704     6.4600    0.000     0.000   -1.00  5.40
0.00  135.0494
Source of log K: SCD3.02 (1993 GMa)                      MTQ3.11
1505802 CaH2PO4+                 -6.0000    20.9230    0.000     0.000    1.00  5.40
0.00  137.0652
Source of log K: NIST46.3                                NIST46.3
5005800 NaHPO4-                   0.0000    13.4450    0.000     0.000   -1.00  5.40
0.00  118.9691
Source of log K: NIST46.3                                MTQ3.11
4105800 KHPO4-                    0.0000    13.2550    0.000     0.000   -1.00  5.40
0.00  135.0776
Source of log K: NIST46.3                                MTQ3.11
3301400 HCO3-                   -14.6000    10.3290    0.000     0.000   -1.00  5.40
0.00   61.0171
Source of log K: NIST46.4                                NIST46.4
3301401 H2CO3 (aq)              -23.7600    16.6810    0.000     0.000    0.00  0.00
0.00   62.0250
Source of log K: NIST46.4                                NIST46.4
9501401 ZnCO3 (aq)                0.0000     4.7600    0.000     0.000    0.00  0.00
0.00  125.3992
Source of log K: NIST46.4                                MTQ3.11
9501400 ZnHCO3+                   0.0000    11.8290    0.000     0.000    1.00  0.00
0.00  126.4071
Source of log K: NIST46.4                                MTQ3.11
2311400 CuCO3 (aq)                0.0000     6.7700    0.000     0.000    0.00  0.00
0.00  123.5552
Source of log K: NIST46.4                                MTQ3.11
2311402 CuHCO3+                   0.0000    12.1290    0.000     0.000    1.00  0.00
0.00  124.5631
Source of log K: NIST46.4                                MTQ3.11
2311401 Cu(CO3)2-2                0.0000    10.2000    0.000     0.000   -2.00  0.00
0.00  183.5644
Source of log K: NIST46.4                                MTQ3.11
2801400 FeHCO3+                   0.0000    11.4290    0.000     0.000    1.00  6.00
0.00  116.8641
Source of log K: NIST46.4                                MTQ3.11
4701400 MnHCO3+                 -10.6000    11.6290    0.000     0.000    1.00  5.00
0.00  115.9551
Source of log K: NIST46.4                                NIST46.4
4601400 MgCO3 (aq)               12.0000     2.9200    0.000     0.000    0.00  0.00
0.00   84.3142
Source of log K: NIST46.3                                NIST46.3
4601401 MgHCO3+                 -10.6000    11.3390    0.000     0.000    1.00  4.00
0.00   85.3221
Source of log K: NIST46.3                                NIST46.3
1501400 CaHCO3+                   5.4000    11.5990    0.000     0.000    1.00  6.00
0.00  101.0951
Source of log K: NIST46.3                                NIST46.3
1501401 CaCO3 (aq)               16.0000     3.2000    0.000     0.000    0.00  0.00
0.00  100.0872
```

Source of log K: NIST46.3		NIST46.3				
5001400 NaCO3-	-20.3500	1.2700	0.000	0.000	-1.00	5.40
0.00 82.9990						
Source of log K: NIST46.3		NIST2.1.1				

Type III - SPECIES WITH FIXED ACTIVITY

ID No Name	Enthalpy	logK	Min logK	Max logK	Charge	DHa
DHb gfw						
2 H2O	0.0000	0.0000	0.000	0.000	0.00	0.00
0.00 18.0153						
Source of log K:						
330 H+1	0.0000	7.8000	0.000	0.000	1.00	9.00
0.00 1.0079						
Source of log K:						
1 E-1	0.0000	5.2000	0.000	0.000	-1.00	0.00
0.00 0.0000						
Source of log K:						
3301403 CO2 (g)	-0.5300	21.6600	0.000	0.000	0.00	0.00
0.00 44.0097						
Source of log K: NIST46.4		NIST46.4				
2802810 Fe+2/Fe+3	-42.7000	13.0320	0.000	0.000	0.00	0.00
0.00 0.0000						
Source of log K: Bard85		Bard85				
4704710 Mn+2/Mn+3	-107.8000	25.3500	0.000	0.000	0.00	0.00
0.00 0.0000						
Source of log K: Bard85		MTQ3.11				
2302310 Cu+1/Cu+2	6.9000	2.6900	0.000	0.000	0.00	0.00
0.00 0.0000						
Source of log K: Bard85		MTQ3.11				
2077002 QUARTZ	-6.2200	4.0060	0.000	0.000	0.00	0.00
0.00 60.0843						
Source of log K: NIST46.4		CODATA89				
2095000 Zn(OH)2 (am)	80.6200	-12.4500	-12.260	-12.480	0.00	0.00
0.00 99.4048						
Source of log K: NIST46.4		NIST46.4				
2028100 FERRIHYDRITE	73.3740	-4.8910	-1.557	-4.996	0.00	0.00
0.00 106.8692						
Source of log K: NIST46.4		NIST13.1				
5015001 CALCITE	2.5850	8.4750	8.560	0.000	0.00	0.00
0.00 100.0872						
Source of log K: NIST46.4		NIST46.4				
8603001 KAOLINITE	35.2800	-5.7260	0.000	0.000	0.00	0.00
0.00 258.1607						
Source of log K: Nord90		Nord90				
9947101 MnPO4,1.5H2O	0.0000	34.7800	0.000	0.000	0.00	0.00
0.00 176.9320						
Source of log K:						
9915002 b-Ca3(PO4)2	0.0000	28.9260	0.000	0.000	0.00	0.00
0.00 310.1830						
Source of log K:						
9923103 Cu(OH)2	0.0000	-2.8000	0.000	0.000	0.00	0.00
0.00 97.5320						
Source of log K:						

Type VI - EXCLUDED SPECIES (not included in mole balance)

ID No Name	Enthalpy	logK	Min logK	Max logK	Charge	DHa
DHb gfw						
3301404 CH4 (g)	-257.1330	41.0452	0.000	0.000	0.00	0.00
0.00 16.0423						
Source of log K: NIST13.1		NIST13.1				
3300021 O2 (g)	571.6600	-83.0894	0.000	0.000	0.00	0.00
0.00 31.9990						
Source of log K: CODATA89		CODATA89				

Charge Balance: UNSPECIATED

Sum of CATIONS= 4.520E-03 Sum of ANIONS = 5.116E-03

PERCENT DIFFERENCE = 6.188E+00 (ANIONS - CATIONS)/(ANIONS + CATIONS)

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:

SO4-2	Log activity guess:	-2.90
CO3-2	Log activity guess:	-6.06

CONSTRAINTS ON COMPONENT ACTIVITIES

As specified, this chemical system is OPEN with respect to the following components:

H2O	H+1	E-1	CO3-2
H4SiO4	Zn+2	Fe+3	Ca+2
Al+3	PO4-3	Cu+2	Fe+2
Cu+1	Mn+3	Mn+2	

Activities of the following components are constrained by the species shown:

COMPONENT	SPECIES	TYPE
Cu+2	Cu(OH)2	3
PO4-3	b-Ca3(PO4)2	3
Mn+3	MnPO4,1.5H2O	3
Al+3	KAOLINITE	3
Ca+2	CALCITE	3
Fe+3	FERRIHYDRITE	3
Zn+2	Zn(OH)2 (am)	3
H4SiO4	QUARTZ	3
Cu+1	Cu+1/Cu+2	3
Mn+2	Mn+2/Mn+3	3
Fe+2	Fe+2/Fe+3	3
CO3-2	CO2 (g)	3
E-1	E-1	3
H+1	H+1	3
H2O	H2O	3

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL mol/L	DIFF FXN	LOG ACTVTY	RESIDUAL
0	Cl-1	1.590E-03	3.966E-07	-2.80000	2.376E-07
1	Cl-1	1.590E-03	2.099E-04	-2.80011	2.098E-04
2	Cl-1	1.590E-03	3.155E-05	-2.85397	3.138E-05
3	Cl-1	1.590E-03	5.463E-06	-2.86250	5.304E-06
4	Cl-1	1.590E-03	9.852E-07	-2.86399	8.262E-07
5	Cl-1	1.590E-03	1.789E-07	-2.86426	1.986E-08

ID No	Name	Total Conc(M)	Conc (M)	log Activity	Diff fxn
492	NO3-1	1.000E-03	9.860E-04	-3.07042	2.047E-08
732	SO4-2	1.260E-03	7.587E-04	-3.37712	6.139E-08
460	Mg+2	1.260E-03	1.206E-03	-3.17589	9.871E-08
500	Na+1	1.000E-03	9.976E-04	-3.06534	2.047E-08
410	K+1	1.000E-03	9.971E-04	-3.06557	2.047E-08
180	Cl-1	1.590E-03	1.585E-03	-2.86431	3.250E-08
2	H2O	0.000E+00	1.050E-02	-0.00005	0.000E+00
330	H+1	1.585E-08	1.838E-08	-7.80000	0.000E+00
1	E-1	6.310E-06	-3.016E-04	-5.20000	0.000E+00
140	CO3-2	0.000E+00	1.575E-06	-6.06005	0.000E+00
280	Fe+2	0.000E+00	3.805E-11	-10.67684	0.000E+00
470	Mn+2	0.000E+00	2.938E-04	-3.78914	0.000E+00
230	Cu+1	0.000E+00	5.681E-16	-15.30990	0.000E+00
770	H4SiO4	0.000E+00	9.807E-05	-4.00610	0.000E+00
950	Zn+2	0.000E+00	1.280E-03	-3.14990	0.000E+00
281	Fe+3	0.000E+00	1.175E-18	-18.50884	0.000E+00
150	Ca+2	0.000E+00	6.957E-03	-2.41481	0.000E+00
30	Al+3	0.000E+00	1.116E-16	-16.53087	0.000E+00
471	Mn+3	0.000E+00	4.361E-24	-23.93914	0.000E+00
580	PO4-3	0.000E+00	5.469E-11	-10.84078	0.000E+00
231	Cu+2	0.000E+00	2.866E-13	-12.79990	0.000E+00

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
330	H+1	1.838E-08	-7.80000	1.00	0.86238	0.064
580	PO4-3	5.469E-11	-10.84078	-3.00	0.26380	0.579
460	Mg+2	1.206E-03	-3.17589	2.00	0.55308	0.257
500	Na+1	9.976E-04	-3.06534	1.00	0.86238	0.064
410	K+1	9.971E-04	-3.06557	1.00	0.86238	0.064
180	Cl-1	1.585E-03	-2.86431	-1.00	0.86238	0.064
732	SO4-2	7.587E-04	-3.37712	-2.00	0.55308	0.257
492	NO3-1	9.860E-04	-3.07042	-1.00	0.86238	0.064
140	CO3-2	1.575E-06	-6.06005	-2.00	0.55308	0.257
280	Fe+2	3.805E-11	-10.67684	2.00	0.55308	0.257
470	Mn+2	2.938E-04	-3.78914	2.00	0.55308	0.257
230	Cu+1	5.681E-16	-15.30990	1.00	0.86238	0.064
281	Fe+3	1.175E-18	-18.50884	3.00	0.26380	0.579
471	Mn+3	4.361E-24	-23.93914	3.00	0.26380	0.579
231	Cu+2	2.866E-13	-12.79990	2.00	0.55308	0.257
30	Al+3	1.116E-16	-16.53087	3.00	0.26380	0.579
770	H4SiO4	9.807E-05	-4.00610	0.00	1.00543	-0.002
150	Ca+2	6.957E-03	-2.41481	2.00	0.55308	0.257
950	Zn+2	1.280E-03	-3.14990	2.00	0.55308	0.257

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
5001401	NaHCO3 (aq)	1.417E-07	-6.84640	0.00	1.00543	10.077
3307701	H2SiO4-2	1.713E-10	-10.02345	-2.00	0.55308	-21.360
3307700	H3SiO4-	8.496E-07	-6.13511	-1.00	0.86238	-9.865
3300020	OH-	7.366E-07	-6.19705	-1.00	0.86238	-13.933
303300	AlOH+2	3.383E-14	-13.72792	2.00	0.55308	-4.740

303301	Al(OH)2+	1.095E-11	-11.02497	1.00	0.86238	-10.030
303303	Al(OH)3 (aq)	1.190E-10	-9.92203	0.00	1.00543	-16.793
303302	Al(OH)4-	1.110E-08	-8.01908	-1.00	0.86238	-22.624
9503300	ZnOH+	5.216E-05	-4.34695	1.00	0.86238	-8.933
9503301	Zn(OH)2 (aq)	4.505E-06	-5.34400	0.00	1.00543	-17.796
9503302	Zn(OH)3-	1.672E-08	-7.84105	-1.00	0.86238	-28.027
9503303	Zn(OH)4-2	6.593E-13	-12.43810	-2.00	0.55308	-40.231
2313300	CuOH+	3.693E-13	-12.49695	1.00	0.86238	-7.433
2313301	Cu(OH)2 (aq)	4.015E-14	-13.39400	0.00	1.00543	-16.196
2313302	Cu(OH)3-	6.099E-17	-16.27905	-1.00	0.86238	-26.815
2313303	Cu(OH)4-2	4.755E-22	-21.58010	-2.00	0.55308	-39.723
2313304	Cu2(OH)2+2	7.914E-21	-20.35884	2.00	0.55308	-10.102
2803300	FeOH+	6.172E-13	-12.27390	1.00	0.86238	-9.333
2803302	Fe(OH)2 (aq)	2.671E-16	-15.57095	0.00	1.00543	-20.496
2803301	Fe(OH)3-	6.256E-17	-16.26800	-1.00	0.86238	-28.927
2813300	FeOH+2	2.298E-13	-12.89590	2.00	0.55308	-1.930
2813301	Fe(OH)2+	3.642E-08	-7.50295	1.00	0.86238	-4.530
2813302	Fe(OH)3 (aq)	2.131E-08	-7.66900	0.00	1.00543	-12.562
2813303	Fe(OH)4-	1.470E-09	-8.89705	-1.00	0.86238	-21.524
2813304	Fe2(OH)2+4	5.716E-24	-24.27179	4.00	0.09357	-1.825
2813305	Fe3(OH)4+5	9.836E-30	-30.61474	5.00	0.02468	-4.680
4703300	MnOH+	3.007E-07	-6.58619	1.00	0.86238	-10.533
4703301	Mn(OH)3-	7.499E-16	-15.18930	-1.00	0.86238	-34.736
4703302	Mn(OH)4-2	2.398E-21	-20.87735	-2.00	0.55308	-48.031
4700020	MnO4-	7.594E-44	-43.18385	-1.00	0.86238	-127.730
4700021	MnO4-2	1.762E-39	-39.01115	-2.00	0.55308	-118.165
4603300	MgOH+	8.014E-08	-7.16044	1.00	0.86238	-11.720
1503300	CaOH+	5.655E-08	-7.31186	1.00	0.86238	-12.633
9501800	ZnCl+	2.819E-06	-5.61421	1.00	0.86238	0.464
9501801	ZnCl2 (aq)	5.238E-09	-8.27852	0.00	1.00543	0.598
9501802	ZnCl3-	6.629E-12	-11.24283	-1.00	0.86238	0.564
9501803	ZnCl4-2	7.064E-15	-14.40814	-2.00	0.55308	0.456
9501804	ZnOHCl (aq)	2.011E-06	-5.69426	0.00	1.00543	-7.482
2311800	CuCl+	3.982E-16	-15.46421	1.00	0.86238	0.264
2311801	CuCl2 (aq)	1.619E-19	-18.78852	0.00	1.00543	-0.262
2311802	CuCl3-	2.407E-24	-23.68283	-1.00	0.86238	-2.226
2311803	CuCl4-2 1	2.571E-29	-28.84714	-2.00	0.55308	-4.333
2301800	CuCl2-	2.791E-16	-15.61852	-1.00	0.86238	5.484
2301801	CuCl3-2	1.272E-19	-19.15283	-2.00	0.55308	5.007
2301802	CuCl (aq)	8.384E-16	-15.07421	0.00	1.00543	3.098
2811800	FeCl+2	2.312E-20	-19.89315	2.00	0.55308	1.737
2811801	FeCl2+	9.054E-23	-22.10746	1.00	0.86238	2.194
2811802	FeCl3 (aq)	1.061E-26	-25.97177	0.00	1.00543	1.128
4701800	MnCl+	3.242E-07	-6.55345	1.00	0.86238	0.164
4701801	MnCl2 (aq)	5.369E-10	-9.26776	0.00	1.00543	0.248
4701802	MnCl3-	2.356E-13	-12.69207	-1.00	0.86238	-0.246
3307320	HSO4-	7.484E-10	-9.19018	-1.00	0.86238	2.051
307320	AlSO4+	1.113E-16	-16.01799	1.00	0.86238	3.954
307321	Al(SO4)2-	5.003E-19	-18.36510	-1.00	0.86238	4.984
9507320	ZnSO4 (aq)	6.466E-05	-4.18701	0.00	1.00543	2.338
9507321	Zn(SO4)2-2	4.296E-07	-6.62413	-2.00	0.55308	3.537
2317320	CuSO4 (aq)	1.516E-14	-13.81701	0.00	1.00543	2.358
2807320	FeSO4 (aq)	2.156E-12	-11.66396	0.00	1.00543	2.388
2817320	FeSO4+	1.692E-18	-17.83596	1.00	0.86238	4.114
2817321	Fe(SO4)2-	1.518E-20	-19.88308	-1.00	0.86238	5.444
4707320	MnSO4 (aq)	1.206E-05	-4.91626	0.00	1.00543	2.248
4607320	MgSO4 (aq)	5.066E-05	-4.29301	0.00	1.00543	2.258
1507320	CaSO4 (aq)	3.679E-04	-3.43193	0.00	1.00543	2.358
5007320	NaSO4-	2.248E-06	-5.71246	-1.00	0.86238	0.794
4107320	KSO4-	2.940E-06	-5.59596	-1.00	0.86238	0.911
2314921	CuNO3+	4.943E-16	-15.37031	1.00	0.86238	0.564
2314922	Cu(NO3)2 (aq)	4.539E-20	-19.34073	0.00	1.00543	-0.402
9504921	ZnNO3+	1.754E-06	-5.82031	1.00	0.86238	0.464
9504922	Zn(NO3)2 (aq)	2.552E-10	-9.59073	0.00	1.00543	-0.302
2814921	FeNO3+2	4.764E-21	-20.57926	2.00	0.55308	1.257
4704921	MnNO3+	2.539E-07	-6.65956	1.00	0.86238	0.264
4704920	Mn(NO3)2 (aq)	4.652E-10	-9.32998	0.00	1.00543	0.598
1504921	CaNO3+	1.200E-05	-4.98523	1.00	0.86238	0.564
3305800	HPO4-2	9.805E-07	-6.26578	-2.00	0.55308	12.632
3305801	H2PO4-	1.572E-07	-6.86778	-1.00	0.86238	19.637
3305802	H3PO4	3.005E-13	-12.51978	0.00	1.00543	21.719
2805800	FeH2PO4+	1.658E-15	-14.84462	1.00	0.86238	22.337
2805801	FeHPO4 (aq)	4.519E-14	-13.34262	0.00	1.00543	15.973
2815801	FeH2PO4+2	1.442E-21	-21.09812	2.00	0.55308	24.109
2815800	FeHPO4+	1.609E-15	-14.85762	1.00	0.86238	22.356
4605800	MgPO4-	5.031E-10	-9.36267	-1.00	0.86238	4.718

4605801	MgH2PO4+	5.055E-09	-8.36057	1.00	0.86238	21.320
4605802	MgHPO4 (aq)	2.270E-07	-6.64167	0.00	1.00543	15.173
1505800	CaHPO4 (aq)	9.485E-07	-6.02059	0.00	1.00543	15.033
1505801	CaPO4-	1.857E-07	-6.79559	-1.00	0.86238	6.524
1505802	CaH2PO4+	1.354E-08	-7.93259	1.00	0.86238	20.987
5005800	NaHPO4-	6.356E-09	-8.26113	-1.00	0.86238	13.509
4105800	KHPO4-	4.102E-09	-8.45136	-1.00	0.86238	13.319
3301400	HCO3-	3.419E-04	-3.53040	-1.00	0.86238	10.394
3301401	H2CO3 (aq)	1.044E-05	-4.97905	0.00	1.00543	16.679
9501401	ZnCO3 (aq)	3.529E-05	-4.44995	0.00	1.00543	4.758
9501400	ZnHCO3+	7.645E-06	-5.18095	1.00	0.86238	11.893
2311400	CuCO3 (aq)	8.085E-13	-12.08995	0.00	1.00543	6.768
2311402	CuHCO3+	3.415E-15	-14.53095	1.00	0.86238	12.193
2311401	Cu(CO3)2-2	3.445E-15	-14.72000	-2.00	0.55308	10.457
2801400	FeHCO3+	9.045E-14	-13.10790	1.00	0.86238	11.493
4701400	MnHCO3+	1.107E-06	-6.02019	1.00	0.86238	11.693
4601400	MgCO3 (aq)	5.513E-07	-6.25628	0.00	1.00543	2.977
4601401	MgHCO3+	2.652E-06	-5.64076	1.00	0.86238	11.459
1501400	CaHCO3+	1.363E-05	-4.92982	1.00	0.86238	11.409
1501401	CaCO3 (aq)	4.735E-06	-5.32236	0.00	1.00543	3.150
5001400	NaCO3-	1.618E-08	-7.85540	-1.00	0.86238	1.334

Type III - SPECIES WITH FIXED ACTIVITY

ID No	Name	Conc (M)	New logK	Enthalpy
2	H2O	1.050E-02	0.000	0.000
330	H+1	-1.802E-02	7.800	0.000
1	E-1	-3.016E-04	5.200	0.000
3301403	CO2 (g)	7.394E-03	21.660	-0.530
2802810	Fe+2/Fe+3	4.096E-11	13.032	-42.700
4704710	Mn+2/Mn+3	3.079E-04	25.350	-107.800
2302310	Cu+1/Cu+2	1.686E-15	2.690	6.900
2077002	QUARTZ	-9.891E-05	4.006	-6.220
2095000	Zn(OH)2 (am)	-1.452E-03	-12.450	80.620
2028100	FERRIHYDRITE	-5.925E-08	-4.891	73.374
5015001	CALCITE	-7.814E-03	8.475	2.585
8603001	KAOLINITE	-5.614E-09	-5.726	35.280
9947101	MnPO4,1.5H2O	-3.079E-04	34.780	0.000
9915002	b-Ca3(PO4)2	1.527E-04	28.926	0.000
9923103	Cu(OH)2	-1.529E-12	-2.800	0.000

Type VI - EXCLUDED SPECIES (not included in mole balance)

ID No	Name	Conc (M)	New logK	Enthalpy
3301404	CH4 (g)	0.000E+00	41.045	-257.133
3300021	O2 (g)	8.138E-32	-83.089	571.660

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

NO3-1				
	98.6	Percent bound in species #	492	NO3-1
	1.2	Percent bound in species #	1504921	CaNO3+
SO4-2				
	60.2	Percent bound in species #	732	SO4-2
	5.1	Percent bound in species #	9507320	ZnSO4 (aq)
	4.0	Percent bound in species #	4607320	MgSO4 (aq)
	29.2	Percent bound in species #	1507320	CaSO4 (aq)
Mg+2				
	95.7	Percent bound in species #	460	Mg+2
	4.0	Percent bound in species #	4607320	MgSO4 (aq)
Na+1				
	99.8	Percent bound in species #	500	Na+1
K+1				
	99.7	Percent bound in species #	410	K+1
Cl-1				
	99.7	Percent bound in species #	180	Cl-1
H2O				
	1.1	Percent bound in species #	3300020	OH-
	80.8	Percent bound in species #	9503300	ZnOH+
	13.9	Percent bound in species #	9503301	Zn(OH)2 (aq)
	3.1	Percent bound in species #	9501804	ZnOHCl (aq)
H+1				
	105.2	Percent bound in species #	3301400	HCO3-
	6.4	Percent bound in species #	3301401	H2CO3 (aq)
	2.4	Percent bound in species #	9501400	ZnHCO3+
	4.2	Percent bound in species #	1501400	CaHCO3+
E-1				
	100.0	Percent bound in species #	4700021	MnO4-2
CO3-2				
	81.5	Percent bound in species #	3301400	HCO3-
	2.5	Percent bound in species #	3301401	H2CO3 (aq)
	8.4	Percent bound in species #	9501401	ZnCO3 (aq)

	1.8	Percent bound in species #9501400	ZnHCO3+
	3.2	Percent bound in species #1501400	CaHCO3+
	1.1	Percent bound in species #1501401	CaCO3 (aq)
Fe+2			
	92.9	Percent bound in species # 280	Fe+2
	1.5	Percent bound in species #2803300	FeOH+
	5.3	Percent bound in species #2807320	FeSO4 (aq)
Mn+2			
	95.4	Percent bound in species # 470	Mn+2
	3.9	Percent bound in species #4707320	MnSO4 (aq)
Cu+1			
	33.7	Percent bound in species # 230	Cu+1
	16.6	Percent bound in species #2301800	CuCl2-
	49.7	Percent bound in species #2301802	CuCl (aq)
H4SiO4			
	99.1	Percent bound in species # 770	H4SiO4
Zn+2			
	88.2	Percent bound in species # 950	Zn+2
	3.6	Percent bound in species #9503300	ZnOH+
	4.5	Percent bound in species #9507320	ZnSO4 (aq)
	2.4	Percent bound in species #9501401	ZnCO3 (aq)
Fe+3			
	61.5	Percent bound in species #2813301	Fe(OH)2+
	36.0	Percent bound in species #2813302	Fe(OH)3 (aq)
	2.5	Percent bound in species #2813303	Fe(OH)4-
Ca+2			
	94.6	Percent bound in species # 150	Ca+2
	5.0	Percent bound in species #1507320	CaSO4 (aq)
Al+3			
	1.1	Percent bound in species # 303303	Al(OH)3 (aq)
	98.8	Percent bound in species # 303302	Al(OH)4-
Mn+3			
	100.0	Percent bound in species # 471	Mn+3
PO4-3			
	38.8	Percent bound in species #3305800	HPO4-2
	6.2	Percent bound in species #3305801	H2PO4-
	9.0	Percent bound in species #4605802	MgHPO4 (aq)
	37.5	Percent bound in species #1505800	CaHPO4 (aq)

7.3	Percent bound in species	#1505801	CaPO4-

Cu+2

18.8	Percent bound in species	# 231	Cu+2
24.2	Percent bound in species	#2313300	CuOH+
2.6	Percent bound in species	#2313301	Cu(OH)2 (aq)
52.9	Percent bound in species	#2311400	CuCO3 (aq)

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
492	NO3-1	1.000E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	1.260E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	1.260E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
500	Na+1	1.000E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	1.000E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
180	Cl-1	1.590E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	6.459E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	3.250E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
1	E-1	-7.049E-39	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	4.197E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
280	Fe+2	4.096E-11	100.0	0.000E+00	0.0	0.000E+00	0.0
470	Mn+2	3.079E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
230	Cu+1	1.686E-15	100.0	0.000E+00	0.0	0.000E+00	0.0
770	H4SiO4	9.892E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
950	Zn+2	1.452E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
281	Fe+3	5.920E-08	100.0	0.000E+00	0.0	0.000E+00	0.0
150	Ca+2	7.356E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
30	Al+3	1.123E-08	100.0	0.000E+00	0.0	0.000E+00	0.0
471	Mn+3	4.361E-24	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	2.528E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
231	Cu+2	1.528E-12	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 2.156E-02 Sum of ANIONS 4.443E-03

PERCENT DIFFERENCE = 6.583E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 2.350E-02

EQUILIBRIUM pH = 7.800

EQUILIBRIUM pe = 5.200 or Eh = 307.60 mv

DATE ID NUMBER: 20000605
TIME ID NUMBER: 14064685

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
95000	Zn metal	-39.338	[1.000]950 [2.000] 1
23000	Cu metal	-11.754	[1.000]230 [1.000] 1
2077000	CHALCEDONY	-0.456	[1.000]770 [-2.000] 2
2077001	CRISTOBALITE	-0.656	[1.000]770 [-2.000] 2
2077002	QUARTZ	-0.006	[1.000]770 [-2.000] 2
2077003	SiO2 (am,gel)	-1.296	[1.000]770 [-2.000] 2
2077004	SiO2 (am,ppt)	-1.266	[1.000]770 [-2.000] 2
2003000	Al(OH)3 (am)	-3.931	[1.000] 30 [3.000] 2 [-3.000]330
2003001	BOEHMITE	-1.709	[-3.000]330 [1.000] 30 [2.000] 2
2003002	DIASPORE	-0.004	[-3.000]330 [1.000] 30 [2.000] 2
2003003	GIBBSITE	-1.422	[1.000] 30 [3.000] 2 [-3.000]330
2095000	Zn(OH)2 (am)	-0.024	[1.000]950 [2.000] 2 [-2.000]330
2095001	Zn(OH)2	0.250	[-2.000]330 [1.000]950 [2.000] 2
2095002	Zn(OH)2 (beta)	0.696	[1.000]950 [2.000] 2 [-2.000]330
2095003	Zn(OH)2 (gamma)	0.716	[1.000]950 [2.000] 2 [-2.000]330
2095004	Zn(OH)2 (epsilon)	0.916	[1.000]950 [2.000] 2 [-2.000]330
2095005	ZnO (active)	1.262	[-2.000]330 [1.000]950 [1.000] 2
2095006	ZINCITE	1.116	[1.000]950 [1.000] 2 [-2.000]330
2023000	CUPRITE	-13.614	[2.000]230 [1.000] 2 [-2.000]330
2023100	Cu(OH)2	-5.874	[1.000]231 [2.000] 2 [-2.000]330
2023101	TENORITE	-4.844	[1.000]231 [1.000] 2 [-2.000]330
2028000	WUSTITE	-6.199	[-2.000]330 [0.947]280 [1.000] 2
2028001	Fe(OH)2	-8.641	[1.000]280 [2.000] 2 [-2.000]330
2028100	FERRIHYDRITE	1.700	[1.000]281 [3.000] 2 [-3.000]330
2028101	Fe3(OH)8	-5.517	[-8.000]330 [2.000]281 [1.000]280 [8.000] 2
2028102	GOETHITE	4.400	[1.000]281 [2.000] 2 [-3.000]330
2047000	PYROLUSITE	-3.569	[1.000]470 [2.000] 2 [-4.000]330 [-2.000] 1
2047001	BIRNESSITE	-5.630	[-4.000]330 [-1.000] 1 [1.000]471 [2.000] 2
2047002	NSUTITE	-5.043	[-4.000]330 [-1.000] 1 [1.000]471 [2.000] 2
2047003	PYROCHROITE	-3.383	[1.000]470 [2.000] 2 [-2.000]330
2047100	MANGANITE	-0.529	[1.000]470 [2.000] 2 [-3.000]330 [-1.000] 1
2046000	BRUCITE	-4.420	[1.000]460 [2.000] 2 [-2.000]330
2046001	PERICLASE	-9.160	[-2.000]330 [1.000]460 [1.000] 2
2046002	Mg(OH)2 (active)	-6.370	[1.000]460 [2.000] 2 [-2.000]330
2015000	LIME	-19.514	[-2.000]330 [1.000]150 [1.000] 2
2015001	PORTLANDITE	-9.619	[1.000]150 [2.000] 2 [-2.000]330
3003000	Al2O3	-5.914	[2.000] 30 [3.000] 2 [-6.000]330
3028000	MAGNETITE	11.302	[-8.000]330 [2.000]281 [1.000]280 [4.000] 2

ID No	Name	SI	Composition by stoich. of components
3028001	HERCYNITE	-4.232	[-8.000]330 [1.000]280 [2.000] 30 [4.000] 2
3028100	HEMATITE	11.200	[2.000]281 [3.000] 2 [-6.000]330
3028101	MAGHEMITE	3.396	[-6.000]330 [2.000]281 [3.000] 2
3028102	LEPIDOCROCITE	3.520	[-3.000]330 [1.000]281 [2.000] 2
3047000	HAUSMANNITE	0.402	[3.000]470 [4.000] 2 [-8.000]330 [-2.000] 1
3047100	BIXBYITE	-0.434	[-6.000]330 [2.000]471 [3.000] 2
3046000	SPINEL	-10.685	[-8.000]330 [1.000]460 [2.000] 30 [4.000] 2
3046001	MAGNESIOFERRITE	5.347	[-8.000]330 [1.000]460 [2.000]281 [4.000] 2
3050000	NATRON	-10.880	[2.000]500 [1.000]140 [10.000] 2
3023000	CUPROUS FERRITE	6.298	[-4.000]330 [1.000]230 [1.000]281 [2.000] 2
3023100	CUPRIC FERRITE	6.594	[-8.000]330 [1.000]231 [2.000]281 [4.000] 2
4195000	ZnCl2	-15.929	[1.000]950 [2.000]180
4195001	Zn2(OH)3Cl	-0.955	[2.000]950 [3.000] 2 [-3.000]330 [1.000]180
4195002	Zn5(OH)8Cl2	2.421	[-8.000]330 [5.000]950 [8.000] 2 [2.000]180
4123000	NANTOKITE	-11.444	[1.000]230 [1.000]180
4123100	MELANOTHALLITE	-24.786	[1.000]231 [2.000]180
4123101	ATACAMITE	-12.455	[2.000]231 [3.000] 2 [-3.000]330 [1.000]180
4128100	Fe(OH)2.7Cl.3	4.732	[-2.700]330 [1.000]281 [2.700] 2 [0.300]180
4147000	MnCl2:4H2O	-12.233	[1.000]470 [2.000]180 [4.000] 2
4150000	HALITE	-7.532	[1.000]500 [1.000]180
5095000	SMITHSONITE	0.790	[1.000]950 [1.000]140
5095001	ZnCO3:1H2O	1.050	[1.000]950 [1.000]140 [1.000] 2
5023100	CuCO3	-7.360	[1.000]231 [1.000]140
5023101	MALACHITE	-10.754	[2.000]231 [2.000] 2 [-2.000]330 [1.000]140
5023102	AZURITE	-18.014	[3.000]231 [2.000] 2 [-2.000]330 [2.000]140
5028000	SIDERITE	-6.497	[1.000]280 [1.000]140
5047000	RHODOCHROSITE	0.731	[1.000]470 [1.000]140
5046000	ARTINITE	-6.412	[-2.000]330 [2.000]460 [1.000]140 [5.000] 2
5046001	HYDROMAGNESITE	-15.754	[5.000]460 [4.000]140 [-2.000]330 [6.000] 2
5046002	MAGNESITE	-1.776	[1.000]460 [1.000]140
5046003	NESQUEHONITE	-4.566	[1.000]460 [1.000]140 [3.000] 2
5015000	ARAGONITE	-0.139	[1.000]150 [1.000]140
5015001	CALCITE	0.000	[1.000]150 [1.000]140
5015002	DOLOMITE (ordered)	-0.621	[1.000]150 [1.000]460 [2.000]140
5015004	DOLOMITE (disordered)	-1.171	[1.000]150 [1.000]460 [2.000]140
5015003	HUNTITE	-6.215	[3.000]460 [1.000]150 [4.000]140
5050001	THERMONATRITE	-12.828	[2.000]500 [1.000]140 [1.000] 2

ID No	Name	SI	Composition by stoich. of components
5195000	Zn(NO3)2:6H2O	-12.606	[1.000]950 [2.000]492 [6.000] 2
5123100	Cu2(OH)3NO3	-14.521	[2.000]231 [3.000] 2 [-3.000]330 [1.000]492
6003000	AlOHSO4	-8.878	[-1.000]330 [1.000] 30 [1.000]732 [1.000] 2
6003001	Al4(OH)10SO4	-14.201	[-10.000]330 [4.000] 30 [1.000]732 [10.000] 2
6095000	Zn2(OH)2SO4	-1.577	[-2.000]330 [2.000]950 [2.000] 2 [1.000]732
6095001	Zn4(OH)6SO4	2.423	[-6.000]330 [4.000]950 [6.000] 2 [1.000]732
6095002	Zn3O(SO4)2	-19.517	[-2.000]330 [3.000]950 [2.000]732 [1.000] 2
6095003	ZINCOSITE	-10.457	[1.000]950 [1.000]732
6095004	ZnSO4:1H2O	-5.889	[1.000]950 [1.000]732 [1.000] 2
6095005	BIANCHITE	-4.762	[1.000]950 [1.000]732 [6.000] 2
6095006	GOSLARITE	-4.516	[1.000]950 [1.000]732 [7.000] 2
6023000	Cu2SO4	-32.047	[2.000]230 [1.000]732
6023100	ANTLERITE	-19.365	[3.000]231 [4.000] 2 [-4.000]330 [1.000]732
6023101	BROCHANTITE	-22.999	[4.000]231 [6.000] 2 [-6.000]330 [1.000]732
6023102	LANGITE	-25.266	[-6.000]330 [4.000]231 [7.000] 2 [1.000]732
6023103	CuOCuSO4	-23.680	[-2.000]330 [2.000]231 [1.000] 2 [1.000]732
6023104	CuSO4	-19.117	[1.000]231 [1.000]732
6023105	CHALCANTHITE	-13.537	[1.000]231 [1.000]732 [5.000] 2
6028000	MELANTERITE	-11.845	[1.000]280 [1.000]732 [7.000] 2
6028100	Fe2(SO4)3	-43.415	[2.000]281 [3.000]732
6028101	H-JAROSITE	-11.181	[-5.000]330 [3.000]281 [2.000]732 [7.000] 2
6050000	Na-JAROSITE	-7.346	[-6.000]330 [1.000]500 [3.000]281 [2.000]732 [6.000] 2
6041002	K-JAROSITE	-3.747	[-6.000]330 [1.000]410 [3.000]281 [2.000]732 [6.000] 2
6047000	MnSO4	-9.749	[1.000]470 [1.000]732
6047100	Mn2(SO4)3	-52.299	[2.000]471 [3.000]732
6046000	EPSOMITE	-4.427	[1.000]460 [1.000]732 [7.000] 2
6015000	ANHYDRITE	-1.432	[1.000]150 [1.000]732
6015001	GYPSUM	-1.182	[1.000]150 [1.000]732 [2.000] 2
6050001	MIRABILITE	-8.394	[2.000]500 [1.000]732 [10.000] 2
6050002	THENARDITE	-9.830	[2.000]500 [1.000]732
6041000	K-ALUM	-21.181	[1.000]410 [1.000] 30 [2.000]732 [12.000] 2
6041001	ALUNITE	-58.013	[1.000]410 [3.000] 30 [2.000]732 [6.000] 2
7095000	Zn3(PO4)2:4H2O	4.289	[3.000]950 [2.000]580 [4.000] 2
7023100	Cu3(PO4)2	-23.231	[3.000]231 [2.000]580
7023101	Cu3(PO4)2:3H2O	-24.961	[3.000]231 [2.000]580 [3.000] 2
7028001	VIVIANITE	-17.713	[3.000]280 [2.000]580 [8.000] 2

ID No	Name	SI	Composition by stoich. of components
7028100	STRENGITE	-2.950	[1.000]281 [1.000]580 [2.000] 2
7047000	Mn3(PO4)2	-9.222	[3.000]470 [2.000]580
7047001	MnHPO4	2.970	[1.000]470 [1.000]580 [1.000]330
7046002	Mg3(PO4)2	-7.929	[3.000]460 [2.000]580
7046001	MgHPO4:3H2O	-3.642	[1.000]460 [1.000]330 [1.000]580 [3.000] 2
7015003	HYDROXYLAPATITE	7.537	[5.000]150 [3.000]580 [1.000] 2 [-1.000]330
7015004	CaHPO4:2H2O	-2.061	[1.000]150 [1.000]330 [1.000]580 [2.000] 2
7015005	CaHPO4	-1.781	[1.000]150 [1.000]330 [1.000]580
7015006	Ca3(PO4)2 (beta)	-0.006	[3.000]150 [2.000]580
7015007	Ca4H(PO4)3:3H2O	-2.902	[4.000]150 [1.000]330 [3.000]580 [3.000] 2
8603000	HALLOYSITE	-3.849	[2.000] 30 [2.000]770 [1.000] 2 [-6.000]330
8603001	KAOLINITE	-1.709	[2.000] 30 [2.000]770 [1.000] 2 [-6.000]330
8628000	GREENALITE	-14.053	[-6.000]330 [3.000]280 [2.000]770 [1.000] 2
8646000	CHRYSOTILE	-2.940	[3.000]460 [2.000]770 [1.000] 2 [-6.000]330
8646003	SEPIOLITE	-2.930	[2.000]460 [3.000]770 [-4.000]330 [-0.500] 2
8646004	SEPIOLITE (A)	-5.950	[-0.500] 2 [2.000]460 [3.000]770 [-4.000]330

Test4.out
MINTEQA2, v4.02
Original database
As distributed by EPA

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 5-JUN-2000 TIME: 14: 6:50

TEST4 - Triple Layer Adsorption model with two adsorbing surfaces.

Component file (COMP.DBS):	comp.dbs	COMP v4.00 09/30/1999
Thermodynamic file (THERMO.UNF):	thermo.unf	THERMO V4.00 09/30/1999
Gaussian DOM file (GAUSSIAN.DBS):	gaussian.dbs	GAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF):	type6.unf	TYPE6 V4.00 09/30/1999

Temperature (Celsius): 25.00
Units of concentration: MOLAL
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed only for those solids specified as ALLOWED
in the input file (if any).
Maximum iterations: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file
Adsorption model: Triple Layer
Number of adsorbing surfaces: 2

```
8.174E+00  129.00 1.200 0.200 81
4.087E+00  600.00 1.400 0.400 82
    330  1.000E-07   -7.00
    410  1.000E-01   -1.00
    492  1.000E-01   -1.00
    813  0.000E+00    0.00
    814  0.000E+00    0.00
    815  0.000E+00    0.00
    811  1.320E-04   -3.88
    823  0.000E+00    0.00
    824  0.000E+00    0.00
    825  0.000E+00    0.00
    821  1.370E-04   -3.86

 H2O has been inserted as a COMPONENT
  3   1
    330      7.0000      0.0000
  6   6
    813      0.0000      0.0000
    814      0.0000      0.0000
    815      0.0000      0.0000
    823      0.0000      0.0000
    824      0.0000      0.0000
    825      0.0000      0.0000
  2   8
8113300 =1SO-            0.0000   -9.3100   0.000   0.000 0.00 0.00 0.00   0.0000
0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
8113301 =1SOH2+          0.0000    7.3300   0.000   0.000 0.00 0.00 0.00   0.0000
0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
8114920 =1SOH2NO3        0.0000    8.3300   0.000   0.000 0.00 0.00 0.00   0.0000
0.00 5   1.000 811   1.000 492   1.000 330   1.000 813  -1.000 814   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
8114100 =1SOK            0.0000   -8.3100   0.000   0.000 0.00 0.00 0.00   0.0000
0.00 5   1.000 811   1.000 410  -1.000 330  -1.000 813   1.000 814   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
8213300 =2SO-            0.0000   -6.5200   0.000   0.000 0.00 0.00 0.00   0.0000
```

```
0.00 3   1.000 821  -1.000 330  -1.000 823   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
8213301 =2SOH2+          0.0000    7.0100   0.000   0.000 0.00 0.00 0.00   0.0000
0.00 3   1.000 821   1.000 330   1.000 823   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
8214100 =2SOK            0.0000   -5.3100   0.000   0.000 0.00 0.00 0.00   0.0000
0.00 5   1.000 821   1.000 410  -1.000 330  -1.000 823   1.000 824   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
8214920 =2SOH2NO3        0.0000    5.3500   0.000   0.000 0.00 0.00 0.00   0.0000
0.00 5   1.000 821   1.000 492   1.000 330   1.000 823  -1.000 824   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
```

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	1.000E-07	-7.000	1.000E-07
410	K+1	1.000E-01	-1.000	1.000E-01
492	NO3-1	1.000E-01	-1.000	1.000E-01
813	ADS1PSIo	1.000E+00	0.000	0.000E+00
814	ADS1PSIb	1.000E+00	0.000	0.000E+00
815	ADS1PSId	1.000E+00	0.000	0.000E+00
811	ADS1TYP1	1.318E-04	-3.880	1.320E-04
823	ADS2PSIo	1.000E+00	0.000	0.000E+00
824	ADS2PSIb	1.000E+00	0.000	0.000E+00
825	ADS2PSId	1.000E+00	0.000	0.000E+00
821	ADS2TYP1	1.380E-04	-3.860	1.370E-04
2	H2O	1.000E+00	0.000	0.000E+00

Charge Balance: UNSPECIATED

Sum of CATIONS= 1.000E-01 Sum of ANIONS = 1.000E-01

PERCENT DIFFERENCE = 5.000E-05 (ANIONS - CATIONS)/(ANIONS + CATIONS)

CONSTRAINTS ON COMPONENT ACTIVITIES

As specified, this chemical system is OPEN with respect to the following components:

H2O H+1

Activities of the following components are constrained by the species shown:

COMPONENT	SPECIES	TYPE
H+1	H+1	3
H2O	H2O	3

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL mol/L	DIFF FXN	LOG ACTVTY	RESIDUAL
0	ADS2PSIb	0.000E+00	6.758E-04	0.00000	6.757E-04
1	ADS2PSId	0.000E+00	4.788E-06	0.00441	4.788E-06
2	ADS2PSId	1.821E-05	1.015E-06	0.01770	1.013E-06
3	ADS2PSId	2.002E-05	8.685E-09	0.01844	6.683E-09

ID No	Name	Total Conc(M)	Conc (M)	log Activity	Diff fxn
821	ADS2TYP1	1.370E-04	1.665E-05	-4.77848	4.261E-12
410	K+1	1.000E-01	9.994E-02	-1.10765	-3.268E-09
492	NO3-1	1.000E-01	9.994E-02	-1.10763	-3.195E-09
813	ADS1PSIo	8.765E-05	3.654E-01	-0.43725	1.628E-10
814	ADS1PSIb	-5.481E-05	4.740E-01	-0.32426	-1.978E-10
815	ADS1PSId	-3.284E-05	8.506E-01	-0.07026	2.531E-11
811	ADS1TYP1	1.320E-04	4.277E-05	-4.36881	5.972E-11
823	ADS2PSIo	-7.844E-05	1.228E+00	0.08907	-1.796E-11
824	ADS2PSIb	5.839E-05	1.127E+00	0.05180	1.132E-11
825	ADS2PSId	2.005E-05	1.043E+00	0.01846	-2.359E-12
2	H2O	0.000E+00	-1.285E-07	-0.00148	0.000E+00
330	H+1	1.000E-07	1.281E-07	-7.00000	0.000E+00

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
330	H+1	1.281E-07	-7.00000	1.00	0.78092	0.107
410	K+1	9.994E-02	-1.10765	1.00	0.78092	0.107
492	NO3-1	9.994E-02	-1.10763	-1.00	0.78092	0.107
811	ADS1TYP1	4.277E-05	-4.36881	0.00	1.00000	0.000
821	ADS2TYP1	1.665E-05	-4.77848	0.00	1.00000	0.000

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
8214920	=2SOH2NO3	3.171E-08	-7.49885	0.00	1.00000	5.350
3300020	OH-	1.285E-07	-6.99848	-1.00	0.78092	-13.890
8113300	=1SO-	5.734E-07	-6.24156	0.00	1.00000	-9.310
8113301	=1SOH2+	3.341E-05	-4.47607	0.00	1.00000	7.330
8114920	=1SOH2NO3	5.503E-05	-4.25944	0.00	1.00000	8.330
8114100	=1SOK	2.121E-07	-6.67347	0.00	1.00000	-8.310
8213300	=2SO-	4.097E-05	-4.38755	0.00	1.00000	-6.520
8213301	=2SOH2+	2.092E-05	-4.67942	0.00	1.00000	7.010
8214100	=2SOK	5.843E-05	-4.23340	0.00	1.00000	-5.310

Type III - SPECIES WITH FIXED ACTIVITY

ID No	Name	Conc (M)	New logK	Enthalpy
2	H2O	-1.285E-07	0.001	0.000
330	H+1	-9.113E-06	7.000	0.000

Type VI - EXCLUDED SPECIES (not included in mole balance)

ID No	Name	Conc (M)	New logK	Enthalpy
823	ADS2PSIo	1.228E+00	0.000	0.000
815	ADS1PSId	8.506E-01	0.000	0.000
814	ADS1PSIb	4.740E-01	0.000	0.000
813	ADS1PSIo	3.654E-01	0.000	0.000
825	ADS2PSId	1.043E+00	0.000	0.000
824	ADS2PSIb	1.127E+00	0.000	0.000

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

ADS2TYP1			
12.2	Percent bound in species #	821	ADS2TYP1
29.9	Percent bound in species #	8213300	=2SO-
15.3	Percent bound in species #	8213301	=2SOH2+
42.6	Percent bound in species #	8214100	=2SOK
K+1			
99.9	Percent bound in species #	410	K+1
NO3-1			
99.9	Percent bound in species #	492	NO3-1
ADS1PSIo			
38.1	Percent bound in species #	8113301	=1SOH2+
62.8	Percent bound in species #	8114920	=1SOH2NO3
ADS1PSIb			
100.4	Percent bound in species #	8114920	=1SOH2NO3
ADS1PSId			
ADS1TYP1			
32.4	Percent bound in species #	811	ADS1TYP1
25.3	Percent bound in species #	8113301	=1SOH2+
41.7	Percent bound in species #	8114920	=1SOH2NO3
ADS2PSIo			
52.2	Percent bound in species #	8213300	=2SO-
74.5	Percent bound in species #	8214100	=2SOK
ADS2PSIb			
100.1	Percent bound in species #	8214100	=2SOK
ADS2PSId			
H2O			
100.0	Percent bound in species #	3300020	OH-
H+1			
1.4	Percent bound in species #	330	H+1
362.7	Percent bound in species #	8113301	=1SOH2+
597.3	Percent bound in species #	8114920	=1SOH2NO3
227.1	Percent bound in species #	8213301	=2SOH2+

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
410	K+1	9.994E-02	99.9	5.864E-05	0.1	0.000E+00	0.0
492	NO3-1	9.994E-02	99.9	5.506E-05	0.1	0.000E+00	0.0
2	H2O	1.285E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	-4.492E-10	0.0	9.214E-06	100.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 9.994E-02 Sum of ANIONS 9.995E-02

PERCENT DIFFERENCE = 1.791E-03 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 9.994E-02

EQUILIBRIUM pH = 7.000

******** TRIPLE LAYER ADSORPTION MODEL ********

**** Parameters For Adsorbent Number 1 ****
Electrostatic Variables: psi0 = 0.025866 sig0 = 0.008021
psib = 0.019182 sigb = -.005016
psid = 0.004156 sigd = -.003005
Adsorbent Concentration (g/l): 8.174
Specific Surface Area (sq. meters/g): 129.00

**** Parameters For Adsorbent Number 2 ****
Electrostatic Variables: psi0 = -.005269 sig0 = -.003086
psib = -.003064 sigb = 0.002298
psid = -.001092 sigd = 0.000789
Adsorbent Concentration (g/l): 4.087
Specific Surface Area (sq. meters/g): 600.00

DATE ID NUMBER: 20000605
TIME ID NUMBER: 14065080

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components

MINTEQ version 4.02

Test1a.inp w/ CNURA modified database

COMPLETE OUTPUT

```
TEST1A - Compute total H+ of a solution of known pH.
This together with TEST1B illustrate a two run set to compute pH.
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 0 0 0 0 1 1 0 0 0
0    0    0
     330  0.000E+00   -2.50                    /H+1
     732  1.580E-03   -2.80                    /SO4-2
     410  7.700E-05   -4.11                    /K+1
     140  0.000E+00  -16.00                    /CO3-2

  3   2
3301403    21.6600    -0.5300                 /CO2 (g)
     330     2.5000     0.0000                 /H+1
```

Test1a.out
Complete output
w/ CNWRA modified database

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:13:38

TEST1A - Compute total H+ of a solution of known pH.
This together with TEST1B illustrate a two run set to compute pH.
Component file (COMP.DBS): comp.dbs COMP v4.02 02/12/2002
Thermodynamic file (THERMO.UNF): thermo.unf THERMO V4.02 02/05/2002
Gaussian DOM file (GAUSSIAN.DBS): gaussian.dbsGAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF): type6.unf TYPE6 V4.02 02/05/2002

Temperature (Celsius): 25.00
Units of concentration: MOLAL
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed only for those solids specified as ALLOWED
in the input file (if any).
Maximum iterations: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

---

330 0.000E+00 -2.50
732 1.580E-03 -2.80
410 7.700E-05 -4.11
140 0.000E+00 -16.00

H2O has been inserted as a COMPONENT
3 2
3301403 21.6600 -0.5300
330 2.5000 0.0000

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	3.162E-03	-2.500	0.000E+00
732	SO4-2	1.585E-03	-2.800	1.580E-03
410	K+1	7.762E-05	-4.110	7.700E-05
140	CO3-2	1.000E-16	-16.000	0.000E+00
2	H2O	1.000E+00	0.000	0.000E+00

Charge Balance: UNSPECIATED

Sum of CATIONS= 7.700E-05 Sum of ANIONS = 3.160E-03

PERCENT DIFFERENCE = 9.524E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:
SO4-2 Log activity guess: -2.92
CO3-2 Log activity guess: -16.66

PART 2 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:13:39

CONSTRAINTS ON COMPONENT ACTIVITIES

As specified, this chemical system is OPEN with respect to the following components:

H2O H+1 CO3-2

Activities of the following components are constrained by the species shown:

COMPONENT	SPECIES	TYPE
CO3-2	co2 (g)	3
H+1	H+1	3
H2O	H2O	3

PART 3 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:13:39

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL mol/L	DIFF FXN	LOG ACTVTY	RESIDUAL
0	SO4-2	1.580E-03	6.594E-07	-2.91757	5.014E-07
1	SO4-2	1.580E-03	4.193E-04	-2.91775	4.192E-04
2	SO4-2	1.580E-03	8.125E-06	-3.01997	7.967E-06
3	SO4-2	1.580E-03	1.693E-07	-3.02220	1.135E-08

ID No	Name	Total Conc(M)	Conc (M)	log Activity	Diff fxn
410	K+1	7.700E-05	7.649E-05	-4.14759	5.093E-11
732	SO4-2	1.580E-03	1.266E-03	-3.02224	3.557E-09
2	H2O	0.000E+00	-1.049E-05	-0.00004	0.000E+00
330	H+1	0.000E+00	3.398E-03	-2.50000	0.000E+00
140	CO3-2	0.000E+00	2.916E-17	-16.66004	0.000E+00

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
330	H+1	3.398E-03	-2.50000	1.00	0.93070	0.031
732	SO4-2	1.266E-03	-3.02224	-2.00	0.75031	0.125
410	K+1	7.649E-05	-4.14759	1.00	0.93070	0.031
140	CO3-2	2.916E-17	-16.66004	-2.00	0.75031	0.125

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
3307320	hso4-	3.132E-04	-3.53530	-1.00	0.93070	2.018
4107320	kso4-	5.106E-07	-6.32310	-1.00	0.93070	0.878
3300020	oh-	3.421E-12	-11.49704	-1.00	0.93070	-13.966
3301400	hco3-	1.588E-09	-8.83038	-1.00	0.93070	10.361
3301401	h2co3 (aq)	1.048E-05	-4.97904	0.00	1.00102	16.681

Type III - SPECIES WITH FIXED ACTIVITY

ID No	Name	Conc (M)	New logK	Enthalpy
2	H2O	-1.049E-05	0.000	0.000
330	H+1	-3.711E-03	2.500	0.000
3301403	co2 (g)	-1.049E-05	21.660	-0.530

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

K+1				
	99.3	Percent bound in species #	410	K+1
SO4-2				
	80.1	Percent bound in species #	732	SO4-2
	19.8	Percent bound in species #	3307320	hso4-
H2O				
	100.0	Percent bound in species #	3300020	oh-
H+1				
	91.0	Percent bound in species #	330	H+1
	8.4	Percent bound in species #	3307320	hso4-
CO3-2				
	100.0	Percent bound in species #	3301401	h2co3 (aq)

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
410	K+1	7.700E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	1.580E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	3.421E-12	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	3.732E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	1.049E-05	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 3.474E-03 Sum of ANIONS 2.846E-03

PERCENT DIFFERENCE = 9.936E+00 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 4.426E-03

EQUILIBRIUM pH = 2.500

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17133906

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components

Test1b.inp
MINTEQA2, ver. 4.02
w/ CNURA modified database

```
TEST1B - Compute equilibrium pH when 0.001 moles gibbsite is added
to the aqueous system of problem TEST1A.
25.00 MOLAL  0.000  0.00000E+00
0 0 1 1 0 0 0 0 1 1 0 0 0
0   0   0
    330  3.732E-03   -7.00                          /H+1
    732  1.580E-03   -2.80                          /SO4-2
    410  7.700E-05   -4.11                          /K+1
    140  0.000E+00  -16.00                          /CO3-2
     30  0.000E+00  -16.00                          /Al+3

  3   1
3301403    21.6600    -0.5300                       /CO2 (g)
  4   1
2003003    -8.7700    22.8000   1.000E-03           /GIBBSITE (C)
```

Test1b.out
Complete Output
w/ CNLWRA modified database

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:13:48

TEST1B - Compute equilibrium pH when 0.001 moles gibbsite is added
to the aqueous system of problem TEST1A.

Component file (COMP.DBS):	comp.dbs	COMP v4.02 02/12/2002
Thermodynamic file (THERMO.UNF):	thermo.unf	THERMO V4.02 02/05/2002
Gaussian DOM file (GAUSSIAN.DBS):	gaussian.dbs	GAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF):	type6.unf	TYPE6 V4.02 02/05/2002

Temperature (Celsius): 25.00
Units of concentration: MOLAL
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
Maximum iterations: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

330	3.732E-03	-7.00
732	1.580E-03	-2.80
410	7.700E-05	-4.11
140	0.000E+00	-16.00
30	0.000E+00	-16.00

H2O has been inserted as a COMPONENT

```
  3   1
3301403    21.6600    -0.5300
  4   1
2003003    -8.7700    22.8000   1.000E-03
```

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	1.000E-07	-7.000	3.732E-03
732	SO4-2	1.585E-03	-2.800	1.580E-03
410	K+1	7.762E-05	-4.110	7.700E-05
140	CO3-2	1.000E-16	-16.000	0.000E+00
30	Al+3	1.000E-16	-16.000	0.000E+00
2	H2O	1.000E+00	0.000	0.000E+00

Charge Balance: UNSPECIATED

Sum of CATIONS= 3.809E-03 Sum of ANIONS = 3.160E-03

PERCENT DIFFERENCE = 9.313E+00 (ANIONS - CATIONS)/(ANIONS + CATIONS)

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:
SO4-2 Log activity guess: -2.80
CO3-2 Log activity guess: -7.66

The following TYPE 4 solids have been pre-dissolved:
gibbsite

CONSTRAINTS ON COMPONENT ACTIVITIES

As specified, this chemical system is OPEN with respect to the following components:

H2O

Activities of the following components are constrained by the species shown:

COMPONENT	SPECIES	TYPE
CO3-2	co2 (g)	3
H2O	H2O	3

PART 3 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:13:48

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL mol/L	DIFF FXN	LOG ACTVTY	RESIDUAL
0	Al+3	1.000E-03	-1.000E-03	-16.00000	9.999E-04
1	Al+3	1.000E-03	-9.999E-04	-8.36062	9.998E-04
2	Al+3	1.000E-03	-6.494E-04	-4.23434	6.493E-04
3	Al+3	1.000E-03	1.245E-04	-3.80217	1.244E-04
4	Al+3	1.000E-03	2.100E-06	-3.83981	2.000E-06
5	Al+3	1.000E-03	-1.655E-07	-3.84058	6.555E-08

ID No	Name	Total Conc(M)	Conc (M)	log Activity	Diff fxn
330	H+1	7.320E-04	6.937E-04	-3.18698	-3.707E-09
732	SO4-2	1.580E-03	7.951E-04	-3.21211	-2.032E-08
410	K+1	7.700E-05	7.667E-05	-4.14351	-3.947E-10
30	Al+3	1.000E-03	2.586E-04	-3.84053	-1.577E-08
2	H2O	3.000E-03	2.987E-03	-0.00003	0.000E+00
140	CO3-2	0.000E+00	6.706E-16	-15.28606	0.000E+00

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
330	H+1	6.937E-04	-3.18698	1.00	0.93729	0.028
732	SO4-2	7.951E-04	-3.21211	-2.00	0.77178	0.113
410	K+1	7.667E-05	-4.14351	1.00	0.93729	0.028
140	CO3-2	6.706E-16	-15.28606	-2.00	0.77178	0.113
30	Al+3	2.586E-04	-3.84053	3.00	0.55828	0.253

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
4107320	kso4-	3.306E-07	-6.50888	-1.00	0.93729	0.875
3300020	oh-	1.652E-11	-10.81004	-1.00	0.93729	-13.969
303300	aloh+2	2.897E-06	-5.65057	2.00	0.77178	-4.884
303301	al(oh)2+	2.934E-08	-7.56062	1.00	0.93729	-10.066
303302	al(oh)4-	1.768E-14	-13.78070	-1.00	0.93729	-22.660
303303	al(oh)3 (aq)	8.492E-12	-11.07066	0.00	1.00081	-16.791
307320	also4+	7.336E-04	-3.16264	1.00	0.93729	3.918
307321	al(so4)2-	4.824E-06	-5.34475	-1.00	0.93729	4.948
3301400	hco3-	7.669E-09	-8.14339	-1.00	0.93729	10.358
3301401	h2co3 (aq)	1.049E-05	-4.97903	0.00	1.00081	16.681
3307320	hso4-	4.130E-05	-4.41215	-1.00	0.93729	2.015

Type III - SPECIES WITH FIXED ACTIVITY

ID No	Name	Conc (M)	New logK	Enthalpy
2	H2O	2.987E-03	0.000	0.000
3301403	co2 (g)	-1.049E-05	21.660	-0.530

Type V - UNDERSATURATED SOLIDS (not present at equilibrium)

ID No	Name	Conc (M)	New logK	Enthalpy
2003003	gibbsite	8.920E-04	-8.770	22.800
6003000	alohso4	2.314E-01	3.230	0.000
6003001	al4(oh)10so4	3.939E-10	-22.700	0.000
6041000	k-alum	5.773E-10	5.170	-30.209
6041001	alunite	2.044E-21	1.400	210.000
2003001	boehmite	1.388E-03	-8.578	117.696
2003002	diaspore	7.037E-02	-6.873	103.052
2003000	al(oh)3 (am)	8.324E-06	-10.800	111.000
3003000	al2o3	6.143E-09	-19.652	258.590

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

H+1				
	92.1	Percent bound in species #	330	H+1
	2.8	Percent bound in species #	3301401	h2co3 (aq)
	5.5	Percent bound in species #	3307320	hso4-
SO4-2				
	50.3	Percent bound in species #	732	SO4-2
	46.4	Percent bound in species #	307320	also4+
	2.6	Percent bound in species #	3307320	hso4-
K+1				
	99.6	Percent bound in species #	410	K+1
Al+3				
	25.9	Percent bound in species #	30	Al+3
	73.4	Percent bound in species #	307320	also4+
H2O				
	98.0	Percent bound in species #	303300	aloh+2
	2.0	Percent bound in species #	303301	al(oh)2+
CO3-2				
	99.9	Percent bound in species #	3301401	h2co3 (aq)

PART 5 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:13:48

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
330	H+1	7.530E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	1.580E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.700E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
30	Al+3	1.000E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	2.956E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	1.049E-05	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 2.286E-03 Sum of ANIONS 1.637E-03

PERCENT DIFFERENCE = 1.655E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 3.535E-03

EQUILIBRIUM pH = 3.187

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17134834

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
3003000	al2o3	-8.212	[2.000] 30 [3.000] 2 [-6.000]330
2003000	al(oh)3 (am)	-5.080	[1.000] 30 [3.000] 2 [-3.000]330
6003000	alohso4	-0.636	[-1.000]330 [1.000] 30 [1.000]732 [1.000] 2
6003001	al4(oh)10so4	-9.405	[-10.000]330 [4.000] 30 [1.000]732 [10.000] 2
6041000	k-alum	-9.239	[1.000]410 [1.000] 30 [2.000]732 [12.000] 2
6041001	alunite	-20.689	[1.000]410 [3.000] 30 [2.000]732 [6.000] 2
2003001	boehmite	-2.858	[-3.000]330 [1.000] 30 [2.000] 2
2003002	diaspore	-1.153	[-3.000]330 [1.000] 30 [2.000] 2
2003003	gibbsite	-2.571	[1.000] 30 [3.000] 2 [-3.000]330

Test2a.in
MINTEQA2, ver. 4.02
w/ CNLWRA modified database
COMPLETE OUTPUT

```
TEST2A - Typical groundwater with Ag+ added as a contaminant.
Solve for speciation at pH 7.0 and pe -3.21
14.00 MG/L   0.000  0.00000E+00
0 0 1 1 2 3 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00                    /H+1
      1  0.000E+00    3.21                    /E- (ENTERED AS PE)
     20  2.230E+00   -4.68                    /Ag+1
     30  2.000E-01   -5.13                    /Al+3
    150  4.800E+01   -2.92                    /Ca+2
    280  1.000E-01   -5.75                    /Fe+2
    281  1.000E-01   -5.75                    /Fe+3
    460  1.400E+02   -2.24                    /Mg+2
    470  4.000E-03   -7.14                    /Mn+2
    471  3.600E-02   -6.18                    /Mn+3
    410  2.900E+00   -4.13                    /K+1
    500  2.200E+01   -3.02                    /Na+1
    140  1.870E+02   -2.51                    /CO3-2
    130  3.000E-01   -5.43                    /Br-1
    180  1.500E+01   -3.37                    /Cl-1
    492  1.000E+00   -4.79                    /NO3-1
    580  9.000E-02   -6.02                    /PO4-3
    730  2.060E-01   -5.21                    /HS-1
    732  2.500E+01   -3.58                    /SO4-2
    992  4.320E+02   -2.14                    /Acetate
    967  1.370E+02   -3.14                    /Citrate
    963  1.370E+02   -2.64                    /EN

  3   5
2802810     0.0000     0.0000                /FE+3/FE+2
4704710     0.0000     0.0000                /MN+3/MN+2
7307320     0.0000     0.0000                /HS-/SO4-2
      1    -3.2100     0.0000                /E- (ENTERED AS PE)
    330     7.0000     0.0000                /H+1
  6   1
3028100     4.0080    30.8450                /HEMATITE
```

Test2a.out
Complete Output
w/CNWRA modified database

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:13:58

TEST2A - Typical groundwater with Ag+ added as a contaminant.
Solve for speciation at pH 7.0 and pe -3.21
Component file (COMP.DBS): comp.dbs COMP v4.02 02/12/2002
Thermodynamic file (THERMO.UNF): thermo.unf THERMO V4.02 02/05/2002
Gaussian DOM file (GAUSSIAN.DBS): gaussian.dbsGAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF): type6.unf TYPE6 V4.02 02/05/2002

Temperature (Celsius): 14.00
Units of concentration: mg/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
Maximum iterations: 500 and use convergence assist measure
The method used to compute activity coefficients is: Davies equation
Intermediate output file

330	0.000E+00	-7.00
1	0.000E+00	3.21
20	2.230E+00	-4.68
30	2.000E-01	-5.13
150	4.800E+01	-2.92
280	1.000E-01	-5.75
281	1.000E-01	-5.75
460	1.400E+02	-2.24
470	4.000E-03	-7.14
471	3.600E-02	-6.18
410	2.900E+00	-4.13
500	2.200E+01	-3.02
140	1.870E+02	-2.51
130	3.000E-01	-5.43
180	1.500E+01	-3.37
492	1.000E+00	-4.79
580	9.000E-02	-6.02
730	2.060E-01	-5.21
732	2.500E+01	-3.58
992	4.320E+02	-2.14
967	1.370E+02	-3.14
963	1.370E+02	-2.64

H2O has been inserted as a COMPONENT

3 5		
2802810	0.0000	0.0000
4704710	0.0000	0.0000
7307320	0.0000	0.0000
1	-3.2100	0.0000
330	7.0000	0.0000
6 1		
3028100	4.0080	30.8450

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	1.000E-07	-7.000	0.000E+00
1	E-1	1.622E+03	3.210	0.000E+00
20	Ag+1	2.089E-05	-4.680	2.230E+00
30	Al+3	7.413E-06	-5.130	2.000E-01
150	Ca+2	1.202E-03	-2.920	4.800E+01
280	Fe+2	1.778E-06	-5.750	1.000E-01
281	Fe+3	1.778E-06	-5.750	1.000E-01
460	Mg+2	5.754E-03	-2.240	1.400E+02
470	Mn+2	7.244E-08	-7.140	4.000E-03
471	Mn+3	6.607E-07	-6.180	3.600E-02
410	K+1	7.413E-05	-4.130	2.900E+00
500	Na+1	9.550E-04	-3.020	2.200E+01
140	CO3-2	3.090E-03	-2.510	1.870E+02
130	Br-1	3.715E-06	-5.430	3.000E-01
180	Cl-1	4.266E-04	-3.370	1.500E+01
492	NO3-1	1.622E-05	-4.790	1.000E+00

580	PO4-3	9.550E-07	-6.020	9.000E-02
730	HS-1	6.166E-06	-5.210	2.060E-01
732	SO4-2	2.630E-04	-3.580	2.500E+01
992	Acetate	7.244E-03	-2.140	4.320E+02
967	Citrate	7.244E-04	-3.140	1.370E+02
963	EtDiAm	2.291E-03	-2.640	1.370E+02
2	H2O	1.000E+00	0.000	0.000E+00

Charge Balance: UNSPECIATED

Sum of CATIONS= 1.502E-02 Sum of ANIONS = 1.671E-02

PERCENT DIFFERENCE = 5.345E+00 (ANIONS - CATIONS)/(ANIONS + CATIONS)

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:

Al+3	Log activity guess:	-9.71
Fe+2	Log activity guess:	-5.45
Fe+3	Log activity guess:	-21.97
Mn+2	Log activity guess:	-6.14
Mn+3	Log activity guess:	-35.42
CO3-2	Log activity guess:	-6.04
PO4-3	Log activity guess:	-11.92
HS-1	Log activity guess:	-6.83
SO4-2	Log activity guess:	-3.57

PART 2 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:13:58

CONSTRAINTS ON COMPONENT ACTIVITIES

As specified, this chemical system is OPEN with respect to the following components:

H2O H+1 E-1

Activities of the following components are constrained by the species shown:

COMPONENT	SPECIES	TYPE
HS-1	hs-/so4-2	3
Mn+2	mn+2/mn+3	3
Fe+2	fe+2/fe+3	3
E-1	E-1	3
H+1	H+1	3
H2O	H2O	3

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL mol/L	DIFF FXN	LOG ACTVTY	RESIDUAL
0	PO4-3	9.487E-07	1.401E-06	-11.92218	1.401E-06
1	PO4-3	9.487E-07	-4.418E-07	-12.23448	4.417E-07
2	PO4-3	9.487E-07	4.295E-07	-12.52920	4.294E-07
3	PO4-3	9.487E-07	-2.794E-07	-12.41112	2.793E-07
4	PO4-3	9.487E-07	-3.103E-08	-12.24860	3.094E-08
5	PO4-3	9.487E-07	-6.764E-10	-12.24089	5.815E-10
6	PO4-3	9.487E-07	2.732E-10	-12.24028	1.783E-10
7	PO4-3	9.487E-07	1.950E-10	-12.23991	1.001E-10
8	PO4-3	9.487E-07	1.117E-10	-12.23977	1.682E-11
9	Ag+1	2.070E-05	-1.869E-05	-12.27957	1.869E-05

ITERATIONS= 10: SOLID acanthite PRECIPITATES

ITERATIONS= 10: SOLID diaspore PRECIPITATES

CONSTRAINTS ON COMPONENT ACTIVITIES

As specified, this chemical system is OPEN with respect to the following components:

H2O H+1 E-1

Activities of the following components are constrained by the species shown:

COMPONENT	SPECIES	TYPE
Al+3	diaspore	4
HS-1	acanthite	4
SO4-2	hs-/so4-2	3
Mn+2	mn+2/mn+3	3
Fe+3	fe+2/fe+3	3
E-1	E-1	3
H+1	H+1	3
H2O	H2O	3

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL mol/L	DIFF FXN	LOG ACTVTY	RESIDUAL
10	Cl-1	4.236E-04	-5.532E-05	-3.43384	5.528E-05
11	Cl-1	4.236E-04	3.154E-04	-3.19082	3.153E-04
12	Cl-1	4.236E-04	1.989E-04	-3.26661	1.988E-04
13	Cl-1	4.236E-04	8.196E-05	-3.35700	8.191E-05
14	Cl-1	4.236E-04	2.480E-06	-3.43090	2.438E-06
15	Cl-1	4.236E-04	-4.881E-08	-3.43343	6.448E-09
16	Na+1	9.580E-04	-5.601E-07	-3.08100	4.643E-07
17	Cl-1	4.236E-04	4.380E-08	-3.43338	1.435E-09
18	Cl-1	4.236E-04	4.145E-06	-3.43342	4.103E-06
19	Cl-1	4.236E-04	-1.931E-06	-3.43765	1.888E-06
20	Cl-1	4.236E-04	-1.109E-06	-3.43567	1.066E-06
21	Cl-1	4.236E-04	-4.608E-07	-3.43453	4.185E-07
22	Cl-1	4.236E-04	-1.715E-07	-3.43406	1.291E-07
***	Temporarily holding ionic strength constant				
23	Mn+3	7.289E-07	-2.155E-10	-35.73196	1.426E-10
***	Releasing temporary hold on ionic strength				

ITERATIONS= 25: SOLID pyrite PRECIPITATES

CONSTRAINTS ON COMPONENT ACTIVITIES

As specified, this chemical system is OPEN with respect to the following components:

H2O H+1 E-1

Activities of the following components are constrained by the species shown:

COMPONENT	SPECIES	TYPE
Fe+2	pyrite	4
Al+3	diaspore	4
HS-1	acanthite	4
SO4-2	hs-/so4-2	3
Mn+2	mn+2/mn+3	3
Fe+3	fe+2/fe+3	3
E-1	E-1	3
H+1	H+1	3
H2O	H2O	3

PART 3 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:13:58

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL mol/L	DIFF FXN	LOG ACTVTY	RESIDUAL
25	Br-1	3.759E-06	-4.909E-07	-5.48573	4.905E-07
26	Br-1	3.759E-06	5.500E-07	-5.42495	5.495E-07
27	Br-1	3.759E-06	1.267E-08	-5.48425	1.229E-08
28	Mn+3	7.289E-07	-7.560E-11	-35.73170	2.709E-12

ID No	Name	Total Conc(M)	Conc (M)	log Activity	Diff fxn
180	Cl-1	4.236E-04	4.236E-04	-3.43382	-2.316E-10
992	Acetate	7.325E-03	6.887E-03	-2.22273	-3.984E-09
20	Ag+1	2.070E-05	2.000E-19	-18.75968	-3.617E-09
492	NO3-1	1.615E-05	1.612E-05	-4.85352	-8.830E-12
150	Ca+2	1.199E-03	9.758E-04	-3.25366	-2.133E-09
967	Citrate	7.253E-04	9.452E-06	-5.57133	-3.625E-10
580	PO4-3	9.487E-07	2.030E-12	-12.23939	-8.472E-13
460	Mg+2	5.767E-03	4.727E-03	-2.56842	-1.039E-08
963	EtDiAm	2.282E-03	3.406E-07	-6.46563	-3.810E-09
471	Mn+3	6.560E-07	6.534E-36	-35.73169	-1.363E-12
410	K+1	7.426E-05	7.398E-05	-4.19165	-4.007E-11
500	Na+1	9.580E-04	9.535E-04	-3.08143	-5.169E-10
140	CO3-2	3.120E-03	1.373E-06	-6.10537	-1.385E-09
130	Br-1	3.759E-06	3.759E-06	-5.48571	-2.056E-12
2	H2O	4.913E-20	3.079E-05	-0.00016	0.000E+00
330	H+1	-7.115E-20	1.150E-07	-7.00000	0.000E+00
1	E-1	1.855E-19	-8.668E-05	3.21000	0.000E+00
281	Fe+3	1.793E-06	1.106E-28	-28.50299	0.000E+00
470	Mn+2	7.289E-08	6.235E-07	-6.44818	0.000E+00
732	SO4-2	2.605E-04	1.882E-04	-3.96845	0.000E+00
730	HS-1	6.236E-06	6.864E-08	-7.22416	0.000E+00
30	Al+3	7.421E-06	1.294E-13	-13.43503	0.000E+00
280	Fe+2	1.793E-06	1.856E-12	-11.97440	0.000E+00

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
330	H+1	1.150E-07	-7.00000	1.00	0.86944	0.061
963	EtDiAm	3.406E-07	-6.46563	0.00	1.00493	-0.002
20	Ag+1	2.000E-19	-18.75968	1.00	0.86944	0.061
30	Al+3	1.294E-13	-13.43503	3.00	0.28390	0.547
150	Ca+2	9.758E-04	-3.25366	2.00	0.57143	0.243
280	Fe+2	1.856E-12	-11.97440	2.00	0.57143	0.243
281	Fe+3	1.106E-28	-28.50299	3.00	0.28390	0.547
460	Mg+2	4.727E-03	-2.56842	2.00	0.57143	0.243
470	Mn+2	6.235E-07	-6.44818	2.00	0.57143	0.243
471	Mn+3	6.534E-36	-35.73169	3.00	0.28390	0.547
410	K+1	7.398E-05	-4.19165	1.00	0.86944	0.061
500	Na+1	9.535E-04	-3.08143	1.00	0.86944	0.061
140	CO3-2	1.373E-06	-6.10537	-2.00	0.57143	0.243
130	Br-1	3.759E-06	-5.48571	-1.00	0.86944	0.061
180	Cl-1	4.236E-04	-3.43382	-1.00	0.86944	0.061
492	NO3-1	1.612E-05	-4.85352	-1.00	0.86944	0.061
580	PO4-3	2.030E-12	-12.23939	-3.00	0.28390	0.547
730	HS-1	6.864E-08	-7.22416	-1.00	0.86944	0.061
732	SO4-2	1.882E-04	-3.96845	-2.00	0.57143	0.243
992	Acetate	6.887E-03	-2.22273	-1.00	0.86944	0.061
967	Citrate	9.452E-06	-5.57133	-3.00	0.28390	0.547

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
5009673	nah[citrate]	7.623E-10	-9.17861	-1.00	0.86944	6.535
5009920	na[acetate]	2.711E-06	-5.56470	0.00	1.00493	-0.263
3307301	s-2	2.440E-18	-17.85572	-2.00	0.57143	-17.389
3300020	oh-	4.887E-08	-7.37174	-1.00	0.86944	-14.311
201300	agbr (aq)	2.252E-20	-19.64539	0.00	1.00493	4.598
201301	agbr2-	6.756E-23	-22.23109	-1.00	0.86944	7.561
201302	agbr3-2	1.337E-27	-27.11680	-2.00	0.57143	8.343

201800	agcl (aq)	1.566E-19	-18.80296	0.00	1.00493	3.388
201801	agcl2-	6.178E-21	-20.26994	-1.00	0.86944	5.418
201802	agcl3-2	2.409E-24	-23.86115	-2.00	0.57143	5.443
201803	agcl4-3	3.646E-27	-26.98497	-3.00	0.28390	6.057
203300	agoh (aq)	1.742E-24	-23.75684	0.00	1.00493	-11.999
203301	ag(oh)2-	1.980E-29	-28.76401	-1.00	0.86944	-23.943
204920	agno3 (aq)	1.358E-24	-23.86488	0.00	1.00493	-0.254
207300	aghs (aq)	6.738E-13	-12.16934	0.00	1.00493	13.812
207301	ag(hs)2-	5.851E-16	-15.29351	-1.00	0.86944	17.975
207320	agso4-	3.900E-22	-21.46974	-1.00	0.86944	1.319
209631	ag[ethylenediamine]	5.808E-21	-20.29676	1.00	0.86944	4.989
209632	ag[ethylenediamine]2	1.663E-24	-23.83993	1.00	0.86944	7.912
209633	agh[ethylenediamine]	3.260E-20	-19.72985	2.00	0.57143	12.738
209634	ag2[ethylenediamine]	5.729E-38	-37.48499	2.00	0.57143	6.743
209635	ag2[ethylenediamine]2	1.393E-37	-37.09914	2.00	0.57143	13.595
209636	ag[hethylenediamine]2	7.311E-21	-20.68283	3.00	0.28390	25.555
209637	agh[ethylenediamine]2	1.872E-30	-29.97082	2.00	0.57143	8.963
209921	ag[acetate]	5.313E-21	-20.27255	0.00	1.00493	0.708
209922	ag[acetate]2	2.989E-23	-22.58528	-1.00	0.86944	0.681
303300	aloh+2	3.090E-12	-11.75308	2.00	0.57143	-5.075
303301	al(oh)2+	3.399E-10	-9.52936	1.00	0.86944	-10.033
303302	al(oh)4-	5.948E-10	-9.28640	-1.00	0.86944	-23.790
303303	al(oh)3 (aq)	5.907E-10	-9.22653	0.00	1.00493	-16.793
307320	also4+	2.287E-14	-13.70141	1.00	0.86944	3.763
307321	al(so4)2-	3.380E-17	-16.53181	-1.00	0.86944	4.901
309671	al[citrate]	9.152E-10	-9.03637	0.00	1.00493	9.968
309672	al[citrate]2	5.877E-10	-9.77770	-3.00	0.28390	15.347
309673	alh[citrate]	8.024E-14	-13.15637	1.00	0.86944	12.911
1501400	cahco3+	1.027E-05	-5.04906	1.00	0.86944	11.371
1501401	caco3 (aq)	5.036E-07	-6.29581	0.00	1.00493	3.061
1503300	caoh+	4.783E-10	-9.38110	1.00	0.86944	-13.067
1504921	cano3+	3.089E-08	-7.57093	1.00	0.86944	0.597
1505800	cahpo4 (aq)	3.630E-08	-7.43791	0.00	1.00493	15.053
1505801	capo4-	8.723E-10	-9.12010	-1.00	0.86944	6.434
1505802	cah2po4+	3.396E-09	-8.52977	1.00	0.86944	21.024
1507320	caso4 (aq)	1.225E-05	-4.90976	0.00	1.00493	2.310
1509631	ca[ethylenediamine]	4.303E-10	-9.60929	2.00	0.57143	0.353
1509671	ca[citrate]	1.452E-04	-3.89883	-1.00	0.86944	4.987
1509672	cah[citrate]	2.745E-07	-6.55938	0.00	1.00493	9.263
1509673	cah2[citrate]	3.110E-11	-10.56799	1.00	0.86944	12.318
1509920	ca[acetate]	5.464E-05	-4.32324	1.00	0.86944	1.214
2801400	fehco3+	2.570E-14	-13.65077	1.00	0.86944	11.490
2803300	feoh+	2.064E-15	-14.74614	1.00	0.86944	-9.711
2803301	fe(oh)3-	1.763E-21	-20.81444	-1.00	0.86944	-29.779
2803302	fe(oh)2 (aq)	5.325E-20	-19.27157	0.00	1.00493	-21.299
2805800	feh2po4+	1.318E-16	-15.94079	1.00	0.86944	22.334
2805801	fehpo4 (aq)	5.742E-16	-15.23879	0.00	1.00493	15.973
2807300	fe(hs)2 (aq)	3.351E-18	-17.47273	0.00	1.00493	8.948
2807301	fe(hs)3-	2.517E-23	-22.65990	-1.00	0.86944	11.048
2807320	feso4 (aq)	2.462E-14	-13.60655	0.00	1.00493	2.334
2809631	fe[ethylenediamine]	1.156E-14	-14.18003	2.00	0.57143	4.503
2809632	fe[ethylenediamine]2	1.168E-17	-17.17567	2.00	0.57143	7.973
2809633	fe[ethylenediamine]3	1.101E-21	-21.20130	2.00	0.57143	10.413
2809671	fe[citrate]	4.121E-12	-11.44573	-1.00	0.86944	6.161
2809672	feh[citrate]	4.489E-15	-14.34573	0.00	1.00493	10.198
2809920	fe[acetate]	1.835E-13	-12.79713	1.00	0.86944	1.461
2811800	fecl+2	4.284E-31	-30.61117	2.00	0.57143	1.569
2811801	fecl2+	6.609E-34	-33.24063	1.00	0.86944	2.191
2811802	fecl3 (aq)	2.106E-38	-37.67445	0.00	1.00493	1.128
2813300	feoh+2	1.872E-24	-23.97076	2.00	0.57143	-2.225
2813301	fe(oh)2+	9.193E-20	-19.09731	1.00	0.86944	-4.533
2813302	fe(oh)3 (aq)	1.729E-21	-20.76014	0.00	1.00493	-13.259
2813303	fe(oh)4-	9.314E-23	-22.09164	-1.00	0.86944	-21.527
2813304	fe2(oh)2+4	5.310E-46	-46.24702	4.00	0.10662	-2.269
2813305	fe3(oh)4+5	1.921E-63	-64.23547	5.00	0.03027	-5.207
2814921	feno3+2	1.364E-32	-32.10818	2.00	0.57143	1.491
2815800	fehpo4+	6.537E-26	-25.24538	1.00	0.86944	22.558
2815801	feh2po4+2	2.250E-31	-30.89087	2.00	0.57143	24.095
2817320	feso4+	2.962E-29	-28.58923	1.00	0.86944	3.943
2817321	fe(so4)2-	7.447E-32	-31.18875	-1.00	0.86944	5.312
2819671	fe[citrate]	1.056E-21	-20.97432	0.00	1.00493	13.098
2819672	feh[citrate]	2.435E-27	-26.67432	1.00	0.86944	14.461
2819920	fe[acetate]	3.473E-27	-26.70232	2.00	0.57143	4.266
2819921	fe[acetate]2	4.837E-26	-25.37615	1.00	0.86944	7.633
2819922	fe[acetate]3	2.591E-26	-25.58448	0.00	1.00493	9.585
3301400	hco3-	2.490E-03	-2.66450	-1.00	0.86944	10.502
3301401	h2co3 (aq)	5.407E-04	-3.26491	0.00	1.00493	16.838
3305800	hpo4-2	3.015E-07	-6.76371	-2.00	0.57143	12.719
3305801	h2po4-	3.275E-07	-6.54558	-1.00	0.86944	19.755
3305802	h3po4	3.526E-12	-11.45060	0.00	1.00493	21.787

3307300	h2s (aq)	7.485E-08	-7.12365	0.00	1.00493	7.098
3307320	hso4-	8.894E-10	-9.11167	-1.00	0.86944	1.918
3309631	h[ethylenediamine]	7.199E-04	-3.20347	1.00	0.86944	10.323
3309632	h2[ethylenediamine]	1.562E-03	-3.04938	2.00	0.57143	17.659
3309671	h[citrate]	1.110E-06	-6.19780	-2.00	0.57143	6.617
3309672	h2[citrate]	4.342E-09	-8.42304	-1.00	0.86944	11.209
3309673	h3[citrate]	5.371E-13	-12.26780	0.00	1.00493	14.301
3309921	h[acetate]	3.384E-05	-4.46848	0.00	1.00493	4.752
4105800	khpo4-	7.669E-11	-10.17604	-1.00	0.86944	13.316
4107320	kso4-	4.580E-08	-7.39992	-1.00	0.86944	0.821
4109671	k[citrate]	3.496E-09	-8.69949	-2.00	0.57143	1.307
4109921	k[acetate]	2.290E-07	-6.63796	0.00	1.00493	-0.226
4601400	mgco3 (aq)	1.700E-06	-5.76750	0.00	1.00493	2.904
4601401	mghco3+	7.363E-05	-4.19373	1.00	0.86944	11.541
4603300	mgoh+	1.890E-08	-7.78430	1.00	0.86944	-12.155
4605800	mgpo4-	6.606E-11	-10.24085	-1.00	0.86944	4.628
4605801	mgh2po4+	3.471E-08	-7.52025	1.00	0.86944	21.348
4605802	mghpo4 (aq)	2.428E-07	-6.61267	0.00	1.00493	15.193
4607320	mgso4 (aq)	4.809E-05	-4.31580	0.00	1.00493	2.219
4609631	mg[ethylenediamine]	3.793E-09	-8.66405	2.00	0.57143	0.613
4609671	mg[citrate]	5.687E-04	-3.30591	-1.00	0.86944	4.895
4609672	mgh[citrate]	5.567E-07	-6.25221	0.00	1.00493	8.885
4609673	mgh2[citrate]	1.321E-10	-9.93975	1.00	0.86944	12.261
4609920	mg[acetate]	3.464E-04	-3.52115	1.00	0.86944	1.331
4700020	mno4-	1.762-100	-99.81473	-1.00	0.86944	-133.255
4700021	mno4-2	5.755E-87	-86.48302	-2.00	0.57143	-122.951
4701400	mnhco3+	1.612E-08	-7.85341	1.00	0.86944	11.761
4701800	mncl+	1.900E-10	-9.78200	1.00	0.86944	0.161
4701801	mncl2 (aq)	8.552E-14	-13.06582	0.00	1.00493	0.248
4701802	mncl3-	1.003E-17	-17.05965	-1.00	0.86944	-0.249
4703300	mnoh+	4.374E-11	-10.41992	1.00	0.86944	-10.911
4703301	mn(oh)3-	6.488E-21	-20.24867	-1.00	0.86944	-34.739
4703302	mn(oh)4-2	3.208E-27	-26.73684	-2.00	0.57143	-48.045
4704920	mn(no3)2 (aq)	2.843E-16	-15.54410	0.00	1.00493	0.609
4704921	mnno3+	9.100E-12	-11.10170	1.00	0.86944	0.261
4707320	mnso4 (aq)	5.927E-09	-8.22502	0.00	1.00493	2.189
4709631	mn[ethylenediamine]	1.406E-10	-10.09518	2.00	0.57143	3.062
4709632	mn[ethylenediamine]2	6.793E-15	-14.41096	2.00	0.57143	5.212
4709671	mn[citrate]	2.095E-08	-7.73951	-1.00	0.86944	4.341
4709672	mnh[citrate]	3.788E-10	-9.41951	0.00	1.00493	9.598
4709920	mn[acetate]	6.164E-08	-7.27091	1.00	0.86944	1.461
5001400	naco3-	1.908E-08	-7.78022	-1.00	0.86944	1.467
5001401	nahco3 (aq)	1.203E-06	-5.91766	0.00	1.00493	10.267
5005800	nahpo4-	1.531E-09	-8.87581	-1.00	0.86944	13.506
5007320	naso4-	5.422E-07	-6.32659	-1.00	0.86944	0.784
5009671	na[citrate]	4.356E-08	-7.60395	-2.00	0.57143	1.292
5009672	na2[citrate]	7.258E-11	-10.19993	-1.00	0.86944	1.595

Type III - SPECIES WITH FIXED ACTIVITY

ID No	Name	Conc (M)	New logK	Enthalpy
2	H2O	3.079E-05	0.000	0.000
330	H+1	-7.601E-03	7.000	0.000
1	E-1	-8.668E-05	-3.210	0.000
2802810	fe+2/fe+3	1.793E-06	13.319	-42.700
4704710	mn+2/mn+3	6.560E-07	26.074	-107.800
7307320	hs-/so4-2	1.143E-05	34.064	-60.140

Type IV - FINITE SOLIDS (present at equilibrium)

ID No	Name	Conc (M)	New logK	Enthalpy
1002000	acanthite	1.035E-05	37.744	-227.000
2003002	diaspore	7.418E-06	-7.565	103.052
1028003	pyrite	3.585E-06	18.843	-49.844

Type V - UNDERSATURATED SOLIDS (not present at equilibrium)

ID No	Name	Conc (M)	New logK	Enthalpy
3003000	al2o3	5.514E-07	-21.388	258.590
2003000	al(oh)3 (am)	1.046E-04	-11.545	111.000
6003000	alohso4	6.704E-08	3.230	0.000
6003001	al4(oh)10so4	3.888E-11	-22.700	0.000
6041000	k-alum	6.415E-21	5.373	-30.209
6041001	alunite	0.000E+00	-0.009	210.000

6015000	anhydrite	1.229E-03	4.312	7.200
5015000	aragonite	7.634E-02	8.242	12.000
5046000	artinite	2.238E-08	-10.407	120.257
2047001	birnessite	9.268E-30	-18.091	0.000
3047100	bixbyite	2.214E-30	-0.191	124.490
2003001	boehmite	1.573E-02	-9.368	117.696
4002000	bromyrite	4.185E-12	12.867	-84.500
2046000	brucite	6.640E-07	-17.609	113.996
7015004	cahpo4:2h2o	4.529E-04	19.149	-23.000
7015005	cahpo4	9.773E-04	19.483	-31.000
7015006	ca3(po4)2 (beta)	1.103E-05	29.282	-54.000
7015007	ca4h(po4)3:3h2o	2.222E-10	47.080	0.000
5015001	calcite	1.149E-01	8.419	8.000
4102000	cerargyrite	9.865E-13	10.188	-65.200
7002000	ag3po4	0.000E+00	17.590	0.000
5015004	dolomite (disordered)	1.570E-02	16.229	46.400
5015002	dolomite (ordered)	6.195E-02	16.825	39.500
6046000	epsomite	4.635E-05	2.204	-11.560
2028001	fe(oh)2	2.892E-12	-13.564	0.000
1028000	fes (ppt)	4.760E-10	2.876	11.000
4128100	fe(oh)2.7cl.3	2.549E-08	3.040	0.000
2028101	fe3(oh)8	6.256E-34	-20.222	0.000
6028100	fe2(so4)3	0.000E+00	2.110	242.028
2028100	ferrihydrite	6.502E-12	-3.683	73.374
2003003	gibbsite	4.298E-02	-8.931	95.395
2028102	goethite	3.973E-09	-0.898	60.584
1028001	greigite	1.439E-25	45.035	0.000
6015001	gypsum	2.479E-03	4.617	-1.000
4150000	halite	8.074E-09	-1.578	-3.700
3047000	hausmannite	2.395E-34	-63.856	421.000
5002000	ag2co3	5.600E-33	11.373	-42.150
3028001	hercynite	1.429E-08	-25.000	313.920
5015003	huntite	7.315E-07	29.245	107.780
5046001	hydromagnesite	1.085E-16	7.300	218.447
7015003	hydroxylapatite	2.220E-02	44.333	0.000
6028101	h-jarosite	0.000E+00	10.551	230.748
6041002	k-jarosite	0.000E+00	13.922	130.875
6050000	na-jarosite	0.000E+00	10.184	151.377
3028102	lepidocrocite	1.336E-09	-1.371	0.000
2015000	lime	5.565E-24	-34.001	193.910
1028002	mackinawite	2.520E-09	3.600	0.000
3028101	maghemite	4.051E-22	-6.386	0.000
3046001	magnesioferrite	4.935E-23	-18.732	278.920
5046002	magnesite	8.326E-02	7.594	-20.000
3028000	magnetite	1.647E-18	-4.802	208.526
2047100	manganite	1.003E-14	-25.340	0.000
6028000	melanterite	2.527E-14	2.347	-20.500
2046002	mg(oh)2 (active)	4.338E-08	-18.794	0.000
7046001	mghpo4:3h2o	2.327E-04	18.175	0.000
7046002	mg3(po4)2	1.247E-09	23.280	0.000
6050001	mirabilite	3.268E-09	1.647	-79.442
4147000	mncl2:4h2o	7.866E-17	-2.788	10.830
7047000	mn3(po4)2	1.157E-20	23.887	-8.870
7047001	mnhpo4	5.157E-01	25.400	0.000
1047000	mns (grn)	8.768E-08	-0.385	32.000
1047001	mns (pnk)	9.720E-11	-3.340	0.000
6047000	mnso4	3.674E-14	-3.018	64.840
6047100	mn2(so4)3	0.000E+00	4.614	163.427
3050000	natron	3.043E-11	1.753	-65.877
5046003	nesquehonite	6.810E-05	4.507	24.221
2047002	nsutite	3.581E-29	-17.504	0.000
2046001	periclase	6.797E-12	-22.599	151.230
2015001	portlandite	1.199E-13	-23.667	128.620
6002000	ag2so4	2.794E-37	4.934	-17.000
2047003	pyrochroite	5.086E-09	-15.845	97.010
2047000	pyrolusite	8.432E-29	-43.206	272.000
5047000	rhodochrosite	1.032E-02	10.567	1.880
5028000	siderite	1.129E-08	10.133	16.000
3046000	spinel	1.286E-13	-39.452	388.012
7028100	strengite	3.931E-15	26.337	9.360
73100	sulfur	2.462E-05	2.036	16.300
6050002	thenardite	3.060E-11	-0.383	9.121
5050001	thermonatrite	1.057E-13	-0.707	10.480
7028001	vivianite	3.951E-25	36.000	0.000
2028000	wustite	1.882E-10	-12.385	103.938
2002000	ag2o	3.984E-37	-12.880	45.620
2000	ag metal	4.643E-02	14.217	-105.790

Type VI - EXCLUDED SPECIES (not included in mole balance)

ID No	Name	Conc (M)	New logK	Enthalpy
3028100	hematite	6.230E-12	3.801	30.845
3300021	o2 (g)	0.000E+00	-86.926	571.660
3301404	ch4 (g)	2.219E-08	42.771	-257.133
3301403	co2 (g)	1.172E-02	18.174	-4.060
3307302	h2s (g)	6.107E-07	8.010	0.000

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

Cl-1			
100.0	Percent bound in species #	180	Cl-1
Acetate			
94.0	Percent bound in species #	992	Acetate
4.7	Percent bound in species #	4609920	mg[acetate]
Ag+1			
99.9	Percent bound in species #	207300	aghs (aq)
NO3-1			
99.8	Percent bound in species #	492	NO3-1
Ca+2			
81.4	Percent bound in species #	150	Ca+2
1.0	Percent bound in species #	1507320	caso4 (aq)
12.1	Percent bound in species #	1509671	ca[citrate]
4.6	Percent bound in species #	1509920	ca[acetate]
Citrate			
1.3	Percent bound in species #	967	Citrate
20.0	Percent bound in species #	1509671	ca[citrate]
78.4	Percent bound in species #	4609671	mg[citrate]
PO4-3			
3.8	Percent bound in species #	1505800	cahpo4 (aq)
31.8	Percent bound in species #	3305800	hpo4-2
34.5	Percent bound in species #	3305801	h2po4-
3.7	Percent bound in species #	4605801	mgh2po4+
25.6	Percent bound in species #	4605802	mghpo4 (aq)
Mg+2			
82.0	Percent bound in species #	460	Mg+2
1.3	Percent bound in species #	4601401	mghco3+
9.9	Percent bound in species #	4609671	mg[citrate]
6.0	Percent bound in species #	4609920	mg[acetate]
EtDiAm			
31.5	Percent bound in species #	3309631	h[ethylenediamine]
68.4	Percent bound in species #	3309632	h2[ethylenediamine]
Mn+3			
100.0	Percent bound in species #	471	Mn+3

K+1			
	99.6	Percent bound in species # 410	K+1
Na+1			
	99.5	Percent bound in species # 500	Na+1
CO3-2			
	79.8	Percent bound in species #3301400	hco3-
	17.3	Percent bound in species #3301401	h2co3 (aq)
	2.4	Percent bound in species #4601401	mghco3+
Br-1			
	100.0	Percent bound in species # 130	Br-1
H2O			
	66.8	Percent bound in species #3300020	oh-
	3.3	Percent bound in species # 303302	al(oh)4-
	2.4	Percent bound in species # 303303	al(oh)3 (aq)
	25.8	Percent bound in species #4603300	mgoh+
H+1			
	33.0	Percent bound in species #3301400	hco3-
	14.3	Percent bound in species #3301401	h2co3 (aq)
	9.6	Percent bound in species #3309631	h[ethylenediamine]
	41.4	Percent bound in species #3309632	h2[ethylenediamine]
E-1			
	100.0	Percent bound in species #4700021	mno4-2
Fe+3			
	97.0	Percent bound in species #2813301	fe(oh)2+
	1.8	Percent bound in species #2813302	fe(oh)3 (aq)
	1.1	Percent bound in species #2819671	fe[citrate]
Mn+2			
	85.5	Percent bound in species # 470	Mn+2
	2.2	Percent bound in species #4701400	mnhco3+
	2.9	Percent bound in species #4709671	mn[citrate]
	8.5	Percent bound in species #4709920	mn[acetate]
SO4-2			
	75.5	Percent bound in species # 732	SO4-2
	4.9	Percent bound in species #1507320	caso4 (aq)
	19.3	Percent bound in species #4607320	mgso4 (aq)
HS-1			
	47.8	Percent bound in species # 730	HS-1
	52.2	Percent bound in species #3307300	h2s (aq)
Al+3			
	11.2	Percent bound in species # 303301	al(oh)2+
	19.6	Percent bound in species # 303302	al(oh)4-

	19.5	Percent bound in species # 303303	al(oh)3 (aq)
	30.2	Percent bound in species # 309671	al[citrate]
	19.4	Percent bound in species # 309672	al[citrate]2
Fe+2			
	29.8	Percent bound in species # 280	Fe+2
	66.1	Percent bound in species #2809671	fe[citrate]
	2.9	Percent bound in species #2809920	fe[acetate]

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
180	Cl-1	4.236E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
992	Acetate	7.325E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
20	Ag+1	6.744E-13	0.0	0.000E+00	0.0	2.069E-05	100.0
492	NO3-1	1.615E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
150	Ca+2	1.199E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
967	Citrate	7.253E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	9.487E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	5.767E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
963	EtDiAm	2.282E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
471	Mn+3	6.534E-36	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.426E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
500	Na+1	9.580E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	3.120E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
130	Br-1	3.759E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	7.312E-08	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	7.538E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
1	E-1	-2.302E-86	100.0	0.000E+00	0.0	0.000E+00	0.0
281	Fe+3	9.481E-20	100.0	0.000E+00	0.0	0.000E+00	0.0
470	Mn+2	7.289E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	2.491E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
730	HS-1	1.435E-07	0.8	0.000E+00	0.0	1.752E-05	99.2
30	Al+3	3.032E-09	0.0	0.000E+00	0.0	7.418E-06	100.0
280	Fe+2	6.230E-12	0.0	0.000E+00	0.0	3.585E-06	100.0

Charge Balance: SPECIATED

Sum of CATIONS = 1.676E-02 Sum of ANIONS 1.095E-02

PERCENT DIFFERENCE = 2.100E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 2.134E-02

EQUILIBRIUM pH = 7.000

EQUILIBRIUM pe = -3.210 or Eh = -182.88 mv

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17135850

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
1002000	acanthite	0.000	[2.000] 20 [-1.000]330 [1.000]730
2000	ag metal	-1.333	[1.000] 20 [1.000] 1
5002000	ag2co3	-32.252	[2.000] 20 [1.000]140
2002000	ag2o	-36.400	[2.000] 20 [1.000] 2 [-2.000]330
7002000	ag3po4	-50.928	[3.000] 20 [1.000]580
6002000	ag2so4	-36.554	[2.000] 20 [1.000]732
3003000	al2o3	-6.259	[2.000] 30 [3.000] 2 [-6.000]330
2003000	al(oh)3 (am)	-3.981	[1.000] 30 [3.000] 2 [-3.000]330
6003000	alohso4	-7.174	[-1.000]330 [1.000] 30 [1.000]732
			[1.000] 2
6003001	al4(oh)10so4	-10.410	[-10.000]330 [4.000] 30 [1.000]732
			[10.000] 2
6041000	k-alum	-20.193	[1.000]410 [1.000] 30 [2.000]732
			[12.000] 2
6041001	alunite	-52.444	[1.000]410 [3.000] 30 [2.000]732
			[6.000] 2
6015000	anhydrite	-2.910	[1.000]150 [1.000]732
5015000	aragonite	-1.117	[1.000]150 [1.000]140
5046000	artinite	-7.650	[-2.000]330 [2.000]460 [1.000]140
			[5.000] 2
2047001	birnessite	-29.033	[-4.000]330 [-1.000] 1 [1.000]471
			[2.000] 2
3047100	bixbyite	-29.655	[-6.000]330 [2.000]471 [3.000] 2
2003001	boehmite	-1.803	[-3.000]330 [1.000] 30 [2.000] 2
4002000	bromyrite	-11.378	[1.000] 20 [1.000]130
2046000	brucite	-6.178	[1.000]460 [2.000] 2 [-2.000]330
7015004	cahpo4:2h2o	-3.344	[1.000]150 [1.000]330 [1.000]580
			[2.000] 2
7015005	cahpo4	-3.010	[1.000]150 [1.000]330 [1.000]580
7015006	ca3(po4)2 (beta)	-4.957	[3.000]150 [2.000]580
7015007	ca4h(po4)3:3h2o	-9.653	[4.000]150 [1.000]330 [3.000]580
			[3.000] 2
5015001	calcite	-0.940	[1.000]150 [1.000]140
4102000	cerargyrite	-12.006	[1.000] 20 [1.000]180
2003002	diaspore	0.000	[-3.000]330 [1.000] 30 [2.000] 2
5015004	dolomite (disordered)	-1.804	[1.000]150 [1.000]460 [2.000]140
5015002	dolomite (ordered)	-1.208	[1.000]150 [1.000]460 [2.000]140
6046000	epsomite	-4.334	[1.000]460 [1.000]732 [7.000] 2
2028001	fe(oh)2	-11.539	[1.000]280 [2.000] 2 [-2.000]330
1028000	fes (ppt)	-9.322	[1.000]280 [1.000]730 [-1.000]330
4128100	fe(oh)2.7cl.3	-7.594	[-2.700]330 [1.000]281 [2.700] 2
			[0.300]180
2028101	fe3(oh)8	-33.204	[-8.000]330 [2.000]281 [1.000]280
			[8.000] 2

ID No	Name	SI	Composition by stoich. of components
6028100	fe2(so4)3	-66.801	[2.000]281 [3.000]732
2028100	ferrihydrite	-11.187	[1.000]281 [3.000] 2 [-3.000]330
2003003	gibbsite	-1.367	[1.000] 30 [3.000] 2 [-3.000]330
2028102	goethite	-8.401	[1.000]281 [2.000] 2 [-3.000]330
1028001	greigite	-24.842	[-4.000]330 [2.000]281 [1.000]280 [4.000]730
6015001	gypsum	-2.606	[1.000]150 [1.000]732 [2.000] 2
4150000	halite	-8.093	[1.000]500 [1.000]180
3047000	hausmannite	-33.621	[3.000]470 [4.000] 2 [-8.000]330 [-2.000] 1
3028100	hematite	-14.454	[2.000]281 [3.000] 2 [-6.000]330
3028001	hercynite	-7.845	[-8.000]330 [1.000]280 [2.000] 30 [4.000] 2
5015003	huntite	-6.136	[3.000]460 [1.000]150 [4.000]140
5046001	hydromagnesite	-15.965	[5.000]460 [4.000]140 [-2.000]330 [6.000] 2
7015003	hydroxylapatite	-1.654	[5.000]150 [3.000]580 [1.000] 2 [-1.000]330
6028101	h-jarosite	-47.896	[-5.000]330 [3.000]281 [2.000]732 [7.000] 2
6041002	k-jarosite	-41.717	[-6.000]330 [1.000]410 [3.000]281 [2.000]732 [6.000] 2
6050000	na-jarosite	-44.344	[-6.000]330 [1.000]500 [3.000]281 [2.000]732 [6.000] 2
3028102	lepidocrocite	-8.874	[-3.000]330 [1.000]281 [2.000] 2
2015000	lime	-23.255	[-2.000]330 [1.000]150 [1.000] 2
1028002	mackinawite	-8.599	[1.000]280 [1.000]730 [-1.000]330
3028101	maghemite	-21.392	[-6.000]330 [2.000]281 [3.000] 2
3046001	magnesioferrite	-22.307	[-8.000]330 [1.000]460 [2.000]281 [4.000] 2
5046002	magnesite	-1.080	[1.000]460 [1.000]140
3028000	magnetite	-17.783	[-8.000]330 [2.000]281 [1.000]280 [4.000] 2
2047100	manganite	-13.999	[1.000]470 [2.000] 2 [-3.000]330 [-1.000] 1
6028000	melanterite	-13.597	[1.000]280 [1.000]732 [7.000] 2
2046002	mg(oh)2 (active)	-7.363	[1.000]460 [2.000] 2 [-2.000]330
7046001	mghpo4:3h2o	-3.633	[1.000]460 [1.000]330 [1.000]580 [3.000] 2
7046002	mg3(po4)2	-8.904	[3.000]460 [2.000]580
6050001	mirabilite	-8.486	[2.000]500 [1.000]732 [10.000] 2
4147000	mncl2:4h2o	-16.104	[1.000]470 [2.000]180 [4.000] 2
7047000	mn3(po4)2	-19.937	[3.000]470 [2.000]580
7047001	mnhpo4	-0.288	[1.000]470 [1.000]580 [1.000]330
1047000	mns (grn)	-7.057	[1.000]470 [1.000]730 [-1.000]330
1047001	mns (pnk)	-10.012	[1.000]470 [1.000]730 [-1.000]330
6047000	mnso4	-13.435	[1.000]470 [1.000]732
6047100	mn2(so4)3	-78.755	[2.000]471 [3.000]732
3050000	natron	-10.517	[2.000]500 [1.000]140 [10.000] 2
5046003	nesquehonite	-4.167	[1.000]460 [1.000]140 [3.000] 2
2047002	nsutite	-28.446	[-4.000]330 [-1.000] 1 [1.000]471 [2.000] 2

ID No	Name	SI	Composition by stoich. of components
2046001	periclase	-11.168	[-2.000]330 [1.000]460 [1.000] 2
2015001	portlandite	-12.921	[1.000]150 [2.000] 2 [-2.000]330
1028003	pyrite	0.000	[-2.000]330 [-2.000] 1 [1.000]280 [2.000]730
2047003	pyrochroite	-8.294	[1.000]470 [2.000] 2 [-2.000]330
2047000	pyrolusite	-28.074	[1.000]470 [2.000] 2 [-4.000]330 [-2.000] 1
5047000	rhodochrosite	-1.986	[1.000]470 [1.000]140
5028000	siderite	-7.947	[1.000]280 [1.000]140
3046000	spinel	-12.891	[-8.000]330 [1.000]460 [2.000] 30 [4.000] 2
7028100	strengite	-14.406	[1.000]281 [1.000]580 [2.000] 2
73100	sulfur	-4.609	[1.000]730 [-1.000]330 [-2.000] 1
6050002	thenardite	-10.514	[2.000]500 [1.000]732
5050001	thermonatrite	-12.976	[2.000]500 [1.000]140 [1.000] 2
7028001	vivianite	-24.403	[3.000]280 [2.000]580 [8.000] 2
2028000	wustite	-9.725	[-2.000]330 [0.947]280 [1.000] 2

Test2b.inp
L) modified CNWRA database
Only parts 1, 5, + 6 of output

```
TEST2B - Typical groundwater with Ag+ added as a comtaminant.
Same as problem TEST2A except ph = 5.0.
14.00 MG/L   0.000  0.00000E+00
0 0 1 1 0 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -5.00                    /H+1
      1  0.000E+00    3.21                    /E- (ENTERED AS PE)
     20  2.230E+00   -4.68                    /Ag+1
     30  2.000E-01   -5.13                    /Al+3
    150  4.800E+01   -2.92                    /Ca+2
    280  1.000E-01   -5.75                    /Fe+2
    281  1.000E-01   -5.75                    /Fe+3
    460  1.400E+02   -2.24                    /Mg+2
    470  4.000E-03   -7.14                    /Mn+2
    471  3.600E-02   -6.18                    /Mn+3
    410  2.900E+00   -4.13                    /K+1
    500  2.200E+01   -3.02                    /Na+1
    140  1.870E+02   -2.51                    /CO3-2
    130  3.000E-01   -5.43                    /Br-1
    180  1.500E+01   -3.37                    /Cl-1
    492  1.000E+00   -4.79                    /NO3-1
    580  9.000E-02   -6.02                    /PO4-3
    730  2.060E-01   -5.21                    /HS-1
    732  2.500E+01   -3.58                    /SO4-2
    992  4.320E+02   -2.14                    /Acetate
    967  1.370E+02   -3.14                    /Citrate
    963  1.370E+02   -2.64                    /EN

  3   5
2802810     0.0000     0.0000                /FE+3/FE+2
4704710     0.0000     0.0000                /MN+3/MN+2
7307320     0.0000     0.0000                /HS-/SO4-2
    330     5.0000     0.0000                /H+1
      1    -3.2100     0.0000                /E- (ENTERED AS PE)
  6   1
3028100     4.0080    30.8450                /HEMATITE
```

Test ●.out
2/13/02 Complete Output Parts 1,5,6
w/CNWRA modified database

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:14:11

TEST2B - Typical groundwater with Ag+ added as a comtaminant.
Same as problem TEST2A except ph = 5.0.
Component file (COMP.DBS): comp.dbs COMP v4.02 02/12/2002
Thermodynamic file (THERMO.UNF): thermo.unf THERMO V4.02 02/05/2002
Gaussian DOM file (GAUSSIAN.DBS): gaussian.dbsGAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF): type6.unf TYPE6 V4.02 02/05/2002

Temperature (Celsius): 14.00
Units of concentration: mg/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
Maximum iterations: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

330	0.000E+00	-5.00
1	0.000E+00	3.21
20	2.230E+00	-4.68
30	2.000E-01	-5.13
150	4.800E+01	-2.92
280	1.000E-01	-5.75
281	1.000E-01	-5.75
460	1.400E+02	-2.24
470	4.000E-03	-7.14
471	3.600E-02	-6.18
410	2.900E+00	-4.13
500	2.200E+01	-3.02
140	1.870E+02	-2.51
130	3.000E-01	-5.43
180	1.500E+01	-3.37
492	1.000E+00	-4.79
580	9.000E-02	-6.02
730	2.060E-01	-5.21
732	2.500E+01	-3.58
992	4.320E+02	-2.14
967	1.370E+02	-3.14
963	1.370E+02	-2.64

H2O has been inserted as a COMPONENT

3	5	
2802810	0.0000	0.0000
4704710	0.0000	0.0000
7307320	0.0000	0.0000
330	5.0000	0.0000
1	-3.2100	0.0000
6	1	
3028100	4.0080	30.8450

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	1.000E-05	-5.000	0.000E+00
1	E-1	1.622E+03	3.210	0.000E+00
20	Ag+1	2.089E-05	-4.680	2.230E+00
30	Al+3	7.413E-06	-5.130	2.000E-01
150	Ca+2	1.202E-03	-2.920	4.800E+01
280	Fe+2	1.778E-06	-5.750	1.000E-01
281	Fe+3	1.778E-06	-5.750	1.000E-01
460	Mg+2	5.754E-03	-2.240	1.400E+02
470	Mn+2	7.244E-08	-7.140	4.000E-03
471	Mn+3	6.607E-07	-6.180	3.600E-02
410	K+1	7.413E-05	-4.130	2.900E+00
500	Na+1	9.550E-04	-3.020	2.200E+01
140	CO3-2	3.090E-03	-2.510	1.870E+02
130	Br-1	3.715E-06	-5.430	3.000E-01
180	Cl-1	4.266E-04	-3.370	1.500E+01
492	NO3-1	1.622E-05	-4.790	1.000E+00

580	PO4-3	9.550E-07	-6.020	9.000E-02
730	HS-1	6.166E-06	-5.210	2.060E-01
732	SO4-2	2.630E-04	-3.580	2.500E+01
992	Acetate	7.244E-03	-2.140	4.320E+02
967	Citrate	7.244E-04	-3.140	1.370E+02
963	EtDiAm	2.291E-03	-2.640	1.370E+02
2	H2O	1.000E+00	0.000	0.000E+00

Charge Balance: UNSPECIATED

Sum of CATIONS= 1.502E-02 Sum of ANIONS = 1.671E-02

PERCENT DIFFERENCE = 5.345E+00 (ANIONS - CATIONS)/(ANIONS + CATIONS)

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:

Al+3	Log activity guess:	-5.49
Fe+2	Log activity guess:	-5.45
Fe+3	Log activity guess:	-21.97
Mn+2	Log activity guess:	-6.14
Mn+3	Log activity guess:	-35.42
CO3-2	Log activity guess:	-9.36
PO4-3	Log activity guess:	-15.72
HS-1	Log activity guess:	-5.68
SO4-2	Log activity guess:	-20.42

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
992	Acetate	7.325E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
492	NO3-1	1.615E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
20	Ag+1	3.981E-11	0.0	0.000E+00	0.0	2.070E-05	100.0
30	Al+3	7.421E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
150	Ca+2	1.199E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
967	Citrate	7.253E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	9.487E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	5.767E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
963	EtDiAm	2.282E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
471	Mn+3	6.641E-36	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.426E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
500	Na+1	9.581E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	3.120E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
130	Br-1	3.759E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
180	Cl-1	4.236E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	1.493E-09	100.0	0.000E+00	0.0	0.000E+00	0.0
1	E-1	-9.000-100	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	1.344E-02	100.0	0.000E+00	0.0	0.000E+00	0.0
281	Fe+3	6.904E-21	100.0	0.000E+00	0.0	0.000E+00	0.0
470	Mn+2	7.289E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	8.310E-21	100.0	0.000E+00	0.0	0.000E+00	0.0
730	HS-1	2.493E-04	93.4	0.000E+00	0.0	1.752E-05	6.6
280	Fe+2	4.754E-11	0.0	0.000E+00	0.0	3.585E-06	100.0

Charge Balance: SPECIATED

Sum of CATIONS = 1.803E-02 Sum of ANIONS 6.041E-03

PERCENT DIFFERENCE = 4.981E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 2.048E-02

EQUILIBRIUM pH = 5.000

EQUILIBRIUM pe = -3.210 or Eh = -182.88 mv

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17141169

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
1002000	acanthite	0.000	[2.000] 20 [-1.000]330 [1.000]730
2000	ag metal	-1.092	[1.000] 20 [1.000] 1
5002000	ag2co3	-35.029	[2.000] 20 [1.000]140
2002000	ag2o	-39.918	[2.000] 20 [1.000] 2 [-2.000]330
7002000	ag3po4	-53.802	[3.000] 20 [1.000]580
6002000	ag2so4	-52.554	[2.000] 20 [1.000]732
3003000	al2o3	-10.458	[2.000] 30 [3.000] 2 [-6.000]330
2003000	al(oh)3 (am)	-6.080	[1.000] 30 [3.000] 2 [-3.000]330
6003000	alohso4	-21.755	[-1.000]330 [1.000] 30 [1.000]732
			[1.000] 2
6003001	al4(oh)10so4	-31.290	[-10.000]330 [4.000] 30 [1.000]732
			[10.000] 2
6041000	k-alum	-49.254	[1.000]410 [1.000] 30 [2.000]732
			[12.000] 2
6041001	alunite	-73.704	[1.000]410 [3.000] 30 [2.000]732
			[6.000] 2
6015000	anhydrite	-19.365	[1.000]150 [1.000]732
5015000	aragonite	-4.349	[1.000]150 [1.000]140
5046000	artinite	-14.846	[-2.000]330 [2.000]460 [1.000]140
			[5.000] 2
2047001	birnessite	-37.017	[-4.000]330 [-1.000] 1 [1.000]471
			[2.000] 2
3047100	bixbyite	-41.623	[-6.000]330 [2.000]471 [3.000] 2
2003001	boehmite	-3.903	[-3.000]330 [1.000] 30 [2.000] 2
4002000	bromyrite	-11.136	[1.000] 20 [1.000]130
2046000	brucite	-10.146	[1.000]460 [2.000] 2 [-2.000]330
7015004	cahpo4:2h2o	-4.912	[1.000]150 [1.000]330 [1.000]580
			[2.000] 2
7015005	cahpo4	-4.578	[1.000]150 [1.000]330 [1.000]580
7015006	ca3(po4)2 (beta)	-12.067	[3.000]150 [2.000]580
7015007	ca4h(po4)3:3h2o	-18.331	[4.000]150 [1.000]330 [3.000]580
			[3.000] 2
5015001	calcite	-4.172	[1.000]150 [1.000]140
4102000	cerargyrite	-11.764	[1.000] 20 [1.000]180
2003002	diaspore	-2.100	[-3.000]330 [1.000] 30 [2.000] 2
5015004	dolomite (disordered)	-8.264	[1.000]150 [1.000]460 [2.000]140
5015002	dolomite (ordered)	-7.667	[1.000]150 [1.000]460 [2.000]140
6046000	epsomite	-20.784	[1.000]460 [1.000]732 [7.000] 2
2028001	fe(oh)2	-14.576	[1.000]280 [2.000] 2 [-2.000]330
1028000	fes (ppt)	-8.841	[1.000]280 [1.000]730 [-1.000]330
4128100	fe(oh)2.7cl.3	-12.030	[-2.700]330 [1.000]281 [2.700] 2
			[0.300]180
2028101	fe3(oh)8	-46.314	[-8.000]330 [2.000]281 [1.000]280
			[8.000] 2

ID No	Name	SI	Composition by stoich. of components
6028100	fe2(so4)3	-114.320	[2.000]281 [3.000]732
2028100	ferrihydrite	-16.224	[1.000]281 [3.000] 2 [-3.000]330
2003003	gibbsite	-3.466	[1.000] 30 [3.000] 2 [-3.000]330
2028102	goethite	-13.438	[1.000]281 [2.000] 2 [-3.000]330
1028001	greigite	-23.879	[-4.000]330 [2.000]281 [1.000]280 [4.000]730
6015001	gypsum	-19.060	[1.000]150 [1.000]732 [2.000] 2
4150000	halite	-8.090	[1.000]500 [1.000]180
3047000	hausmannite	-49.572	[3.000]470 [4.000] 2 [-8.000]330 [-2.000] 1
3028100	hematite	-24.528	[2.000]281 [3.000] 2 [-6.000]330
3028001	hercynite	-15.081	[-8.000]330 [1.000]280 [2.000] 30 [4.000] 2
5015003	huntite	-19.050	[3.000]460 [1.000]150 [4.000]140
5046001	hydromagnesite	-32.844	[5.000]460 [4.000]140 [-2.000]330 [6.000] 2
7015003	hydroxylapatite	-14.304	[5.000]150 [3.000]580 [1.000] 2 [-1.000]330
6028101	h-jarosite	-87.969	[-5.000]330 [3.000]281 [2.000]732 [7.000] 2
6041002	k-jarosite	-83.789	[-6.000]330 [1.000]410 [3.000]281 [2.000]732 [6.000] 2
6050000	na-jarosite	-86.416	[-6.000]330 [1.000]500 [3.000]281 [2.000]732 [6.000] 2
3028102	lepidocrocite	-13.911	[-3.000]330 [1.000]281 [2.000] 2
2015000	lime	-27.227	[-2.000]330 [1.000]150 [1.000] 2
1028002	mackinawite	-8.117	[1.000]280 [1.000]730 [-1.000]330
3028101	maghemite	-31.466	[-6.000]330 [2.000]281 [3.000] 2
3046001	magnesioferrite	-36.349	[-8.000]330 [1.000]460 [2.000]281 [4.000] 2
5046002	magnesite	-4.307	[1.000]460 [1.000]140
3028000	magnetite	-30.894	[-8.000]330 [2.000]281 [1.000]280 [4.000] 2
2047100	manganite	-19.982	[1.000]470 [2.000] 2 [-3.000]330 [-1.000] 1
6028000	melanterite	-29.116	[1.000]280 [1.000]732 [7.000] 2
2046002	mg(oh)2 (active)	-11.331	[1.000]460 [2.000] 2 [-2.000]330
7046001	mghpo4:3h2o	-5.197	[1.000]460 [1.000]330 [1.000]580 [3.000] 2
7046002	mg3(po4)2	-16.001	[3.000]460 [2.000]580
6050001	mirabilite	-24.963	[2.000]500 [1.000]732 [10.000] 2
4147000	mncl2:4h2o	-16.086	[1.000]470 [2.000]180 [4.000] 2
7047000	mn3(po4)2	-27.079	[3.000]470 [2.000]580
7047001	mnhpo4	-1.867	[1.000]470 [1.000]580 [1.000]330
1047000	mns (grn)	-7.523	[1.000]470 [1.000]730 [-1.000]330
1047001	mns (pnk)	-10.478	[1.000]470 [1.000]730 [-1.000]330
6047000	mnso4	-29.900	[1.000]470 [1.000]732
6047100	mn2(so4)3	-128.167	[2.000]471 [3.000]732
3050000	natron	-13.772	[2.000]500 [1.000]140 [10.000] 2
5046003	nesquehonite	-7.394	[1.000]460 [1.000]140 [3.000] 2
2047002	nsutite	-36.430	[-4.000]330 [-1.000] 1 [1.000]471 [2.000] 2

ID No	Name	SI	Composition by stoich. of components
2046001	periclase	-15.136	[-2.000]330 [1.000]460 [1.000] 2
2015001	portlandite	-16.894	[1.000]150 [2.000] 2 [-2.000]330
1028003	pyrite	0.000	[-2.000]330 [-2.000] 1 [1.000]280 [2.000]730
2047003	pyrochroite	-12.277	[1.000]470 [2.000] 2 [-2.000]330
2047000	pyrolusite	-36.058	[1.000]470 [2.000] 2 [-4.000]330 [-2.000] 1
5047000	rhodochrosite	-5.229	[1.000]470 [1.000]140
5028000	siderite	-10.243	[1.000]280 [1.000]140
3046000	spinel	-21.058	[-8.000]330 [1.000]460 [2.000] 30 [4.000] 2
7028100	strengite	-17.038	[1.000]281 [1.000]580 [2.000] 2
73100	sulfur	-5.090	[1.000]730 [-1.000]330 [-2.000] 1
6050002	thenardite	-26.992	[2.000]500 [1.000]732
5050001	thermonatrite	-16.231	[2.000]500 [1.000]140 [1.000] 2
7028001	vivianite	-28.705	[3.000]280 [2.000]580 [8.000] 2
2028000	wustite	-12.813	[-2.000]330 [0.947]280 [1.000] 2

ID No	Name	SI	Composition by stoich. of components
2046001	periclase	-15.136	[-2.000]330 [1.000]460 [1.000] 2
2015001	portlandite	-16.894	[1.000]150 [2.000] 2 [-2.000]330
1028003	pyrite	0.000	[-2.000]330 [-2.000] 1 [1.000]280 [2.000]730
2047003	pyrochroite	-12.277	[1.000]470 [2.000] 2 [-2.000]330
2047000	pyrolusite	-36.058	[1.000]470 [2.000] 2 [-4.000]330 [-2.000] 1
5047000	rhodochrosite	-5.229	[1.000]470 [1.000]140
5028000	siderite	-10.243	[1.000]280 [1.000]140
3046000	spinel	-21.058	[-8.000]330 [1.000]460 [2.000] 30 [4.000] 2
7028100	strengite	-17.038	[1.000]281 [1.000]580 [2.000] 2
73100	sulfur	-5.090	[1.000]730 [-1.000]330 [-2.000] 1
6050002	thenardite	-26.992	[2.000]500 [1.000]732
5050001	thermonatrite	-16.231	[2.000]500 [1.000]140 [1.000] 2
7028001	vivianite	-28.705	[3.000]280 [2.000]580 [8.000] 2
2028000	wustite	-12.813	[-2.000]330 [0.947]280 [1.000] 2

Test 2c.inp
w/ modified CNWRA database
Only parts 1 & 5 of output for each pH sweep.

```
TEST2A - Typical groundwater with Ag+ added as a contaminant.
Sweep pH from 7.0 to 5.0 in increments of -0.5 pH units.
14.00 MG/L   0.000  0.00000E+00
0 0 1 1 0 0 0 0 1 2 1 2 1
 5 H+1                    ACTIVITY   mol/L
1 330   1.000
  7.00  -0.50
TEST2C.PRN         20      732
0   0   0
    330  0.000E+00   -7.00                    /H+1
      1  0.000E+00    3.21                    /E- (ENTERED AS PE)
     20  2.230E+00   -4.68                    /Ag+1
     30  2.000E-01   -5.13                    /Al+3
    150  4.800E+01   -2.92                    /Ca+2
    280  1.000E-01   -5.75                    /Fe+2
    281  1.000E-01   -5.75                    /Fe+3
    460  1.400E+02   -2.24                    /Mg+2
    470  4.000E-03   -7.14                    /Mn+2
    471  3.600E-02   -6.18                    /Mn+3
    410  2.900E+00   -4.13                    /K+1
    500  2.200E+01   -3.02                    /Na+1
    140  1.870E+02   -2.51                    /CO3-2
    130  3.000E-01   -5.43                    /Br-1
    180  1.500E+01   -3.37                    /Cl-1
    492  1.000E+00   -4.79                    /NO3-1
    580  9.000E-02   -6.02                    /PO4-3
    730  2.060E-01   -5.21                    /HS-1
    732  2.500E+01   -3.58                    /SO4-2
    992  4.320E+02   -2.14                    /Acetate
    967  1.370E+02   -3.14                    /Citrate
    963  1.370E+02   -2.64                    /EN

  3   5
2802810     0.0000     0.0000                /FE+3/FE+2
4704710     0.0000     0.0000                /MN+3/MN+2
7307320     0.0000     0.0000                /HS-/SO4-2
    330     9.0000     0.0000                /H+1
      1    -3.2100     0.0000                /E- (ENTERED AS PE)
  6   1
3028100     4.0080    30.8450                /HEMATITE
```

Test2c.out
Parts 1,5,6 Output
Test2c.prn
4) CNURA modified database

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:14:20

TEST2A - Typical groundwater with Ag+ added as a contaminant.
Sweep pH from 7.0 to 5.0 in increments of -0.5 pH units.
Component file (COMP.DBS): comp.dbs COMP v4.02 02/12/2002
Thermodynamic file (THERMO.UNF): thermo.unf THERMO V4.02 02/05/2002
Gaussian DOM file (GAUSSIAN.DBS): gaussian.dbsGAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF): type6.unf TYPE6 V4.02 02/05/2002

Temperature (Celsius): 14.00
Units of concentration: mg/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
Maximum iterations: 200
The method used to compute activity coefficients is: Davies equation
Abbreviated output file

330	0.000E+00	-7.00
1	0.000E+00	3.21
20	2.230E+00	-4.68
30	2.000E-01	-5.13
150	4.800E+01	-2.92
280	1.000E-01	-5.75
281	1.000E-01	-5.75
460	1.400E+02	-2.24
470	4.000E-03	-7.14
471	3.600E-02	-6.18
410	2.900E+00	-4.13
500	2.200E+01	-3.02
140	1.870E+02	-2.51
130	3.000E-01	-5.43
180	1.500E+01	-3.37
492	1.000E+00	-4.79
580	9.000E-02	-6.02
730	2.060E-01	-5.21
732	2.500E+01	-3.58
992	4.320E+02	-2.14
967	1.370E+02	-3.14
963	1.370E+02	-2.64

H2O has been inserted as a COMPONENT

3	5	
2802810	0.0000	0.0000
4704710	0.0000	0.0000
7307320	0.0000	0.0000
330	9.0000	0.0000
1	-3.2100	0.0000
6	1	
3028100	4.0080	30.8450

Charge Balance: UNSPECIATED

Sum of CATIONS= 1.502E-02 Sum of ANIONS = 1.671E-02

PERCENT DIFFERENCE = 5.345E+00 (ANIONS - CATIONS)/(ANIONS + CATIONS)

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:

Al+3	Log activity guess:	-17.28
Fe+2	Log activity guess:	-5.52
Fe+3	Log activity guess:	-22.05
Mn+2	Log activity guess:	-6.14
Mn+3	Log activity guess:	-35.43
CO3-2	Log activity guess:	-3.96
PO4-3	Log activity guess:	-9.51
HS-1	Log activity guess:	-24.83

SO4-2 Log activity guess: -3.57

```
--------------------------------------------------------------------------------
*** TITRATION: H+1
*** Titration point  1 in the series of  5 ***
    The series of  5 fixed pH values are:
        7.00   6.50   6.00   5.50   5.00
*** The fixed pH for this point is:    7.00

--------------------------------------------------------------------------------
```

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:14:20

TEST2A - Typical groundwater with Ag+ added as a contaminant.
Sweep pH from 7.0 to 5.0 in increments of -0.5 pH units.

Component file (COMP.DBS):	comp.dbs	COMP v4.02 02/12/2002
Thermodynamic file (THERMO.UNF):	thermo.unf	THERMO V4.02 02/05/2002
Gaussian DOM file (GAUSSIAN.DBS):	gaussian.dbs	GAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF):	type6.unf	TYPE6 V4.02 02/05/2002

Temperature (Celsius): 14.00
Units of concentration: mg/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
Maximum iterations: 200
The method used to compute activity coefficients is: Davies equation
Abbreviated output file

330	0.000E+00	-7.00
1	0.000E+00	3.21
20	2.230E+00	-4.68
30	2.000E-01	-5.13
150	4.800E+01	-2.92
280	1.000E-01	-5.75
281	1.000E-01	-5.75
460	1.400E+02	-2.24
470	4.000E-03	-7.14
471	3.600E-02	-6.18
410	2.900E+00	-4.13
500	2.200E+01	-3.02
140	1.870E+02	-2.51
130	3.000E-01	-5.43
180	1.500E+01	-3.37
492	1.000E+00	-4.79
580	9.000E-02	-6.02
730	2.060E-01	-5.21
732	2.500E+01	-3.58
992	4.320E+02	-2.14
967	1.370E+02	-3.14
963	1.370E+02	-2.64

H2O has been inserted as a COMPONENT

3	5	
2802810	0.0000	0.0000
4704710	0.0000	0.0000
7307320	0.0000	0.0000
330	9.0000	0.0000
1	-3.2100	0.0000
6	1	
3028100	4.0080	30.8450

Charge Balance: UNSPECIATED

Sum of CATIONS= 1.502E-02 Sum of ANIONS = 1.671E-02

PERCENT DIFFERENCE = 5.345E+00 (ANIONS - CATIONS)/(ANIONS + CATIONS)

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:

Al+3	Log activity guess:	-17.28
Fe+2	Log activity guess:	-5.52
Fe+3	Log activity guess:	-22.05
Mn+2	Log activity guess:	-6.14
Mn+3	Log activity guess:	-35.43
CO3-2	Log activity guess:	-3.96
PO4-3	Log activity guess:	-9.51
HS-1	Log activity guess:	-24.83
SO4-2	Log activity guess:	-3.57

*** TITRATION: H+1
*** Titration point 1 in the series of 5 ***
The series of 5 fixed pH values are:
7.00 6.50 6.00 5.50 5.00
*** The fixed pH for this point is: 7.00

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
992	Acetate	7.325E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
180	Cl-1	4.236E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
20	Ag+1	6.744E-13	0.0	0.000E+00	0.0	2.069E-05	100.0
492	NO3-1	1.615E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
150	Ca+2	1.199E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
967	Citrate	7.253E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	9.487E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	5.767E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
963	EtDiAm	2.282E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
471	Mn+3	6.534E-36	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.426E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
500	Na+1	9.580E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	3.120E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
130	Br-1	3.759E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	7.312E-08	100.0	0.000E+00	0.0	0.000E+00	0.0
1	E-1	-2.302E-86	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	7.538E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
281	Fe+3	9.481E-20	100.0	0.000E+00	0.0	0.000E+00	0.0
470	Mn+2	7.289E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	2.491E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
730	HS-1	1.435E-07	0.8	0.000E+00	0.0	1.752E-05	99.2
30	Al+3	3.032E-09	0.0	0.000E+00	0.0	7.418E-06	100.0
280	Fe+2	6.230E-12	0.0	0.000E+00	0.0	3.585E-06	100.0

Charge Balance: SPECIATED

Sum of CATIONS = 1.676E-02 Sum of ANIONS 1.095E-02

PERCENT DIFFERENCE = 2.100E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 2.134E-02

EQUILIBRIUM pH = 7.000

EQUILIBRIUM pe = -3.210 or Eh = -182.88 mv

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17142058
ACCESSORY OUTPUT FILE: TEST2C.PRN

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:14:20

*** TITRATION: H+1
*** Titration point 2 in the series of 5 ***
*** The fixed pH for this point is: 6.50

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
992	Acetate	7.325E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
180	Cl-1	4.236E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
20	Ag+1	5.716E-11	0.0	0.000E+00	0.0	2.070E-05	100.0
492	NO3-1	1.615E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
150	Ca+2	1.199E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
967	Citrate	7.253E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	9.487E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	5.767E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
963	EtDiAm	2.282E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
471	Mn+3	6.638E-36	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.426E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
500	Na+1	9.580E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	3.120E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
130	Br-1	3.759E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	2.639E-08	100.0	0.000E+00	0.0	0.000E+00	0.0
1	E-1	-2.336E-90	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	8.939E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
281	Fe+3	1.625E-25	100.0	0.000E+00	0.0	0.000E+00	0.0
470	Mn+2	7.289E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	6.293E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
730	HS-1	2.430E-04	93.3	0.000E+00	0.0	1.752E-05	6.7
30	Al+3	4.818E-08	0.6	0.000E+00	0.0	7.373E-06	99.4
280	Fe+2	1.303E-16	0.0	0.000E+00	0.0	3.585E-06	100.0

Charge Balance: SPECIATED

Sum of CATIONS = 1.734E-02 Sum of ANIONS 9.880E-03

PERCENT DIFFERENCE = 2.741E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 2.143E-02

EQUILIBRIUM pH = 6.500

EQUILIBRIUM pe = -3.210 or Eh = -182.88 mv

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17142064
ACCESSORY OUTPUT FILE: TEST2C.PRN

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:14:20

*** TITRATION: H+1
*** Titration point 3 in the series of 5 ***
*** The fixed pH for this point is: 6.00

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
992	Acetate	7.325E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
180	Cl-1	4.236E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
20	Ag+1	4.707E-11	0.0	0.000E+00	0.0	2.070E-05	100.0
492	NO3-1	1.615E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
150	Ca+2	1.199E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
967	Citrate	7.253E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	9.487E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	5.767E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
963	EtDiAm	2.282E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
471	Mn+3	6.673E-36	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.426E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
500	Na+1	9.580E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	3.120E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
130	Br-1	3.759E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	1.599E-08	100.0	0.000E+00	0.0	0.000E+00	0.0
1	E-1	-2.354E-94	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	1.027E-02	100.0	0.000E+00	0.0	0.000E+00	0.0
281	Fe+3	2.069E-24	100.0	0.000E+00	0.0	0.000E+00	0.0
470	Mn+2	7.289E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	7.638E-11	100.0	0.000E+00	0.0	0.000E+00	0.0
730	HS-1	2.493E-04	93.4	0.000E+00	0.0	1.752E-05	6.6
30	Al+3	1.407E-06	19.0	0.000E+00	0.0	6.014E-06	81.0
280	Fe+2	6.788E-15	0.0	0.000E+00	0.0	3.585E-06	100.0

Charge Balance: SPECIATED

Sum of CATIONS = 1.759E-02 Sum of ANIONS 8.787E-03

PERCENT DIFFERENCE = 3.338E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 2.125E-02

EQUILIBRIUM pH = 6.000

EQUILIBRIUM pe = -3.210 or Eh = -182.88 mv

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17142069
ACCESSORY OUTPUT FILE: TEST2C.PRN

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:14:20

*** TITRATION: H+1
*** Titration point 4 in the series of 5 ***
*** The fixed pH for this point is: 5.50

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
992	Acetate	7.325E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
180	Cl-1	4.236E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
20	Ag+1	4.173E-11	0.0	0.000E+00	0.0	2.070E-05	100.0
492	NO3-1	1.615E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
150	Ca+2	1.199E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
967	Citrate	7.253E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	9.487E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	5.767E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
963	EtDiAm	2.282E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
471	Mn+3	6.677E-36	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.426E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
500	Na+1	9.580E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	3.120E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
130	Br-1	3.759E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
30	Al+3	7.421E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	7.155E-09	100.0	0.000E+00	0.0	0.000E+00	0.0
1	E-1	-2.416E-98	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	1.161E-02	100.0	0.000E+00	0.0	0.000E+00	0.0
281	Fe+3	9.686E-23	100.0	0.000E+00	0.0	0.000E+00	0.0
470	Mn+2	7.289E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	8.116E-16	100.0	0.000E+00	0.0	0.000E+00	0.0
730	HS-1	2.493E-04	93.4	0.000E+00	0.0	1.752E-05	6.6
280	Fe+2	5.508E-13	0.0	0.000E+00	0.0	3.585E-06	100.0

Charge Balance: SPECIATED

Sum of CATIONS = 1.777E-02 Sum of ANIONS 7.612E-03

PERCENT DIFFERENCE = 4.003E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 2.092E-02

EQUILIBRIUM pH = 5.500

EQUILIBRIUM pe = -3.210 or Eh = -182.88 mv

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17142080
ACCESSORY OUTPUT FILE: TEST2C.PRN

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:14:20

*** TITRATION: H+1
*** Titration point 5 in the series of 5 ***
*** The fixed pH for this point is: 5.00

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
992	Acetate	7.325E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
180	Cl-1	4.236E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
20	Ag+1	3.982E-11	0.0	0.000E+00	0.0	2.069E-05	100.0
492	NO3-1	1.615E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
150	Ca+2	1.199E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
967	Citrate	7.253E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	9.487E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	5.767E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
963	EtDiAm	2.282E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
471	Mn+3	6.640E-36	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.426E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
500	Na+1	9.580E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	3.120E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
130	Br-1	3.759E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
30	Al+3	7.421E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	1.493E-09	100.0	0.000E+00	0.0	0.000E+00	0.0
1	E-1	-9.000-100	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	1.344E-02	100.0	0.000E+00	0.0	0.000E+00	0.0
281	Fe+3	6.904E-21	100.0	0.000E+00	0.0	0.000E+00	0.0
470	Mn+2	7.289E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	8.310E-21	100.0	0.000E+00	0.0	0.000E+00	0.0
730	HS-1	2.493E-04	93.4	0.000E+00	0.0	1.752E-05	6.6
280	Fe+2	4.754E-11	0.0	0.000E+00	0.0	3.585E-06	100.0

Charge Balance: SPECIATED

Sum of CATIONS = 1.803E-02 Sum of ANIONS 6.041E-03

PERCENT DIFFERENCE = 4.980E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 2.048E-02

EQUILIBRIUM pH = 5.000

EQUILIBRIUM pe = -3.210 or Eh = -182.88 mv

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17142086
ACCESSORY OUTPUT FILE: TEST2C.PRN

Test 2c.prn

20020213	17142058	330	7.00	1	-3.21	20	0.0	0.0	100.0	732	100.0	0.0	0.0
20020213	17142064	330	6.50	1	-3.21	20	0.0	0.0	100.0	732	100.0	0.0	0.0
20020213	17142069	330	6.00	1	-3.21	20	0.0	0.0	100.0	732	100.0	0.0	0.0
20020213	17142080	330	5.50	1	-3.21	20	0.0	0.0	100.0	732	100.0	0.0	0.0
20020213	17142086	330	5.00	1	-3.21	20	0.0	0.0	100.0	732	100.0	0.0	0.0

Test3.inp
MINTEQA2, Ver 4.02
w/CNWRA modified database
COMPLETE OUTPUT

```
TEST3 - Metal activities controlled by solid phases.
Illustrates the defining of species not in the database.
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 0 0 0 0 1 0 0 0 0
0   0   0
    330  1.585E-08   -7.80                    /H+1
      1  6.310E-06   -5.20                    /E- (ENTERED AS PE)
    460  1.260E-03   -2.90                    /Mg+2
    500  1.000E-03   -3.00                    /Na+1
    410  1.000E-03   -3.00                    /K+1
    180  1.590E-03   -2.80                    /Cl-1
    732  1.260E-03   -2.90                    /SO4-2
    492  1.000E-03   -3.00                    /NO3-1
    140  0.000E+00   -6.00                    /CO3-2
    280  0.000E+00  -12.00                    /Fe+2
    470  0.000E+00  -12.00                    /Mn+2
    230  0.000E+00   -9.00                    /Cu+1
    281  0.000E+00  -16.00                    /Fe+3
    471  0.000E+00  -16.00                    /Mn+3
    231  0.000E+00   -7.00                    /Cu+2
     30  0.000E+00  -16.00                    /Al+3
    770  0.000E+00   -7.00                    /H4SiO4
    150  0.000E+00   -6.00                    /Ca+2
    950  0.000E+00  -10.00                    /Zn+2
    580  0.000E+00  -12.00                    /PO4-3

  3  11
3301403    21.6600    -0.5300                /CO2 (g)
2802810     0.0000     0.0000                /FE+3/FE+2
4704710     0.0000     0.0000                /MN+3/MN+2
2302310     0.0000     0.0000                /CU+1/CU+2
8603001    -5.7260    35.2800                /KAOLINITE
2077002     4.0060    -6.2200                /QUARTZ
2028100    -4.8910     0.0000                /FERRIHYDRITE
5015001     8.4750     2.5850                /CALCITE
2095000   -12.4500     0.0000                /ZN(OH)2 (A)
      1     5.2000     0.0000                /E- (ENTERED AS PE)
    330     7.8000     0.0000                /H+1

  3   3
9947101 MnPO4,1.5H2O     0.0000   34.7800   0.000   0.000 0.00 0.00 0.00 176.9320
 0.00 3   1.000 580   1.000 471   1.500   2   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
9915002 b-Ca3(PO4)2      0.0000   28.9260   0.000   0.000 0.00 0.00 0.00 310.1830
 0.00 2   2.000 580   3.000 150   0.000   0   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
9923103 Cu(OH)2          0.0000   -2.8000   0.000   0.000 0.00 0.00 0.00  97.5320
 0.00 3   2.000   2   1.000 231  -2.000 330   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
```

Test3.out
Complete Output
w/CNWRA modified database

PART 1 of OUTPUT FILE
MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:14:33

TEST3 - Metal activities controlled by solid phases.
Illustrates the defining of species not in the database.
Component file (COMP.DBS): comp.dbs COMP v4.02 02/12/2002
Thermodynamic file (THERMO.UNF): thermo.unf THERMO V4.02 02/05/2002
Gaussian DOM file (GAUSSIAN.DBS): gaussian.dbsGAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF): type6.unf TYPE6 V4.02 02/05/2002

Temperature (Celsius): 25.00
Units of concentration: MOLAL
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed only for those solids specified as ALLOWED
in the input file (if any).
Maximum iterations: 200
The method used to compute activity coefficients is: Davies equation
Full output file

330	1.585E-08	-7.80
1	6.310E-06	-5.20
460	1.260E-03	-2.90
500	1.000E-03	-3.00
410	1.000E-03	-3.00
180	1.590E-03	-2.80
732	1.260E-03	-2.90
492	1.000E-03	-3.00
140	0.000E+00	-6.00
280	0.000E+00	-12.00
470	0.000E+00	-12.00
230	0.000E+00	-9.00
281	0.000E+00	-16.00
471	0.000E+00	-16.00
231	0.000E+00	-7.00
30	0.000E+00	-16.00
770	0.000E+00	-7.00
150	0.000E+00	-6.00
950	0.000E+00	-10.00
580	0.000E+00	-12.00

H2O has been inserted as a COMPONENT
3 11
3301403 21.6600 -0.5300
2802810 0.0000 0.0000
4704710 0.0000 0.0000
2302310 0.0000 0.0000
8603001 -5.7260 35.2800
2077002 4.0060 -6.2200
2028100 -4.8910 0.0000
5015001 8.4750 2.5850
2095000 -12.4500 0.0000
1 5.2000 0.0000
330 7.8000 0.0000
3 3
9947101 MnPO4,1.5H2O 0.0000 34.7800 0.000 0.000 0.00 0.00 0.00 176.9320
0.00 3 1.000 580 1.000 471 1.500 2 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0

0.000 0 0.000 0 0.000 0
9915002 b-Ca3(PO4)2 0.0000 28.9260 0.000 0.000 0.00 0.00 0.00 310.1830
0.00 2 2.000 580 3.000 150 0.000 0 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0

0.000 0 0.000 0 0.000 0
9923103 Cu(OH)2 0.0000 -2.8000 0.000 0.000 0.00 0.00 0.00 97.5320
0.00 3 2.000 2 1.000 231 -2.000 330 0.000 0 0.000 0 0.000 0
0.000 0 0.000 0 0.000 0 0.000 0 0.000 0 0.000 0

0.000 0 0.000 0 0.000 0

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	1.585E-08	-7.800	1.585E-08
1	E-1	6.310E-06	-5.200	6.310E-06
460	Mg+2	1.259E-03	-2.900	1.260E-03
500	Na+1	1.000E-03	-3.000	1.000E-03
410	K+1	1.000E-03	-3.000	1.000E-03
180	Cl-1	1.585E-03	-2.800	1.590E-03
732	SO4-2	1.259E-03	-2.900	1.260E-03
492	NO3-1	1.000E-03	-3.000	1.000E-03
140	CO3-2	1.000E-06	-6.000	0.000E+00
280	Fe+2	1.000E-12	-12.000	0.000E+00
470	Mn+2	1.000E-12	-12.000	0.000E+00
230	Cu+1	1.000E-09	-9.000	0.000E+00
281	Fe+3	1.000E-16	-16.000	0.000E+00
471	Mn+3	1.000E-16	-16.000	0.000E+00
231	Cu+2	1.000E-07	-7.000	0.000E+00
30	Al+3	1.000E-16	-16.000	0.000E+00
770	H4SiO4	1.000E-07	-7.000	0.000E+00
150	Ca+2	1.000E-06	-6.000	0.000E+00
950	Zn+2	1.000E-10	-10.000	0.000E+00
580	PO4-3	1.000E-12	-12.000	0.000E+00
2	H2O	1.000E+00	0.000	0.000E+00

PART 2 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:14:33

ALL SPECIES CONSIDERED IN THIS PROBLEM

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID No	Name	Enthalpy	logK	Min logK	Max logK	Charge	DHa	DHb	gfw
330	H+1	0.0000	0.0000	0.000	0.000	1.00	9.00	0.00	1.0079
Source of log K:									
580	PO4-3	0.0000	0.0000	0.000	0.000	-3.00	5.00	0.00	94.9714
Source of log K:									
460	Mg+2	0.0000	0.0000	0.000	0.000	2.00	6.50	0.20	24.3050
Source of log K:									
500	Na+1	0.0000	0.0000	0.000	0.000	1.00	4.00	0.08	22.9898
Source of log K:									
410	K+1	0.0000	0.0000	0.000	0.000	1.00	3.00	0.01	39.0983
Source of log K:									
180	Cl-1	0.0000	0.0000	0.000	0.000	-1.00	3.00	0.01	35.4530
Source of log K:									
732	SO4-2	0.0000	0.0000	0.000	0.000	-2.00	4.00	-0.04	96.0630
Source of log K:									
492	NO3-1	0.0000	0.0000	0.000	0.000	-1.00	3.00	0.00	62.0049
Source of log K:									
140	CO3-2	0.0000	0.0000	0.000	0.000	-2.00	5.40	0.00	60.0094
Source of log K:									
280	Fe+2	0.0000	0.0000	0.000	0.000	2.00	6.00	0.00	55.8470
Source of log K:									
470	Mn+2	0.0000	0.0000	0.000	0.000	2.00	6.00	0.00	54.9380
Source of log K:									
230	Cu+1	0.0000	0.0000	0.000	0.000	1.00	2.50	0.00	63.5460
Source of log K:									
281	Fe+3	0.0000	0.0000	0.000	0.000	3.00	9.00	0.00	55.8470
Source of log K:									
471	Mn+3	0.0000	0.0000	0.000	0.000	3.00	9.00	0.00	54.9380
Source of log K:									
231	Cu+2	0.0000	0.0000	0.000	0.000	2.00	6.00	0.00	63.5460
Source of log K:									
30	Al+3	0.0000	0.0000	0.000	0.000	3.00	9.00	0.00	26.9815
Source of log K:									
770	H4SiO4	0.0000	0.0000	0.000	0.000	0.00	0.00	0.00	96.1149
Source of log K:									
150	Ca+2	0.0000	0.0000	0.000	0.000	2.00	6.00	0.17	40.0780
Source of log K:									
950	Zn+2	0.0000	0.0000	0.000	0.000	2.00	6.00	0.00	65.3900
Source of log K:									

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID No	Name	Enthalpy	logK	Min logK	Max logK	Charge	DHa	DHb	gfw
9504922	zn(no3)2 (aq)	0.0000	-0.3000	0.000	0.000	0.00	0.00		

```
0.00  189.3998
Source of log K: nist46.4                          mtq3.11
9507320 znso4 (aq)              6.2000     2.3400    0.000     0.000    0.00  0.00
0.00  161.4530
Source of log K: nist46.3                          nist46.3
9507321 zn(so4)2-2              0.0000     3.2800    0.000     0.000   -2.00  0.00
0.00  257.5160
Source of log K: mtq3.11                           mtq3.11
3300020 oh-                    55.8100   -13.9970    0.000     0.000   -1.00  3.50
0.00   17.0074
Source of log K: nist46.4                          nist46.4
 303300 aloh+2                 47.8100    -4.9970    0.000     0.000    2.00  5.40
0.00   43.9889
Source of log K: nist46.3                          nist46.3
 303301 al(oh)2+                0.0000   -10.0940    0.000     0.000    1.00  5.40
0.00   60.9963
Source of log K: nist46.3                          mtq3.11
 303302 al(oh)4-              173.2400   -22.6880    0.000     0.000   -1.00  4.50
0.00   95.0111
Source of log K: nist46.3                          nist46.3
 303303 al(oh)3 (aq)            0.0000   -16.7910    0.000     0.000    0.00  0.00
0.00   78.0037
Source of log K: nist46.3                          mtq3.11
 307320 also4+                 28.0000     3.8900    0.000     0.000    1.00  4.50
0.00  123.0445
Source of log K: nist46.3                          nist46.3
 307321 al(so4)2-              11.9000     4.9200    0.000     0.000   -1.00  4.50
0.00  219.1075
Source of log K: nord90                            nord90
1501400 cahco3+                 5.4000    11.5990    0.000     0.000    1.00  6.00
0.00  101.0951
Source of log K: nist46.3                          nist46.3
1501401 caco3 (aq)             16.0000     3.2000    0.000     0.000    0.00  0.00
0.00  100.0872
Source of log K: nist46.3                          nist46.3
1503300 caoh+                  64.1100   -12.6970    0.000     0.000    1.00  6.00
0.00   57.0854
Source of log K: nist46.3                          nist46.3
1504921 cano3+                 -5.4000     0.5000    0.000     0.000    1.00  0.00
0.00  102.0829
Source of log K: nist46.4                          nist46.4
1505800 cahpo4 (aq)            -3.0000    15.0350    0.000     0.000    0.00  0.00
0.00  136.0573
Source of log K: nist46.3                          nist46.3
1505801 capo4-                 12.9704     6.4600    0.000     0.000   -1.00  5.40
0.00  135.0494
Source of log K: scd3.02 (1993 gma)                mtq3.11
1505802 cah2po4+               -6.0000    20.9230    0.000     0.000    1.00  5.40
0.00  137.0652
Source of log K: nist46.3                          nist46.3
1507320 caso4 (aq)              7.1000     2.3600    0.000     0.000    0.00  0.00
0.00  136.1410
Source of log K: nist46.3                          nist46.3
2301800 cucl2-                 -1.7573     5.4200    0.000     0.000   -1.00  4.00
0.00  134.4520
Source of log K: nist46.3                          mtq3.11
2301801 cucl3-2                 1.0878     4.7500    0.000     0.000   -2.00  5.00
0.00  169.9050
Source of log K: nist46.3                          mtq3.11
2301802 cucl (aq)               0.0000     3.1000    0.000     0.000    0.00  0.00
0.00   98.9990
Source of log K: nist46.4                          mtq3.11
2311400 cuco3 (aq)              0.0000     6.7700    0.000     0.000    0.00  0.00
0.00  123.5552
Source of log K: nist46.4                          mtq3.11
2311401 cu(co3)2-2              0.0000    10.2000    0.000     0.000   -2.00  0.00
0.00  183.5644
Source of log K: nist46.4                          mtq3.11
2311402 cuhco3+                 0.0000    12.1290    0.000     0.000    1.00  0.00
0.00  124.5631
Source of log K: nist46.4                          mtq3.11
2311800 cucl+                   8.3000     0.2000    0.000     0.000    1.00  4.00
0.00   98.9990
Source of log K: nist46.3                          nist46.3
2311801 cucl2 (aq)             44.1830    -0.2600    0.000     0.000    0.00  0.00
0.00  134.4520
Source of log K: scd3.02 (1989 ipa)                mtq3.11
2311802 cucl3-                 57.2790    -2.2900    0.000     0.000   -1.00  4.00
0.00  169.9050
Source of log K: mtq3.11                           mtq3.11
```

2311803 cucl4-2 1	32.5515	-4.5900	0.000	0.000	-2.00	5.00
0.00 205.3580						
Source of log K: mtq3.11		mtq3.11				
2313300 cuoh+	35.8100	-7.4970	0.000	0.000	1.00	4.00
0.00 80.5534						
Source of log K: nist46.3		nist46.3				
2313301 cu(oh)2 (aq)	0.0000	-16.1940	0.000	0.000	0.00	0.00
0.00 97.5608						
Source of log K: nist46.3		mtq3.11				
2313302 cu(oh)3-	0.0000	-26.8790	0.000	0.000	-1.00	0.00
0.00 114.5682						
Source of log K: nist46.3		mtq3.11				
2313303 cu(oh)4-2	0.0000	-39.9800	0.000	0.000	-2.00	0.00
0.00 131.5756						
Source of log K: nist46.3		mtq3.11				
2313304 cu2(oh)2+2	76.6200	-10.5940	0.000	0.000	2.00	0.00
0.00 161.1068						
Source of log K: nist46.3		nist46.3				
2314921 cuno3+	-4.1000	0.5000	0.000	0.000	1.00	0.00
0.00 125.5509						
Source of log K: nist46.4		nist46.4				
2314922 cu(no3)2 (aq)	0.0000	-0.4000	0.000	0.000	0.00	0.00
0.00 187.5558						
Source of log K: nist46.4		mtq3.11				
2317320 cuso4 (aq)	8.7000	2.3600	0.000	0.000	0.00	0.00
0.00 159.6090						
Source of log K: nist46.3		nist46.3				
2801400 fehco3+	0.0000	11.4290	0.000	0.000	1.00	6.00
0.00 116.8641						
Source of log K: nist46.4		mtq3.11				
2803300 feoh+	55.8100	-9.3970	0.000	0.000	1.00	5.00
0.00 72.8544						
Source of log K: nist46.3		nist46.3				
2803301 fe(oh)3-	126.4300	-28.9910	0.000	0.000	-1.00	5.00
0.00 106.8692						
Source of log K: nist46.3		nist46.3				
2803302 fe(oh)2 (aq)	119.6200	-20.4940	0.000	0.000	0.00	0.00
0.00 89.8618						
Source of log K: nist46.3		nist46.3				
2805800 feh2po4+	0.0000	22.2730	0.000	0.000	1.00	5.40
0.00 152.8342						
Source of log K: nist46.3		mtq3.11				
2805801 fehpo4 (aq)	0.0000	15.9750	0.000	0.000	0.00	0.00
0.00 151.8263						
Source of log K: nist46.3		mtq3.11				
2807320 feso4 (aq)	8.0000	2.3900	0.000	0.000	0.00	0.00
0.00 151.9100						
Source of log K: nist46.3		nist46.3				
2811800 fecl+2	23.0000	1.4800	0.000	0.000	2.00	5.00
0.00 91.3000						
Source of log K: nist46.3		nist46.3				
2811801 fecl2+	0.0000	2.1300	0.000	0.000	1.00	5.00
0.00 126.7530						
Source of log K: nist46.3		mtq3.11				
2811802 fecl3 (aq)	0.0000	1.1300	0.000	0.000	0.00	0.00
0.00 162.2060						
Source of log K: nord90		mtq3.11				
2813300 feoh+2	41.8100	-2.1870	0.000	0.000	2.00	5.00
0.00 72.8544						
Source of log K: nist46.3		nist46.3				
2813301 fe(oh)2+	0.0000	-4.5940	0.000	0.000	1.00	5.40
0.00 89.8618						
Source of log K: nist46.3		mtq3.11				
2813302 fe(oh)3 (aq)	103.8000	-12.5600	0.000	0.000	0.00	0.00
0.00 106.8692						
Source of log K: nord90		nord90				
2813303 fe(oh)4-	0.0000	-21.5880	0.000	0.000	-1.00	5.40
0.00 123.8766						
Source of log K: nist46.3		mtq3.11				
2813304 fe2(oh)2+4	57.6200	-2.8540	0.000	0.000	4.00	0.00
0.00 145.7088						
Source of log K: nist46.3		nist46.3				
2813305 fe3(oh)4+5	65.2400	-6.2880	0.000	0.000	5.00	0.00
0.00 235.5706						
Source of log K: nist46.3		nist46.3				
2814921 feno3+2	-37.0000	1.0000	0.000	0.000	2.00	0.00
0.00 117.8519						
Source of log K: nist46.4		nist46.4				
2815800 fehpo4+	-30.5432	22.2920	0.000	0.000	1.00	5.40
0.00 151.8263						

```
Source of log K: nist46.3                                    mtq3.11
2815801 feh2po4+2                0.0000    23.8515    0.000    0.000    2.00  5.40
0.00  152.8342
Source of log K: nist46.3                                    mtq3.11
2817320 feso4+                  25.0000     4.0500    0.000    0.000    1.00  5.00
0.00  151.9100
Source of log K: nist46.3                                    nist46.3
2817321 fe(so4)2-               19.2000     5.3800    0.000    0.000   -1.00  0.00
0.00  247.9730
Source of log K: nord90                                      nord90
3301400 hco3-                  -14.6000    10.3290    0.000    0.000   -1.00  5.40
0.00   61.0171
Source of log K: nist46.4                                    nist46.4
3301401 h2co3 (aq)             -23.7600    16.6810    0.000    0.000    0.00  0.00
0.00   62.0250
Source of log K: nist46.4                                    nist46.4
3305800 hpo4-2                 -15.0000    12.3750    0.000    0.000   -2.00  5.00
0.00   95.9793
Source of log K: nist46.3                                    nist46.3
3305801 h2po4-                 -18.0000    19.5730    0.000    0.000   -1.00  5.40
0.00   96.9872
Source of log K: nist46.3                                    nist46.3
3305802 h3po4                  -10.1000    21.7210    0.000    0.000    0.00  0.00
0.00   97.9951
Source of log K: nist46.3                                    nist46.3
3307320 hso4-                   22.0000     1.9900    0.000    0.000   -1.00  4.50
0.00   97.0709
Source of log K: nist46.3                                    nist46.3
3307700 h3sio4-                 20.0000    -9.8400    0.000    0.000   -1.00  4.00
0.00   95.1070
Source of log K: nist46.4                                    nist46.4
3307701 h2sio4-2                61.0000   -23.0400    0.000    0.000   -2.00  5.40
0.00   94.0991
Source of log K: nist46.4                                    nist46.4
4105800 khpo4-                   0.0000    13.2550    0.000    0.000   -1.00  5.40
0.00  135.0776
Source of log K: nist46.3                                    mtq3.11
4107320 kso4-                    4.1000     0.8500    0.000    0.000   -1.00  5.40
0.00  135.1613
Source of log K: nist46.3                                    nist46.3
4601400 mgco3 (aq)              12.0000     2.9200    0.000    0.000    0.00  0.00
0.00   84.3142
Source of log K: nist46.3                                    nist46.3
4601401 mghco3+                -10.6000    11.3390    0.000    0.000    1.00  4.00
0.00   85.3221
Source of log K: nist46.3                                    nist46.3
4603300 mgoh+                   67.8100   -11.3970    0.000    0.000    1.00  6.50
0.00   41.3124
Source of log K: nist46.3                                    nist46.3
4605800 mgpo4-                  12.9704     4.6540    0.000    0.000   -1.00  5.40
0.00  119.2764
Source of log K: scd3.02 (1993 gma)                          mtq3.11
4605801 mgh2po4+                -4.6861    21.2561    0.000    0.000    1.00  5.40
0.00  121.2922
Source of log K: nist46.3                                    mtq3.11
4605802 mghpo4 (aq)             -3.0000    15.1750    0.000    0.000    0.00  0.00
0.00  120.2843
Source of log K: nist46.3                                    nist46.3
4607320 mgso4 (aq)               5.8000     2.2600    0.000    0.000    0.00  0.00
0.00  120.3680
Source of log K: nist46.3                                    nist46.3
4700020 mno4-                  822.6699  -127.7945    0.000    0.000   -1.00  3.00
0.00  118.9360
Source of log K: nist2.1.1                                   nist2.1.1
4700021 mno4-2                 711.0699  -118.4218    0.000    0.000   -2.00  5.00
0.00  118.9360
Source of log K: nist2.1.1                                   nist2.1.1
4701400 mnhco3+                -10.6000    11.6290    0.000    0.000    1.00  5.00
0.00  115.9551
Source of log K: nist46.4                                    nist46.4
4701800 mncl+                    0.0000     0.1000    0.000    0.000    1.00  5.00
0.00   90.3910
Source of log K: nist46.3                                    mtq3.11
4701801 mncl2 (aq)               0.0000     0.2500    0.000    0.000    0.00  0.00
0.00  125.8440
Source of log K: nord90                                      mtq3.11
4701802 mncl3-                   0.0000    -0.3100    0.000    0.000   -1.00  5.00
0.00  161.2970
Source of log K: nord90                                      mtq3.11
4703300 mnoh+                   55.8100   -10.5970    0.000    0.000    1.00  5.00
```

```
0.00   71.9454
Source of log K: nist46.3                          nist46.3
4703301 mn(oh)3-                0.0000   -34.8000    0.000     0.000    -1.00   5.00
0.00  105.9602
Source of log K: mtq3.11                           mtq3.11
4703302 mn(oh)4-2               0.0000   -48.2880    0.000     0.000    -2.00   5.00
0.00  122.9676
Source of log K: nist46.4                          mtq3.11
4704920 mn(no3)2 (aq)          -1.6569     0.6000    0.000     0.000     0.00   0.00
0.00  178.9478
Source of log K: nist46.3                          mtq3.11
4704921 mnno3+                  0.0000     0.2000    0.000     0.000     1.00   0.00
0.00  116.9429
Source of log K: nist46.4                          mtq3.11
4707320 mnso4 (aq)              8.7000     2.2500    0.000     0.000     0.00   0.00
0.00  151.0010
Source of log K: nist46.3                          nist46.3
5001400 naco3-                -20.3500     1.2700    0.000     0.000    -1.00   5.40
0.00   82.9990
Source of log K: nist46.3                          nist2.1.1
5001401 nahco3 (aq)           -28.3301    10.0790    0.000     0.000     0.00   0.00
0.00   84.0069
Source of log K: nist46.3                          nist2.1.1
5005800 nahpo4-                 0.0000    13.4450    0.000     0.000    -1.00   5.40
0.00  118.9691
Source of log K: nist46.3                          mtq3.11
5007320 naso4-                  1.0000     0.7300    0.000     0.000    -1.00   5.40
0.00  119.0528
Source of log K: nist46.3                          nist46.3
9501400 znhco3+                 0.0000    11.8290    0.000     0.000     1.00   0.00
0.00  126.4071
Source of log K: nist46.4                          mtq3.11
9501401 znco3 (aq)              0.0000     4.7600    0.000     0.000     0.00   0.00
0.00  125.3992
Source of log K: nist46.4                          mtq3.11
9501800 zncl+                   5.4000     0.4000    0.000     0.000     1.00   4.00
0.00  100.8430
Source of log K: nist46.3                          nist46.3
9501801 zncl2 (aq)             37.0000     0.6000    0.000     0.000     0.00   0.00
0.00  136.2960
Source of log K: nist46.3                          nist46.3
9501802 zncl3-                 39.9990     0.5000    0.000     0.000    -1.00   4.00
0.00  171.7490
Source of log K: mtq3.11                           mtq3.11
9501803 zncl4-2                45.8566     0.1990    0.000     0.000    -2.00   5.00
0.00  207.2020
Source of log K: mtq3.11                           mtq3.11
9501804 znohcl (aq)             0.0000    -7.4800    0.000     0.000     0.00   0.00
0.00  117.8504
Source of log K: mtq3.11                           mtq3.11
9503300 znoh+                  55.8100    -8.9970    0.000     0.000     1.00   0.00
0.00   82.3974
Source of log K: nist46.3                          nist46.3
9503301 zn(oh)2 (aq)            0.0000   -17.7940    0.000     0.000     0.00   0.00
0.00   99.4048
Source of log K: nist46.3                          mtq3.11
9503302 zn(oh)3-                0.0000   -28.0910    0.000     0.000    -1.00   0.00
0.00  116.4122
Source of log K: nist46.3                          mtq3.11
9503303 zn(oh)4-2               0.0000   -40.4880    0.000     0.000    -2.00   0.00
0.00  133.4196
Source of log K: nist46.3                          mtq3.11
9504921 znno3+                 -4.6000     0.4000    0.000     0.000     1.00   0.00
0.00  127.3949
Source of log K: nist46.4                          nist46.4
```

Type III - SPECIES WITH FIXED ACTIVITY

```
  ID No      Name                 Enthalpy      logK    Min logK  Max logK  Charge  DHa
DHb     gfw
      2 H2O                         0.0000     0.0000    0.000     0.000     0.00   0.00
0.00   18.0153
Source of log K:
    330 H+1                         0.0000     7.8000    0.000     0.000     1.00   9.00
0.00    1.0079
Source of log K:
      1 E-1                         0.0000     5.2000    0.000     0.000    -1.00   0.00
0.00    0.0000
```

Source of log K:						
3301403 co2 (g)	-0.5300	21.6600	0.000	0.000	0.00	0.00
0.00 44.0097						
Source of log K: nist46.4		nist46.4				
2802810 fe+2/fe+3	-42.7000	13.0320	0.000	0.000	0.00	0.00
0.00 0.0000						
Source of log K: bard85		bard85				
4704710 mn+2/mn+3	-107.8000	25.3500	0.000	0.000	0.00	0.00
0.00 0.0000						
Source of log K: bard85		mtq3.11				
2302310 cu+1/cu+2	6.9000	2.6900	0.000	0.000	0.00	0.00
0.00 0.0000						
Source of log K: bard85		mtq3.11				
5015001 calcite	2.5850	8.4750	8.560	0.000	0.00	0.00
0.00 100.0872						
Source of log K: nist46.4		nist46.4				
2028100 ferrihydrite	73.3740	-4.8910	-1.557	-4.996	0.00	0.00
0.00 106.8692						
Source of log K: nist46.4		nist13.1				
8603001 kaolinite	35.2800	-5.7260	0.000	0.000	0.00	0.00
0.00 258.1607						
Source of log K: nord90		nord90				
2077002 quartz	-6.2200	4.0060	0.000	0.000	0.00	0.00
0.00 60.0843						
Source of log K: nist46.4		codata89				
2095000 zn(oh)2 (am)	80.6200	-12.4500	-12.260	-12.480	0.00	0.00
0.00 99.4048						
Source of log K: nist46.4		nist46.4				
9947101 MnPO4,1.5H2O	0.0000	34.7800	0.000	0.000	0.00	0.00
0.00 176.9320						
Source of log K:						
9915002 b-Ca3(PO4)2	0.0000	28.9260	0.000	0.000	0.00	0.00
0.00 310.1830						
Source of log K:						
9923103 Cu(OH)2	0.0000	-2.8000	0.000	0.000	0.00	0.00
0.00 97.5320						
Source of log K:						

Type VI - EXCLUDED SPECIES (not included in mole balance)

ID No Name	Enthalpy	logK	Min logK	Max logK	Charge	DHa
DHb gfw						
3301404 ch4 (g)	-257.1330	41.0452	0.000	0.000	0.00	0.00
0.00 16.0423						
Source of log K: nist13.1		nist13.1				
3300021 o2 (g)	571.6600	-83.0894	0.000	0.000	0.00	0.00
0.00 31.9990						
Source of log K: codata89		codata89				

Charge Balance: UNSPECIATED

Sum of CATIONS= 4.520E-03 Sum of ANIONS = 5.116E-03

PERCENT DIFFERENCE = 6.188E+00 (ANIONS - CATIONS)/(ANIONS + CATIONS)

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:

SO4-2	Log activity guess: -2.90
CO3-2	Log activity guess: -6.06

CONSTRAINTS ON COMPONENT ACTIVITIES

As specified, this chemical system is OPEN with respect to the following components:

H2O	H+1	E-1	CO3-2
Ca+2	Fe+3	H4SiO4	Zn+2
PO4-3	Cu+2	Fe+2	Cu+1
Al+3	Mn+3	Mn+2	

Activities of the following components are constrained by the species shown:

COMPONENT	SPECIES	TYPE
Cu+2	Cu(OH)2	3
PO4-3	b-Ca3(PO4)2	3
Mn+3	MnPO4,1.5H2O	3
Zn+2	zn(oh)2 (am)	3
H4SiO4	quartz	3
Al+3	kaolinite	3
Fe+3	ferrihydrite	3
Ca+2	calcite	3
Cu+1	cu+1/cu+2	3
Mn+2	mn+2/mn+3	3
Fe+2	fe+2/fe+3	3
CO3-2	co2 (g)	3
E-1	E-1	3
H+1	H+1	3
H2O	H2O	3

PART 3 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:14:33

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL mol/L	DIFF FXN	LOG ACTVTY	RESIDUAL
0	Cl-1	1.590E-03	3.966E-07	-2.80000	2.376E-07
1	Cl-1	1.590E-03	2.099E-04	-2.80011	2.098E-04
2	Cl-1	1.590E-03	3.155E-05	-2.85397	3.138E-05
3	Cl-1	1.590E-03	5.463E-06	-2.86250	5.304E-06
4	Cl-1	1.590E-03	9.852E-07	-2.86399	8.262E-07
5	Cl-1	1.590E-03	1.789E-07	-2.86426	1.986E-08

ID No	Name	Total Conc(M)	Conc (M)	log Activity	Diff fxn
492	NO3-1	1.000E-03	9.860E-04	-3.07042	2.047E-08
732	SO4-2	1.260E-03	7.587E-04	-3.37712	6.139E-08
460	Mg+2	1.260E-03	1.206E-03	-3.17589	9.871E-08
500	Na+1	1.000E-03	9.976E-04	-3.06534	2.047E-08
410	K+1	1.000E-03	9.971E-04	-3.06557	2.047E-08
180	Cl-1	1.590E-03	1.585E-03	-2.86431	3.250E-08
2	H2O	0.000E+00	1.050E-02	-0.00005	0.000E+00
330	H+1	1.585E-08	1.838E-08	-7.80000	0.000E+00
1	E-1	6.310E-06	-3.016E-04	-5.20000	0.000E+00
140	CO3-2	0.000E+00	1.575E-06	-6.06005	0.000E+00
280	Fe+2	0.000E+00	3.805E-11	-10.67684	0.000E+00
470	Mn+2	0.000E+00	2.938E-04	-3.78914	0.000E+00
230	Cu+1	0.000E+00	5.681E-16	-15.30990	0.000E+00
150	Ca+2	0.000E+00	6.957E-03	-2.41481	0.000E+00
281	Fe+3	0.000E+00	1.175E-18	-18.50884	0.000E+00
30	Al+3	0.000E+00	1.116E-16	-16.53087	0.000E+00
770	H4SiO4	0.000E+00	9.807E-05	-4.00610	0.000E+00
950	Zn+2	0.000E+00	1.280E-03	-3.14990	0.000E+00
471	Mn+3	0.000E+00	4.361E-24	-23.93914	0.000E+00
580	PO4-3	0.000E+00	5.469E-11	-10.84078	0.000E+00
231	Cu+2	0.000E+00	2.866E-13	-12.79990	0.000E+00

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
330	H+1	1.838E-08	-7.80000	1.00	0.86238	0.064
580	PO4-3	5.469E-11	-10.84078	-3.00	0.26380	0.579
460	Mg+2	1.206E-03	-3.17589	2.00	0.55308	0.257
500	Na+1	9.976E-04	-3.06534	1.00	0.86238	0.064
410	K+1	9.971E-04	-3.06557	1.00	0.86238	0.064
180	Cl-1	1.585E-03	-2.86431	-1.00	0.86238	0.064
732	SO4-2	7.587E-04	-3.37712	-2.00	0.55308	0.257
492	NO3-1	9.860E-04	-3.07042	-1.00	0.86238	0.064
140	CO3-2	1.575E-06	-6.06005	-2.00	0.55308	0.257
280	Fe+2	3.805E-11	-10.67684	2.00	0.55308	0.257
470	Mn+2	2.938E-04	-3.78914	2.00	0.55308	0.257
230	Cu+1	5.681E-16	-15.30990	1.00	0.86238	0.064
281	Fe+3	1.175E-18	-18.50884	3.00	0.26380	0.579
471	Mn+3	4.361E-24	-23.93914	3.00	0.26380	0.579
231	Cu+2	2.866E-13	-12.79990	2.00	0.55308	0.257
30	Al+3	1.116E-16	-16.53087	3.00	0.26380	0.579
770	H4SiO4	9.807E-05	-4.00610	0.00	1.00543	-0.002
150	Ca+2	6.957E-03	-2.41481	2.00	0.55308	0.257
950	Zn+2	1.280E-03	-3.14990	2.00	0.55308	0.257

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
9504922	zn(no3)2 (aq)	2.552E-10	-9.59073	0.00	1.00543	-0.302
9507320	znso4 (aq)	6.466E-05	-4.18701	0.00	1.00543	2.338
9507321	zn(so4)2-2	4.296E-07	-6.62413	-2.00	0.55308	3.537
3300020	oh-	7.366E-07	-6.19705	-1.00	0.86238	-13.933
303300	aloh+2	3.383E-14	-13.72792	2.00	0.55308	-4.740
303301	al(oh)2+	1.095E-11	-11.02497	1.00	0.86238	-10.030
303302	al(oh)4-	1.110E-08	-8.01908	-1.00	0.86238	-22.624
303303	al(oh)3 (aq)	1.190E-10	-9.92203	0.00	1.00543	-16.793
307320	also4+	1.113E-16	-16.01799	1.00	0.86238	3.954

307321	al(so4)2-	5.003E-19	-18.36510	-1.00	0.86238	4.984
1501400	cahco3+	1.363E-05	-4.92982	1.00	0.86238	11.409
1501401	caco3 (aq)	4.735E-06	-5.32236	0.00	1.00543	3.150
1503300	caoh+	5.655E-08	-7.31186	1.00	0.86238	-12.633
1504921	cano3+	1.200E-05	-4.98523	1.00	0.86238	0.564
1505800	cahpo4 (aq)	9.485E-07	-6.02059	0.00	1.00543	15.033
1505801	capo4-	1.857E-07	-6.79559	-1.00	0.86238	6.524
1505802	cah2po4+	1.354E-08	-7.93259	1.00	0.86238	20.987
1507320	caso4 (aq)	3.679E-04	-3.43193	0.00	1.00543	2.358
2301800	cucl2-	2.791E-16	-15.61852	-1.00	0.86238	5.484
2301801	cucl3-2	1.272E-19	-19.15283	-2.00	0.55308	5.007
2301802	cucl (aq)	8.384E-16	-15.07421	0.00	1.00543	3.098
2311400	cuco3 (aq)	8.085E-13	-12.08995	0.00	1.00543	6.768
2311401	cu(co3)2-2	3.445E-15	-14.72000	-2.00	0.55308	10.457
2311402	cuhco3+	3.415E-15	-14.53095	1.00	0.86238	12.193
2311800	cucl+	3.982E-16	-15.46421	1.00	0.86238	0.264
2311801	cucl2 (aq)	1.619E-19	-18.78852	0.00	1.00543	-0.262
2311802	cucl3-	2.407E-24	-23.68283	-1.00	0.86238	-2.226
2311803	cucl4-2 1	2.571E-29	-28.84714	-2.00	0.55308	-4.333
2313300	cuoh+	3.693E-13	-12.49695	1.00	0.86238	-7.433
2313301	cu(oh)2 (aq)	4.015E-14	-13.39400	0.00	1.00543	-16.196
2313302	cu(oh)3-	6.099E-17	-16.27905	-1.00	0.86238	-26.815
2313303	cu(oh)4-2	4.755E-22	-21.58010	-2.00	0.55308	-39.723
2313304	cu2(oh)2+2	7.914E-21	-20.35884	2.00	0.55308	-10.102
2314921	cuno3+	4.943E-16	-15.37031	1.00	0.86238	0.564
2314922	cu(no3)2 (aq)	4.539E-20	-19.34073	0.00	1.00543	-0.402
2317320	cuso4 (aq)	1.516E-14	-13.81701	0.00	1.00543	2.358
2801400	fehco3+	9.045E-14	-13.10790	1.00	0.86238	11.493
2803300	feoh+	6.172E-13	-12.27390	1.00	0.86238	-9.333
2803301	fe(oh)3-	6.256E-17	-16.26800	-1.00	0.86238	-28.927
2803302	fe(oh)2 (aq)	2.671E-16	-15.57095	0.00	1.00543	-20.496
2805800	feh2po4+	1.658E-15	-14.84462	1.00	0.86238	22.337
2805801	fehpo4 (aq)	4.519E-14	-13.34262	0.00	1.00543	15.973
2807320	feso4 (aq)	2.156E-12	-11.66396	0.00	1.00543	2.388
2811800	fecl+2	2.312E-20	-19.89315	2.00	0.55308	1.737
2811801	fecl2+	9.054E-23	-22.10746	1.00	0.86238	2.194
2811802	fecl3 (aq)	1.061E-26	-25.97177	0.00	1.00543	1.128
2813300	feoh+2	2.298E-13	-12.89590	2.00	0.55308	-1.930
2813301	fe(oh)2+	3.642E-08	-7.50295	1.00	0.86238	-4.530
2813302	fe(oh)3 (aq)	2.131E-08	-7.66900	0.00	1.00543	-12.562
2813303	fe(oh)4-	1.470E-09	-8.89705	-1.00	0.86238	-21.524
2813304	fe2(oh)2+4	5.716E-24	-24.27179	4.00	0.09357	-1.825
2813305	fe3(oh)4+5	9.836E-30	-30.61474	5.00	0.02468	-4.680
2814921	feno3+2	4.764E-21	-20.57926	2.00	0.55308	1.257
2815800	fehpo4+	1.609E-15	-14.85762	1.00	0.86238	22.356
2815801	feh2po4+2	1.442E-21	-21.09812	2.00	0.55308	24.109
2817320	feso4+	1.692E-18	-17.83596	1.00	0.86238	4.114
2817321	fe(so4)2-	1.518E-20	-19.88308	-1.00	0.86238	5.444
3301400	hco3-	3.419E-04	-3.53040	-1.00	0.86238	10.394
3301401	h2co3 (aq)	1.044E-05	-4.97905	0.00	1.00543	16.679
3305800	hpo4-2	9.805E-07	-6.26578	-2.00	0.55308	12.632
3305801	h2po4-	1.572E-07	-6.86778	-1.00	0.86238	19.637
3305802	h3po4	3.005E-13	-12.51978	0.00	1.00543	21.719
3307320	hso4-	7.484E-10	-9.19018	-1.00	0.86238	2.051
3307700	h3sio4-	8.496E-07	-6.13511	-1.00	0.86238	-9.865
3307701	h2sio4-2	1.713E-10	-10.02345	-2.00	0.55308	-21.360
4105800	khpo4-	4.102E-09	-8.45136	-1.00	0.86238	13.319
4107320	kso4-	2.940E-06	-5.59596	-1.00	0.86238	0.911
4601400	mgco3 (aq)	5.513E-07	-6.25628	0.00	1.00543	2.977
4601401	mghco3+	2.652E-06	-5.64076	1.00	0.86238	11.459
4603300	mgoh+	8.014E-08	-7.16044	1.00	0.86238	-11.720
4605800	mgpo4-	5.031E-10	-9.36267	-1.00	0.86238	4.718
4605801	mgh2po4+	5.055E-09	-8.36057	1.00	0.86238	21.320
4605802	mghpo4 (aq)	2.270E-07	-6.64167	0.00	1.00543	15.173
4607320	mgso4 (aq)	5.066E-05	-4.29301	0.00	1.00543	2.258
4700020	mno4-	7.594E-44	-43.18385	-1.00	0.86238	-127.730
4700021	mno4-2	1.762E-39	-39.01115	-2.00	0.55308	-118.165
4701400	mnhco3+	1.107E-06	-6.02019	1.00	0.86238	11.693
4701800	mncl+	3.242E-07	-6.55345	1.00	0.86238	0.164
4701801	mncl2 (aq)	5.369E-10	-9.26776	0.00	1.00543	0.248
4701802	mncl3-	2.356E-13	-12.69207	-1.00	0.86238	-0.246
4703300	mnoh+	3.007E-07	-6.58619	1.00	0.86238	-10.533
4703301	mn(oh)3-	7.499E-16	-15.18930	-1.00	0.86238	-34.736
4703302	mn(oh)4-2	2.398E-21	-20.87735	-2.00	0.55308	-48.031
4704920	mn(no3)2 (aq)	4.652E-10	-9.32998	0.00	1.00543	0.598
4704921	mnno3+	2.539E-07	-6.65956	1.00	0.86238	0.264
4707320	mnso4 (aq)	1.206E-05	-4.91626	0.00	1.00543	2.248
5001400	naco3-	1.618E-08	-7.85540	-1.00	0.86238	1.334
5001401	nahco3 (aq)	1.417E-07	-6.84640	0.00	1.00543	10.077
5005800	nahpo4-	6.356E-09	-8.26113	-1.00	0.86238	13.509

5007320	naso4-	2.248E-06	-5.71246	-1.00	0.86238	0.794
9501400	znhco3+	7.645E-06	-5.18095	1.00	0.86238	11.893
9501401	znco3 (aq)	3.529E-05	-4.44995	0.00	1.00543	4.758
9501800	zncl+	2.819E-06	-5.61421	1.00	0.86238	0.464
9501801	zncl2 (aq)	5.238E-09	-8.27852	0.00	1.00543	0.598
9501802	zncl3-	6.629E-12	-11.24283	-1.00	0.86238	0.564
9501803	zncl4-2	7.064E-15	-14.40814	-2.00	0.55308	0.456
9501804	znohcl (aq)	2.011E-06	-5.69426	0.00	1.00543	-7.482
9503300	znoh+	5.216E-05	-4.34695	1.00	0.86238	-8.933
9503301	zn(oh)2 (aq)	4.505E-06	-5.34400	0.00	1.00543	-17.796
9503302	zn(oh)3-	1.672E-08	-7.84105	-1.00	0.86238	-28.027
9503303	zn(oh)4-2	6.593E-13	-12.43810	-2.00	0.55308	-40.231
9504921	znno3+	1.754E-06	-5.82031	1.00	0.86238	0.464

Type III - SPECIES WITH FIXED ACTIVITY

ID No	Name	Conc (M)	New logK	Enthalpy
2	H2O	1.050E-02	0.000	0.000
330	H+1	-1.802E-02	7.800	0.000
1	E-1	-3.016E-04	5.200	0.000
3301403	co2 (g)	7.394E-03	21.660	-0.530
2802810	fe+2/fe+3	4.096E-11	13.032	-42.700
4704710	mn+2/mn+3	3.079E-04	25.350	-107.800
2302310	cu+1/cu+2	1.686E-15	2.690	6.900
5015001	calcite	-7.814E-03	8.475	2.585
2028100	ferrihydrite	-5.925E-08	-4.891	73.374
8603001	kaolinite	-5.614E-09	-5.726	35.280
2077002	quartz	-9.891E-05	4.006	-6.220
2095000	zn(oh)2 (am)	-1.452E-03	-12.450	80.620
9947101	MnPO4,1.5H2O	-3.079E-04	34.780	0.000
9915002	b-Ca3(PO4)2	1.527E-04	28.926	0.000
9923103	Cu(OH)2	-1.529E-12	-2.800	0.000

Type VI - EXCLUDED SPECIES (not included in mole balance)

ID No	Name	Conc (M)	New logK	Enthalpy
3301404	ch4 (g)	0.000E+00	41.045	-257.133
3300021	o2 (g)	8.138E-32	-83.089	571.660

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

NO3-1			
	98.6	Percent bound in species # 492	NO3-1
	1.2	Percent bound in species #1504921	cano3+
SO4-2			
	60.2	Percent bound in species # 732	SO4-2
	5.1	Percent bound in species #9507320	znso4 (aq)
	29.2	Percent bound in species #1507320	caso4 (aq)
	4.0	Percent bound in species #4607320	mgso4 (aq)
Mg+2			
	95.7	Percent bound in species # 460	Mg+2
	4.0	Percent bound in species #4607320	mgso4 (aq)
Na+1			
	99.8	Percent bound in species # 500	Na+1
K+1			
	99.7	Percent bound in species # 410	K+1
Cl-1			
	99.7	Percent bound in species # 180	Cl-1
H2O			
	1.1	Percent bound in species #3300020	oh-
	3.1	Percent bound in species #9501804	znohcl (aq)
	80.8	Percent bound in species #9503300	znoh+
	13.9	Percent bound in species #9503301	zn(oh)2 (aq)
H+1			
	4.2	Percent bound in species #1501400	cahco3+
	105.2	Percent bound in species #3301400	hco3-
	6.4	Percent bound in species #3301401	h2co3 (aq)
	2.4	Percent bound in species #9501400	znhco3+
E-1			
	100.0	Percent bound in species #4700021	mno4-2
CO3-2			
	3.2	Percent bound in species #1501400	cahco3+
	1.1	Percent bound in species #1501401	caco3 (aq)
	81.5	Percent bound in species #3301400	hco3-
	2.5	Percent bound in species #3301401	h2co3 (aq)
	1.8	Percent bound in species #9501400	znhco3+

	8.4	Percent bound in species #9501401	znco3 (aq)
Fe+2			
	92.9	Percent bound in species # 280	Fe+2
	1.5	Percent bound in species #2803300	feoh+
	5.3	Percent bound in species #2807320	feso4 (aq)
Mn+2			
	95.4	Percent bound in species # 470	Mn+2
	3.9	Percent bound in species #4707320	mnso4 (aq)
Cu+1			
	33.7	Percent bound in species # 230	Cu+1
	16.6	Percent bound in species #2301800	cucl2-
	49.7	Percent bound in species #2301802	cucl (aq)
Ca+2			
	94.6	Percent bound in species # 150	Ca+2
	5.0	Percent bound in species #1507320	caso4 (aq)
Fe+3			
	61.5	Percent bound in species #2813301	fe(oh)2+
	36.0	Percent bound in species #2813302	fe(oh)3 (aq)
	2.5	Percent bound in species #2813303	fe(oh)4-
Al+3			
	98.8	Percent bound in species # 303302	al(oh)4-
	1.1	Percent bound in species # 303303	al(oh)3 (aq)
H4SiO4			
	99.1	Percent bound in species # 770	H4SiO4
Zn+2			
	88.2	Percent bound in species # 950	Zn+2
	4.5	Percent bound in species #9507320	znso4 (aq)
	2.4	Percent bound in species #9501401	znco3 (aq)
	3.6	Percent bound in species #9503300	znoh+
Mn+3			
	100.0	Percent bound in species # 471	Mn+3
PO4-3			
	37.5	Percent bound in species #1505800	cahpo4 (aq)
	7.3	Percent bound in species #1505801	capo4-
	38.8	Percent bound in species #3305800	hpo4-2
	6.2	Percent bound in species #3305801	h2po4-
	9.0	Percent bound in species #4605802	mghpo4 (aq)
Cu+2			
	18.8	Percent bound in species # 231	Cu+2
	52.9	Percent bound in species #2311400	cuco3 (aq)

24.2	Percent bound in species #2313300	cuoh+
2.6	Percent bound in species #2313301	cu(oh)2 (aq)

PART 5 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:14:33

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
492	NO3-1	1.000E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	1.260E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	1.260E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
500	Na+1	1.000E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	1.000E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
180	Cl-1	1.590E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	6.459E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	3.250E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
1	E-1	-7.049E-39	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	4.197E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
280	Fe+2	4.096E-11	100.0	0.000E+00	0.0	0.000E+00	0.0
470	Mn+2	3.079E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
230	Cu+1	1.686E-15	100.0	0.000E+00	0.0	0.000E+00	0.0
150	Ca+2	7.356E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
281	Fe+3	5.920E-08	100.0	0.000E+00	0.0	0.000E+00	0.0
30	Al+3	1.123E-08	100.0	0.000E+00	0.0	0.000E+00	0.0
770	H4SiO4	9.892E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
950	Zn+2	1.452E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
471	Mn+3	4.361E-24	100.0	0.000E+00	0.0	0.000E+00	0.0
580	PO4-3	2.528E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
231	Cu+2	1.528E-12	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 2.156E-02 Sum of ANIONS 4.443E-03

PERCENT DIFFERENCE = 6.583E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 2.350E-02

EQUILIBRIUM pH = 7.800

EQUILIBRIUM pe = 5.200 or Eh = 307.60 mv

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17143393

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
3003000	al2o3	-5.914	[2.000] 30 [3.000] 2 [-6.000]330
2003000	al(oh)3 (am)	-3.931	[1.000] 30 [3.000] 2 [-3.000]330
6003000	alohso4	-8.878	[-1.000]330 [1.000] 30 [1.000]732 [1.000] 2
6003001	al4(oh)10so4	-14.201	[-10.000]330 [4.000] 30 [1.000]732 [10.000] 2
6041000	k-alum	-21.181	[1.000]410 [1.000] 30 [2.000]732 [12.000] 2
6041001	alunite	-58.013	[1.000]410 [3.000] 30 [2.000]732 [6.000] 2
6015000	anhydrite	-1.432	[1.000]150 [1.000]732
6023100	antlerite	-19.365	[3.000]231 [4.000] 2 [-4.000]330 [1.000]732
5015000	aragonite	-0.139	[1.000]150 [1.000]140
5046000	artinite	-6.412	[-2.000]330 [2.000]460 [1.000]140 [5.000] 2
4123101	atacamite	-12.455	[2.000]231 [3.000] 2 [-3.000]330 [1.000]180
5023102	azurite	-18.014	[3.000]231 [2.000] 2 [-2.000]330 [2.000]140
6095005	bianchite	-4.762	[1.000]950 [1.000]732 [6.000] 2
2047001	birnessite	-5.630	[-4.000]330 [-1.000] 1 [1.000]471 [2.000] 2
3047100	bixbyite	-0.434	[-6.000]330 [2.000]471 [3.000] 2
2003001	boehmite	-1.709	[-3.000]330 [1.000] 30 [2.000] 2
6023101	brochantite	-22.999	[4.000]231 [6.000] 2 [-6.000]330 [1.000]732
2046000	brucite	-4.420	[1.000]460 [2.000] 2 [-2.000]330
7015004	cahpo4:2h2o	-2.061	[1.000]150 [1.000]330 [1.000]580 [2.000] 2
7015005	cahpo4	-1.781	[1.000]150 [1.000]330 [1.000]580
7015006	ca3(po4)2 (beta)	-0.006	[3.000]150 [2.000]580
7015007	ca4h(po4)3:3h2o	-2.902	[4.000]150 [1.000]330 [3.000]580 [3.000] 2
5015001	calcite	0.000	[1.000]150 [1.000]140
6023105	chalcanthite	-13.537	[1.000]231 [1.000]732 [5.000] 2
2077000	chalcedony	-0.456	[1.000]770 [-2.000] 2
8646000	chrysotile	-2.940	[3.000]460 [2.000]770 [1.000] 2 [-6.000]330
2077001	cristobalite	-0.656	[1.000]770 [-2.000] 2
23000	cu metal	-11.754	[1.000]230 [1.000] 1
6023000	cu2so4	-32.047	[2.000]230 [1.000]732
5023100	cuco3	-7.360	[1.000]231 [1.000]140

ID No	Name	SI	Composition by stoich. of components
5123100	cu2(oh)3no3	-14.521	[2.000]231 [3.000] 2 [-3.000]330 [1.000]492
2023100	cu(oh)2	-5.874	[1.000]231 [2.000] 2 [-2.000]330
7023100	cu3(po4)2	-23.231	[3.000]231 [2.000]580
7023101	cu3(po4)2:3h2o	-24.961	[3.000]231 [2.000]580 [3.000] 2
6023103	cuocuso4	-23.680	[-2.000]330 [2.000]231 [1.000] 2 [1.000]732
6023104	cuso4	-19.117	[1.000]231 [1.000]732
3023100	cupric ferrite	6.594	[-8.000]330 [1.000]231 [2.000]281 [4.000] 2
2023000	cuprite	-13.614	[2.000]230 [1.000] 2 [-2.000]330
3023000	cuprous ferrite	6.298	[-4.000]330 [1.000]230 [1.000]281 [2.000] 2
2003002	diaspore	-0.004	[-3.000]330 [1.000] 30 [2.000] 2
5015004	dolomite (disordered)	-1.171	[1.000]150 [1.000]460 [2.000]140
5015002	dolomite (ordered)	-0.621	[1.000]150 [1.000]460 [2.000]140
6046000	epsomite	-4.427	[1.000]460 [1.000]732 [7.000] 2
2028001	fe(oh)2	-8.641	[1.000]280 [2.000] 2 [-2.000]330
4128100	fe(oh)2.7cl.3	4.732	[-2.700]330 [1.000]281 [2.700] 2 [0.300]180
2028101	fe3(oh)8	-5.517	[-8.000]330 [2.000]281 [1.000]280 [8.000] 2
6028100	fe2(so4)3	-43.415	[2.000]281 [3.000]732
2028100	ferrihydrite	1.700	[1.000]281 [3.000] 2 [-3.000]330
2003003	gibbsite	-1.422	[1.000] 30 [3.000] 2 [-3.000]330
2028102	goethite	4.400	[1.000]281 [2.000] 2 [-3.000]330
6095006	goslarite	-4.516	[1.000]950 [1.000]732 [7.000] 2
8628000	greenalite	-14.053	[-6.000]330 [3.000]280 [2.000]770 [1.000] 2
6015001	gypsum	-1.182	[1.000]150 [1.000]732 [2.000] 2
4150000	halite	-7.532	[1.000]500 [1.000]180
8603000	halloysite	-3.849	[2.000] 30 [2.000]770 [1.000] 2 [-6.000]330
3047000	hausmannite	0.402	[3.000]470 [4.000] 2 [-8.000]330 [-2.000] 1
3028100	hematite	11.200	[2.000]281 [3.000] 2 [-6.000]330
3028001	hercynite	-4.232	[-8.000]330 [1.000]280 [2.000] 30 [4.000] 2
5015003	huntite	-6.215	[3.000]460 [1.000]150 [4.000]140
5046001	hydromagnesite	-15.754	[5.000]460 [4.000]140 [-2.000]330 [6.000] 2
7015003	hydroxylapatite	7.537	[5.000]150 [3.000]580 [1.000] 2 [-1.000]330
6028101	h-jarosite	-11.181	[-5.000]330 [3.000]281 [2.000]732 [7.000] 2
6041002	k-jarosite	-3.747	[-6.000]330 [1.000]410 [3.000]281 [2.000]732 [6.000] 2
6050000	na-jarosite	-7.346	[-6.000]330 [1.000]500 [3.000]281 [2.000]732 [6.000] 2
8603001	kaolinite	-1.709	[2.000] 30 [2.000]770 [1.000] 2 [-6.000]330

ID No	Name	SI	Composition by stoich. of components
6023102	langite	-25.266	[-6.000]330 [4.000]231 [7.000] 2 [1.000]732
3028102	lepidocrocite	3.520	[-3.000]330 [1.000]281 [2.000] 2
2015000	lime	-19.514	[-2.000]330 [1.000]150 [1.000] 2
3028101	maghemite	3.396	[-6.000]330 [2.000]281 [3.000] 2
3046001	magnesioferrite	5.347	[-8.000]330 [1.000]460 [2.000]281 [4.000] 2
5046002	magnesite	-1.776	[1.000]460 [1.000]140
3028000	magnetite	11.302	[-8.000]330 [2.000]281 [1.000]280 [4.000] 2
5023101	malachite	-10.754	[2.000]231 [2.000] 2 [-2.000]330 [1.000]140
2047100	manganite	-0.529	[1.000]470 [2.000] 2 [-3.000]330 [-1.000] 1
4123100	melanothallite	-24.786	[1.000]231 [2.000]180
6028000	melanterite	-11.845	[1.000]280 [1.000]732 [7.000] 2
2046002	mg(oh)2 (active)	-6.370	[1.000]460 [2.000] 2 [-2.000]330
7046001	mghpo4:3h2o	-3.642	[1.000]460 [1.000]330 [1.000]580 [3.000] 2
7046002	mg3(po4)2	-7.929	[3.000]460 [2.000]580
6050001	mirabilite	-8.394	[2.000]500 [1.000]732 [10.000] 2
4147000	mncl2:4h2o	-12.233	[1.000]470 [2.000]180 [4.000] 2
7047000	mn3(po4)2	-9.222	[3.000]470 [2.000]580
7047001	mnhpo4	2.970	[1.000]470 [1.000]580 [1.000]330
6047000	mnso4	-9.749	[1.000]470 [1.000]732
6047100	mn2(so4)3	-52.299	[2.000]471 [3.000]732
4123000	nantokite	-11.444	[1.000]230 [1.000]180
3050000	natron	-10.880	[2.000]500 [1.000]140 [10.000] 2
5046003	nesquehonite	-4.566	[1.000]460 [1.000]140 [3.000] 2
2047002	nsutite	-5.043	[-4.000]330 [-1.000] 1 [1.000]471 [2.000] 2
2046001	periclase	-9.160	[-2.000]330 [1.000]460 [1.000] 2
2015001	portlandite	-9.619	[1.000]150 [2.000] 2 [-2.000]330
2047003	pyrochroite	-3.383	[1.000]470 [2.000] 2 [-2.000]330
2047000	pyrolusite	-3.569	[1.000]470 [2.000] 2 [-4.000]330 [-2.000] 1
2077002	quartz	-0.006	[1.000]770 [-2.000] 2
5047000	rhodochrosite	0.731	[1.000]470 [1.000]140
8646003	sepiolite	-2.930	[2.000]460 [3.000]770 [-4.000]330 [-0.500] 2
8646004	sepiolite (a)	-5.950	[-0.500] 2 [2.000]460 [3.000]770 [-4.000]330
5028000	siderite	-6.497	[1.000]280 [1.000]140
2077004	sio2 (am,ppt)	-1.266	[1.000]770 [-2.000] 2
2077003	sio2 (am,gel)	-1.296	[1.000]770 [-2.000] 2
5095000	smithsonite	0.790	[1.000]950 [1.000]140
3046000	spinel	-10.685	[-8.000]330 [1.000]460 [2.000] 30 [4.000] 2
7028100	strengite	-2.950	[1.000]281 [1.000]580 [2.000] 2
2023101	tenorite	-4.844	[1.000]231 [1.000] 2 [-2.000]330
6050002	thenardite	-9.830	[2.000]500 [1.000]732

ID No	Name	SI	Composition by stoich. of components
5050001	thermonatrite	-12.828	[2.000]500 [1.000]140 [1.000] 2
7028001	vivianite	-17.713	[3.000]280 [2.000]580 [8.000] 2
2028000	wustite	-6.199	[-2.000]330 [0.947]280 [1.000] 2
2095006	zincite	1.116	[1.000]950 [1.000] 2 [-2.000]330
6095003	zincosite	-10.457	[1.000]950 [1.000]732
95000	zn metal	-39.338	[1.000]950 [2.000] 1
5095001	znco3:1h2o	1.050	[1.000]950 [1.000]140 [1.000] 2
4195000	zncl2	-15.929	[1.000]950 [2.000]180
4195001	zn2(oh)3cl	-0.955	[2.000]950 [3.000] 2 [-3.000]330 [1.000]180
4195002	zn5(oh)8cl2	2.421	[-8.000]330 [5.000]950 [8.000] 2 [2.000]180
5195000	zn(no3)2:6h2o	-12.606	[1.000]950 [2.000]492 [6.000] 2
2095005	zno (active)	1.262	[-2.000]330 [1.000]950 [1.000] 2
2095000	zn(oh)2 (am)	-0.024	[1.000]950 [2.000] 2 [-2.000]330
2095001	zn(oh)2	0.250	[-2.000]330 [1.000]950 [2.000] 2
2095002	zn(oh)2 (beta)	0.696	[1.000]950 [2.000] 2 [-2.000]330
2095003	zn(oh)2 (gamma)	0.716	[1.000]950 [2.000] 2 [-2.000]330
2095004	zn(oh)2 (epsilon)	0.916	[1.000]950 [2.000] 2 [-2.000]330
7095000	zn3(po4)2:4h2o	4.289	[3.000]950 [2.000]580 [4.000] 2
6095000	zn2(oh)2so4	-1.577	[-2.000]330 [2.000]950 [2.000] 2 [1.000]732
6095001	zn4(oh)6so4	2.423	[-6.000]330 [4.000]950 [6.000] 2 [1.000]732
6095002	zn3o(so4)2	-19.517	[-2.000]330 [3.000]950 [2.000]732 [1.000] 2
6095004	znso4:1h2o	-5.889	[1.000]950 [1.000]732 [1.000] 2

Test30.inp
4) Modified CNCIRA database

```
Test30 for error in subroutine SOLID, version 4.01, 4.02. March 2000.

25.00 MG/L   0.000  0.00000E+00
0 1 1 1 1 0 0 0 1 1 0 0 0
   33.00     0.0   0.00  0.000      0.00
0    0    0
     330  0.000E+00   -7.52 y                    /H+1
       1  0.000E+00   -1.21 y                    /E- (ENTERED AS EH)
     490  1.360E+01   -4.96 y                    /NH4+1
     140  6.383E+02   -2.69 y                    /CO3-2
     180  1.170E+04   -1.65 y                    /Cl-1
     270  1.100E-00   -4.98 y                    /F-1
     492  4.500E+01   -4.25 y                    /NO3-1
     491  2.000E-02   -5.98 y                    /NO2-1
     580  2.910E-00   -5.55 y                    /PO4-3
     732  2.180E+03   -2.59 y                    /SO4-2
     730  1.030E-01  -28.00 y                    /HS-1
     144  0.000E+00   -6.00 y                    /DOM1
     100  3.700E-01   -6.27 y                    /Ba+2
     150  8.540E+02   -2.29 y                    /Ca+2
     280  2.000E-02   -6.32 y                    /Fe+2
     460  8.120E+02   -2.62 y                    /Mg+2
     470  1.000E-00   -5.34 y                    /Mn+2
     410  4.480E+01   -3.36 y                    /K+1
     500  6.680E+03   -1.86 y                    /Na+1
     281  9.800E-01  -11.75 y                    /Fe+3

  3   2
     330     6.9100     0.0000                   /H+1
2802810    13.0320   -42.7000                    /Fe+2/Fe+3
```

Test30.
Parts 1,5,6 of Output
w/CNWRA modified database

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:14:43

Test30 for error in subroutine SOLID, version 4.01, 4.02. March 2000.

```
Component file (COMP.DBS):           comp.dbs     COMP v4.02 02/12/2002
Thermodynamic file (THERMO.UNF):     thermo.unf   THERMO V4.02 02/05/2002
Gaussian DOM file (GAUSSIAN.DBS):    gaussian.dbsGAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF):             type6.unf    TYPE6 V4.02 02/05/2002
```

```
 Temperature (Celsius):  25.00
 Units of concentration: mg/L
 Ionic strength to be computed.
 If specified, carbonate concentration represents total inorganic carbon.
 Do not automatically terminate if charge imbalance exceeds 30%
 Precipitation is allowed for all solids in the thermodynamic database and
   the print option for solids is set to: 1
 Maximum iterations: 200
 The method used to compute activity coefficients is: Davies equation
 Intermediate output file
```

```
    330  0.000E+00   -7.52 y
      1  0.000E+00   -1.21 y
    490  1.360E+01   -4.96 y
    140  6.383E+02   -2.69 y
    180  1.170E+04   -1.65 y
    270  1.100E+00   -4.98 y
    492  4.500E+01   -4.25 y
    491  2.000E-02   -5.98 y
    580  2.910E+00   -5.55 y
    732  2.180E+03   -2.59 y
    730  1.030E-01  -28.00 y
    144  0.000E+00   -6.00 y
    100  3.700E-01   -6.27 y
    150  8.540E+02   -2.29 y
    280  2.000E-02   -6.32 y
    460  8.120E+02   -2.62 y
    470  1.000E+00   -5.34 y
    410  4.480E+01   -3.36 y
    500  6.680E+03   -1.86 y
    281  9.800E-01  -11.75 y

 H2O has been inserted as a COMPONENT
  3   2
    330     6.9100     0.0000
2802810    13.0320   -42.7000
```

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	3.020E-08	-7.520	0.000E+00
1	E-1	6.166E-02	-1.210	0.000E+00
490	NH4+1	1.096E-05	-4.960	1.360E+01
140	CO3-2	2.042E-03	-2.690	6.383E+02
180	Cl-1	2.239E-02	-1.650	1.170E+04
270	F-1	1.047E-05	-4.980	1.100E+00
492	NO3-1	5.623E-05	-4.250	4.500E+01
491	NO2-1	1.047E-06	-5.980	2.000E-02
580	PO4-3	2.818E-06	-5.550	2.910E+00
732	SO4-2	2.570E-03	-2.590	2.180E+03
730	HS-1	1.000E-28	-28.000	1.030E-01
144	DOM1	1.000E-06	-6.000	0.000E+00
100	Ba+2	5.370E-07	-6.270	3.700E-01
150	Ca+2	5.129E-03	-2.290	8.540E+02
280	Fe+2	4.786E-07	-6.320	2.000E-02
460	Mg+2	2.399E-03	-2.620	8.120E+02
470	Mn+2	4.571E-06	-5.340	1.000E+00
410	K+1	4.365E-04	-3.360	4.480E+01
500	Na+1	1.380E-02	-1.860	6.680E+03
281	Fe+3	1.778E-12	-11.750	9.800E-01
2	H2O	1.000E+00	0.000	0.000E+00

*** SPECIAL PARAMETERS for Dissolved Organic Matter:
DOC (mg/l): 33.00
Charge on DOM species are determined from fixed database values

** DOC COMPONENT 144:
Total Acidity (umol/mgC): 1.00
Total site concentration (mol/l): 3.300E-05

Charge Balance: UNSPECIATED

Sum of CATIONS= 4.114E-01 Sum of ANIONS = 4.070E-01

PERCENT DIFFERENCE = 5.439E-01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:

CO3-2	Log activity guess:	-5.49
PO4-3	Log activity guess:	-10.44
SO4-2	Log activity guess:	-1.63
HS-1	Log activity guess:	-5.81
Fe+2	Log activity guess:	-4.74
Mn+2	Log activity guess:	-4.73
Fe+3	Log activity guess:	-16.56

PART 5 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:14:44

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED		SORBED		PRECIPITATED	
		mol/L	percent	mol/L	percent	mol/L	percent
410	K+1	1.173E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
500	Na+1	2.974E-01	100.0	0.000E+00	0.0	2.352E-06	0.0
490	NH4+1	7.717E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
470	Mn+2	1.863E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
180	Cl-1	3.378E-01	100.0	0.000E+00	0.0	5.498E-06	0.0
270	F-1	4.306E-05	72.7	0.000E+00	0.0	1.620E-05	27.3
492	NO3-1	7.428E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
491	NO2-1	4.450E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
460	Mg+2	3.005E-02	87.9	0.000E+00	0.0	4.149E-03	12.1
732	SO4-2	2.322E-02	100.0	0.000E+00	0.0	2.643E-06	0.0
730	HS-1	5.009E-20	0.0	0.000E+00	0.0	3.188E-06	100.0
144	DOM1	3.300E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
150	Ca+2	1.760E-02	80.7	0.000E+00	0.0	4.209E-03	19.3
2	H2O	2.542E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	2.907E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
280	Fe+2	7.143E-14	100.0	0.000E+00	0.0	0.000E+00	0.0
1	E-1	6.742E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
281	Fe+3	7.520E-13	0.0	0.000E+00	0.0	1.833E-05	100.0
580	PO4-3	4.353E-09	0.0	0.000E+00	0.0	3.136E-05	100.0
100	Ba+2	1.147E-07	4.2	0.000E+00	0.0	2.643E-06	95.8
140	CO3-2	2.582E-03	23.7	0.000E+00	0.0	8.305E-03	76.3

Charge Balance: SPECIATED

Sum of CATIONS = 3.756E-01 Sum of ANIONS 3.683E-01

PERCENT DIFFERENCE = 9.821E-01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 4.240E-01

EQUILIBRIUM pH = 6.910

EQUILIBRIUM pe = 5.308 or Eh = 313.97 mv

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17144431

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
6015000	anhydrite	-0.510	[1.000]150 [1.000]732
5015000	aragonite	-0.332	[1.000]150 [1.000]140
5046000	artinite	-6.361	[-2.000]330 [2.000]460 [1.000]140 [5.000] 2
4210000	baf2	-11.260	[1.000]100 [2.000]270
7010001	bahpo4	-9.676	[1.000]100 [1.000]330 [1.000]580
2010001	ba(oh)2:8h2o	-18.118	[1.000]100 [10.000] 2 [-2.000]330
1010001	bas	-36.430	[1.000]100 [-1.000]330 [1.000]730
6010000	barite(baso4)	0.000	[1.000]100 [1.000]732
2046000	brucite	-5.167	[1.000]460 [2.000] 2 [-2.000]330
7015004	cahpo4:2h2o	-5.357	[1.000]150 [1.000]330 [1.000]580 [2.000] 2
7015005	cahpo4	-5.066	[1.000]150 [1.000]330 [1.000]580
7015006	ca3(po4)2 (beta)	-8.321	[3.000]150 [2.000]580
7015007	ca4h(po4)3:3h2o	-14.518	[4.000]150 [1.000]330 [3.000]580 [3.000] 2
5015001	calcite	-0.194	[1.000]150 [1.000]140
5015004	dolomite (disordered)	-0.550	[1.000]150 [1.000]460 [2.000]140
5015002	dolomite (ordered)	0.000	[1.000]150 [1.000]460 [2.000]140
6046000	epsomite	-2.534	[1.000]460 [1.000]732 [7.000] 2
7015002	fco3apatite	0.000	[9.316]150 [0.360]500 [0.144]460 [4.800]580 [1.200]140 [2.480]270
2028001	fe(oh)2	-13.531	[1.000]280 [2.000] 2 [-2.000]330
1028000	fes (ppt)	-23.586	[1.000]280 [1.000]730 [-1.000]330
4128100	fe(oh)2.7cl.3	0.000	[-2.700]330 [1.000]281 [2.700] 2 [0.300]180
2028101	fe3(oh)8	-21.761	[-8.000]330 [2.000]281 [1.000]280 [8.000] 2
6028100	fe2(so4)3	-46.737	[2.000]281 [3.000]732
2028100	ferrihydrite	-3.977	[1.000]281 [3.000] 2 [-3.000]330
4215000	fluorite	-1.021	[1.000]150 [2.000]270
2028102	goethite	-1.272	[1.000]281 [2.000] 2 [-3.000]330
1028001	greigite	-62.782	[-4.000]330 [2.000]281 [1.000]280 [4.000]730
6015001	gypsum	-0.270	[1.000]150 [1.000]732 [2.000] 2
4150000	halite	-2.881	[1.000]500 [1.000]180
3047000	hausmannite	-11.336	[3.000]470 [4.000] 2 [-8.000]330 [-2.000] 1
3028100	hematite	-0.138	[2.000]281 [3.000] 2 [-6.000]330
5015003	huntite	-3.965	[3.000]460 [1.000]150 [4.000]140
5046001	hydromagnesite	-13.265	[5.000]460 [4.000]140 [-2.000]330 [6.000] 2
7015003	hydroxylapatite	-5.813	[5.000]150 [3.000]580 [1.000] 2 [-1.000]330

ID No	Name	SI	Composition by stoich. of components
6028101	h-jarosite	-22.869	[-5.000]330 [3.000]281 [2.000]732 [7.000] 2
6041002	k-jarosite	-16.331	[-6.000]330 [1.000]410 [3.000]281 [2.000]732 [6.000] 2
6050000	na-jarosite	-17.525	[-6.000]330 [1.000]500 [3.000]281 [2.000]732 [6.000] 2
3028102	lepidocrocite	-2.152	[-3.000]330 [1.000]281 [2.000] 2
2015000	lime	-21.264	[-2.000]330 [1.000]150 [1.000] 2
1028002	mackinawite	-22.936	[1.000]280 [1.000]730 [-1.000]330
3028101	maghemite	-7.942	[-6.000]330 [2.000]281 [3.000] 2
3046001	magnesioferrite	-6.734	[-8.000]330 [1.000]460 [2.000]281 [4.000] 2
5046002	magnesite	-0.962	[1.000]460 [1.000]140
3028000	magnetite	-4.920	[-8.000]330 [2.000]281 [1.000]280 [4.000] 2
2047100	manganite	-4.706	[1.000]470 [2.000] 2 [-3.000]330 [-1.000] 1
6028000	melanterite	-14.095	[1.000]280 [1.000]732 [7.000] 2
4246001	mgf2	-3.593	[1.000]460 [2.000]270
2046002	mg(oh)2 (active)	-7.117	[1.000]460 [2.000] 2 [-2.000]330
7046001	mghpo4:3h2o	-5.935	[1.000]460 [1.000]330 [1.000]580 [3.000] 2
7046002	mg3(po4)2	-13.220	[3.000]460 [2.000]580
6050001	mirabilite	-2.772	[2.000]500 [1.000]732 [10.000] 2
4147000	mncl2:4h2o	-9.346	[1.000]470 [2.000]180 [4.000] 2
7047000	mn3(po4)2	-22.457	[3.000]470 [2.000]580
7047001	mnhpo4	-1.955	[1.000]470 [1.000]580 [1.000]330
1047000	mns (grn)	-18.324	[1.000]470 [1.000]730 [-1.000]330
1047001	mns (pnk)	-21.494	[1.000]470 [1.000]730 [-1.000]330
6047000	mnso4	-10.467	[1.000]470 [1.000]732
3050000	natron	-6.374	[2.000]500 [1.000]140 [10.000] 2
5046003	nesquehonite	-3.768	[1.000]460 [1.000]140 [3.000] 2
2046001	periclase	-9.902	[-2.000]330 [1.000]460 [1.000] 2
2015001	portlandite	-11.374	[1.000]150 [2.000] 2 [-2.000]330
1028003	pyrite	-10.173	[-2.000]330 [-2.000] 1 [1.000]280 [2.000]730
2047003	pyrochroite	-6.778	[1.000]470 [2.000] 2 [-2.000]330
2047000	pyrolusite	-8.529	[1.000]470 [2.000] 2 [-4.000]330 [-2.000] 1
5047000	rhodochrosite	-1.103	[1.000]470 [1.000]140
5028000	siderite	-9.825	[1.000]280 [1.000]140
7028100	strengite	-10.163	[1.000]281 [1.000]580 [2.000] 2
73100	sulfur	0.000	[1.000]730 [-1.000]330 [-2.000] 1
6050002	thenardite	-4.154	[2.000]500 [1.000]732
5050001	thermonatrite	-8.274	[2.000]500 [1.000]140 [1.000] 2
7028001	vivianite	-35.475	[3.000]280 [2.000]580 [8.000] 2
5010000	witherite	-5.209	[1.000]100 [1.000]140
2028000	wustite	-10.919	[-2.000]330 [0.947]280 [1.000] 2

Test4.inp
MINTEQA2, ver. 4.02
USCNWRA modified database
COMPLETE OUTPUT

```
TEST4 - Triple Layer Adsorption model with two adsorbing
surfaces.
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 0 0 0 0 1 1 0 0 0
3   2   6
8.174E+00  129.00 1.200 0.200 81
4.087E+00  600.00 1.400 0.400 82
    330  1.000E-07   -7.00                    /H+1
    410  1.000E-01   -1.00                    /K+1
    492  1.000E-01   -1.00                    /NO3-1
    813  0.000E+00    0.00                    /ADS1PSIo
    814  0.000E+00    0.00                    /ADS1PSIb
    815  0.000E+00    0.00                    /ADS1PSId
    811  1.320E-04   -3.88                    /ADS1TYP1
    823  0.000E+00    0.00                    /ADS2PSIo
    824  0.000E+00    0.00                    /ADS2PSIb
    825  0.000E+00    0.00                    /ADS2PSId
    821  1.370E-04   -3.86                    /ADS2TYP1

  3   1
    330      7.0000      0.0000               /H+1
  6   6
    813      0.0000      0.0000               /ADS1PSIo
    814      0.0000      0.0000               /ADS1PSIb
    815      0.0000      0.0000               /ADS1PSId
    823      0.0000      0.0000               /ADS2PSIo
    824      0.0000      0.0000               /ADS2PSIb
    825      0.0000      0.0000               /ADS2PSId

  2   8
8113300 =1SO-            0.0000   -9.3100   0.000   0.000 0.00 0.00 0.00    0.0000
 0.00 3    1.000 811  -1.000 330  -1.000 813    0.000    0    0.000    0    0.000    0
  0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8113301 =1SOH2+          0.0000    7.3300   0.000   0.000 0.00 0.00 0.00    0.0000
 0.00 3    1.000 811    1.000 330    1.000 813    0.000    0    0.000    0    0.000    0
  0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8114920 =1SOH2NO3        0.0000    8.3300   0.000   0.000 0.00 0.00 0.00    0.0000
 0.00 5    1.000 811    1.000 492    1.000 330    1.000 813   -1.000 814    0.000    0
  0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8114100 =1SOK            0.0000   -8.3100   0.000   0.000 0.00 0.00 0.00    0.0000
 0.00 5    1.000 811    1.000 410   -1.000 330   -1.000 813    1.000 814    0.000    0
  0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8213300 =2SO-            0.0000   -6.5200   0.000   0.000 0.00 0.00 0.00    0.0000
 0.00 3    1.000 821  -1.000 330  -1.000 823    0.000    0    0.000    0    0.000    0
  0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8213301 =2SOH2+          0.0000    7.0100   0.000   0.000 0.00 0.00 0.00    0.0000
 0.00 3    1.000 821    1.000 330    1.000 823    0.000    0    0.000    0    0.000    0
  0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8214100 =2SOK            0.0000   -5.3100   0.000   0.000 0.00 0.00 0.00    0.0000
 0.00 5    1.000 821    1.000 410   -1.000 330   -1.000 823    1.000 824    0.000    0
  0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8214920 =2SOH2NO3        0.0000    5.3500   0.000   0.000 0.00 0.00 0.00    0.0000
 0.00 5    1.000 821    1.000 492    1.000 330    1.000 823   -1.000 824    0.000    0
  0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
```

Test.out
Complete Output
4) CNWRA modified database

PART 1 of OUTPUT FILE
MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:14:55

TEST4 - Triple Layer Adsorption model with two adsorbing surfaces.

Component file (COMP.DBS):	comp.dbs	COMP v4.02 02/12/2002
Thermodynamic file (THERMO.UNF):	thermo.unf	THERMO V4.02 02/05/2002
Gaussian DOM file (GAUSSIAN.DBS):	gaussian.dbs	GAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF):	type6.unf	TYPE6 V4.02 02/05/2002

Temperature (Celsius): 25.00
Units of concentration: MOLAL
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed only for those solids specified as ALLOWED
in the input file (if any).
Maximum iterations: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file
Adsorption model: Triple Layer
Number of adsorbing surfaces: 2

```
8.174E+00  129.00 1.200 0.200 81
4.087E+00  600.00 1.400 0.400 82
    330  1.000E-07   -7.00
    410  1.000E-01   -1.00
    492  1.000E-01   -1.00
    813  0.000E+00    0.00
    814  0.000E+00    0.00
    815  0.000E+00    0.00
    811  1.320E-04   -3.88
    823  0.000E+00    0.00
    824  0.000E+00    0.00
    825  0.000E+00    0.00
    821  1.370E-04   -3.86

 H2O has been inserted as a COMPONENT
  3   1
    330      7.0000      0.0000
  6   6
    813      0.0000      0.0000
    814      0.0000      0.0000
    815      0.0000      0.0000
    823      0.0000      0.0000
    824      0.0000      0.0000
    825      0.0000      0.0000
  2   8
8113300 =1SO-            0.0000   -9.3100   0.000   0.000 0.00 0.00 0.00   0.0000
0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
8113301 =1SOH2+          0.0000    7.3300   0.000   0.000 0.00 0.00 0.00   0.0000
0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
8114920 =1SOH2NO3        0.0000    8.3300   0.000   0.000 0.00 0.00 0.00   0.0000
0.00 5   1.000 811   1.000 492   1.000 330   1.000 813  -1.000 814   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
8114100 =1SOK            0.0000   -8.3100   0.000   0.000 0.00 0.00 0.00   0.0000
0.00 5   1.000 811   1.000 410  -1.000 330  -1.000 813   1.000 814   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
8213300 =2SO-            0.0000   -6.5200   0.000   0.000 0.00 0.00 0.00   0.0000
0.00 3   1.000 821  -1.000 330  -1.000 823   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
```

```
8213301 =2SOH2+          0.0000    7.0100   0.000   0.000 0.00 0.00 0.00   0.0000
0.00 3   1.000 821   1.000 330   1.000 823   0.000   0   0.000   0   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
8214100 =2SOK            0.0000   -5.3100   0.000   0.000 0.00 0.00 0.00   0.0000
0.00 5   1.000 821   1.000 410  -1.000 330  -1.000 823   1.000 824   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
8214920 =2SOH2NO3        0.0000    5.3500   0.000   0.000 0.00 0.00 0.00   0.0000
0.00 5   1.000 821   1.000 492   1.000 330   1.000 823  -1.000 824   0.000   0
 0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0

  0.000   0   0.000   0   0.000   0
```

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	1.000E-07	-7.000	1.000E-07
410	K+1	1.000E-01	-1.000	1.000E-01
492	NO3-1	1.000E-01	-1.000	1.000E-01
813	ADS1PSIo	1.000E+00	0.000	0.000E+00
814	ADS1PSIb	1.000E+00	0.000	0.000E+00
815	ADS1PSId	1.000E+00	0.000	0.000E+00
811	ADS1TYP1	1.318E-04	-3.880	1.320E-04
823	ADS2PSIo	1.000E+00	0.000	0.000E+00
824	ADS2PSIb	1.000E+00	0.000	0.000E+00
825	ADS2PSId	1.000E+00	0.000	0.000E+00
821	ADS2TYP1	1.380E-04	-3.860	1.370E-04
2	H2O	1.000E+00	0.000	0.000E+00

Charge Balance: UNSPECIATED

Sum of CATIONS= 1.000E-01 Sum of ANIONS = 1.000E-01

PERCENT DIFFERENCE = 5.000E-05 (ANIONS - CATIONS)/(ANIONS + CATIONS)

CONSTRAINTS ON COMPONENT ACTIVITIES

As specified, this chemical system is OPEN with respect to the following components:

H2O H+1

Activities of the following components are constrained by the species shown:

COMPONENT	SPECIES	TYPE
H+1	H+1	3
H2O	H2O	3

PART 3 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:14:55

PARAMETERS OF THE COMPONENT MOST OUT OF BALANCE:

ITER	NAME	TOTAL mol/L	DIFF FXN	LOG ACTVTY	RESIDUAL
0	ADS2PSIb	0.000E+00	6.758E-04	0.00000	6.757E-04
1	ADS2PSId	0.000E+00	4.788E-06	0.00441	4.788E-06
2	ADS2PSId	1.821E-05	1.015E-06	0.01770	1.013E-06
3	ADS2PSId	2.002E-05	8.685E-09	0.01844	6.683E-09

ID No	Name	Total Conc(M)	Conc (M)	log Activity	Diff fxn
821	ADS2TYP1	1.370E-04	1.665E-05	-4.77848	4.261E-12
410	K+1	1.000E-01	9.994E-02	-1.10765	-3.268E-09
492	NO3-1	1.000E-01	9.994E-02	-1.10763	-3.195E-09
813	ADS1PSIo	8.765E-05	3.654E-01	-0.43725	1.628E-10
814	ADS1PSIb	-5.481E-05	4.740E-01	-0.32426	-1.978E-10
815	ADS1PSId	-3.284E-05	8.506E-01	-0.07026	2.531E-11
811	ADS1TYP1	1.320E-04	4.277E-05	-4.36881	5.972E-11
823	ADS2PSIo	-7.844E-05	1.228E+00	0.08907	-1.796E-11
824	ADS2PSIb	5.839E-05	1.127E+00	0.05180	1.132E-11
825	ADS2PSId	2.005E-05	1.043E+00	0.01846	-2.359E-12
2	H2O	0.000E+00	-1.285E-07	-0.00148	0.000E+00
330	H+1	1.000E-07	1.281E-07	-7.00000	0.000E+00

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
330	H+1	1.281E-07	-7.00000	1.00	0.78092	0.107
410	K+1	9.994E-02	-1.10765	1.00	0.78092	0.107
492	NO3-1	9.994E-02	-1.10763	-1.00	0.78092	0.107
811	ADS1TYP1	4.277E-05	-4.36881	0.00	1.00000	0.000
821	ADS2TYP1	1.665E-05	-4.77848	0.00	1.00000	0.000

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID No	Name	Conc (M)	log Act	Charge	Act Coef	New logK
8214920	=2SOH2NO3	3.171E-08	-7.49885	0.00	1.00000	5.350
3300020	oh-	1.285E-07	-6.99848	-1.00	0.78092	-13.890
8113300	=1SO-	5.734E-07	-6.24156	0.00	1.00000	-9.310
8113301	=1SOH2+	3.341E-05	-4.47607	0.00	1.00000	7.330
8114920	=1SOH2NO3	5.503E-05	-4.25944	0.00	1.00000	8.330
8114100	=1SOK	2.121E-07	-6.67347	0.00	1.00000	-8.310
8213300	=2SO-	4.097E-05	-4.38755	0.00	1.00000	-6.520
8213301	=2SOH2+	2.092E-05	-4.67942	0.00	1.00000	7.010
8214100	=2SOK	5.843E-05	-4.23340	0.00	1.00000	-5.310

Type III - SPECIES WITH FIXED ACTIVITY

ID No	Name	Conc (M)	New logK	Enthalpy
2	H2O	-1.285E-07	0.001	0.000
330	H+1	-9.113E-06	7.000	0.000

Type VI - EXCLUDED SPECIES (not included in mole balance)

ID No	Name	Conc (M)	New logK	Enthalpy
823	ADS2PSIo	1.228E+00	0.000	0.000
815	ADS1PSId	8.506E-01	0.000	0.000
814	ADS1PSIb	4.740E-01	0.000	0.000
813	ADS1PSIo	3.654E-01	0.000	0.000
825	ADS2PSId	1.043E+00	0.000	0.000
824	ADS2PSIb	1.127E+00	0.000	0.000

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

ADS2TYP1			
12.2	Percent bound in species #	821	ADS2TYP1
29.9	Percent bound in species #	8213300	=2SO-
15.3	Percent bound in species #	8213301	=2SOH2+
42.6	Percent bound in species #	8214100	=2SOK
K+1			
99.9	Percent bound in species #	410	K+1
NO3-1			
99.9	Percent bound in species #	492	NO3-1
ADS1PSIo			
38.1	Percent bound in species #	8113301	=1SOH2+
62.8	Percent bound in species #	8114920	=1SOH2NO3
ADS1PSIb			
100.4	Percent bound in species #	8114920	=1SOH2NO3
ADS1PSId			
ADS1TYP1			
32.4	Percent bound in species #	811	ADS1TYP1
25.3	Percent bound in species #	8113301	=1SOH2+
41.7	Percent bound in species #	8114920	=1SOH2NO3
ADS2PSIo			
52.2	Percent bound in species #	8213300	=2SO-
74.5	Percent bound in species #	8214100	=2SOK
ADS2PSIb			
100.1	Percent bound in species #	8214100	=2SOK
ADS2PSId			
H2O			
100.0	Percent bound in species #	3300020	oh-
H+1			
1.4	Percent bound in species #	330	H+1
362.7	Percent bound in species #	8113301	=1SOH2+
597.3	Percent bound in species #	8114920	=1SOH2NO3
227.1	Percent bound in species #	8213301	=2SOH2+

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
410	K+1	9.994E-02	99.9	5.864E-05	0.1	0.000E+00	0.0
492	NO3-1	9.994E-02	99.9	5.506E-05	0.1	0.000E+00	0.0
2	H2O	1.285E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	-4.492E-10	0.0	9.214E-06	100.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 9.994E-02 Sum of ANIONS 9.995E-02

PERCENT DIFFERENCE = 1.791E-03 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 9.994E-02

EQUILIBRIUM pH = 7.000

******** TRIPLE LAYER ADSORPTION MODEL ********

**** Parameters For Adsorbent Number 1 ****
Electrostatic Variables: psi0 = 0.025866 sig0 = 0.008021
psib = 0.019182 sigb = -.005016
psid = 0.004156 sigd = -.003005
Adsorbent Concentration (g/l): 8.174
Specific Surface Area (sq. meters/g): 129.00

**** Parameters For Adsorbent Number 2 ****
Electrostatic Variables: psi0 = -.005269 sig0 = -.003086
psib = -.003064 sigb = 0.002298
psid = -.001092 sigd = 0.000789
Adsorbent Concentration (g/l): 4.087
Specific Surface Area (sq. meters/g): 600.00

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17145530

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components

Test5a.inp
w/ CNLBRA modified database
only parts 1, 5, and 6 of output

```
Like TEST1B, except titrate with 1 mmol
rather that specifying 1 mmol as finite solid
25.00 MOLAL  0.000  0.00000E+00
0 0 1 1 0 0 0 0 1 1 2 0 0
 1 GIBBSITE (C)          TOTAL CONC mol/L
3 330  -3.000   30   1.000    2   3.000
  1.000E-03
0   0   0
    330  3.733E-03   -4.00                    /H+1
    732  1.580E-03   -2.80                    /SO4-2
    410  7.700E-05   -4.11                    /K+1
    140  0.000E+00   -7.00                    /CO3-2
     30  0.000E+00   -7.00                    /Al+3

  3   1
3301403    21.6600    -0.5300                /CO2 (g)
  5   1
2003003    -8.7700    22.8000                /GIBBSITE (C)
```

Test5a.out
Parts 1, 5, & of output
4) CNURA modified database

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:15: 6

Like TEST1B, except titrate with 1 mmol
rather that specifying 1 mmol as finite solid
Component file (COMP.DBS): comp.dbs COMP v4.02 02/12/2002
Thermodynamic file (THERMO.UNF): thermo.unf THERMO V4.02 02/05/2002
Gaussian DOM file (GAUSSIAN.DBS): gaussian.dbsGAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF): type6.unf TYPE6 V4.02 02/05/2002

Temperature (Celsius): 25.00
Units of concentration: MOLAL
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
Maximum iterations: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

330	3.733E-03	-4.00
732	1.580E-03	-2.80
410	7.700E-05	-4.11
140	0.000E+00	-7.00
30	0.000E+00	-7.00

H2O has been inserted as a COMPONENT
3 1
3301403 21.6600 -0.5300
5 1
2003003 -8.7700 22.8000

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	1.000E-04	-4.000	3.733E-03
732	SO4-2	1.585E-03	-2.800	1.580E-03
410	K+1	7.762E-05	-4.110	7.700E-05
140	CO3-2	1.000E-07	-7.000	0.000E+00
30	Al+3	1.000E-07	-7.000	0.000E+00
2	H2O	1.000E+00	0.000	0.000E+00

Charge Balance: UNSPECIATED

Sum of CATIONS= 3.810E-03 Sum of ANIONS = 3.160E-03

PERCENT DIFFERENCE = 9.326E+00 (ANIONS - CATIONS)/(ANIONS + CATIONS)

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:
SO4-2 Log activity guess: -2.81
CO3-2 Log activity guess: -13.66

*** TITRATION: GIBBSITE (C)
*** Titration point 1 in the series of 1 ***
The series of titrant total concentrations (mol/L) are:
1.000E-03
*** The total concentration of titrant for this point is: 1.000E-03 mol/L

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
330	H+1	7.540E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	1.580E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.700E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
30	Al+3	1.000E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	2.952E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	1.049E-05	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 2.287E-03 Sum of ANIONS 1.637E-03

PERCENT DIFFERENCE = 1.657E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 3.535E-03

EQUILIBRIUM pH = 3.186

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17150667

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
3003000	al2o3	-8.215	[2.000] 30 [3.000] 2 [-6.000]330
2003000	al(oh)3 (am)	-5.081	[1.000] 30 [3.000] 2 [-3.000]330
6003000	alohso4	-0.636	[-1.000]330 [1.000] 30 [1.000]732 [1.000] 2
6003001	al4(oh)10so4	-9.411	[-10.000]330 [4.000] 30 [1.000]732 [10.000] 2
6041000	k-alum	-9.239	[1.000]410 [1.000] 30 [2.000]732 [12.000] 2
6041001	alunite	-20.689	[1.000]410 [3.000] 30 [2.000]732 [6.000] 2
2003001	boehmite	-2.859	[-3.000]330 [1.000] 30 [2.000] 2
2003002	diaspore	-1.154	[-3.000]330 [1.000] 30 [2.000] 2
2003003	gibbsite	-2.572	[1.000] 30 [3.000] 2 [-3.000]330

Test 5b.inp
U) modified LLNL database
only Parts 1, 5, +6 of output

```
Like TEST1B, except titrate with 0.5 mmol, 1 mmol, 5 mmol gibbsite
rather that specifying 1 mmol as finite solid
25.00 MOLAL  0.000  0.00000E+00
0 0 1 1 0 1 0 0 1 1 2 0 0
 3 GIBBSITE (C)          TOTAL CONC mol/L
3 330  -3.000   30   1.000    2   3.000
  5.000E-04  1.000E-03  5.000E-03
0   0   0
    330  3.733E-03   -4.00                    /H+1
    732  1.580E-03   -2.80                    /SO4-2
    410  7.700E-05   -4.11                    /K+1
    140  0.000E+00   -7.00                    /CO3-2
     30  0.000E+00   -7.00                    /Al+3

  3   1
3301403    21.6600    -0.5300                 /CO2 (g)
  5   1
2003003    -8.7700    22.8000                 /GIBBSITE (C)
```

Test 5b.out
Parts 1,5,6 all sweeps
4/CNDRA modified database

PART 1 of OUTPUT FILE
MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:15:16

Like TEST1B, except titrate with 0.5 mmol, 1 mmol, 5 mmol gibbsite
rather that specifying 1 mmol as finite solid
Component file (COMP.DBS): comp.dbs COMP v4.02 02/12/2002
Thermodynamic file (THERMO.UNF): thermo.unf THERMO V4.02 02/05/2002
Gaussian DOM file (GAUSSIAN.DBS): gaussian.dbsGAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF): type6.unf TYPE6 V4.02 02/05/2002

Temperature (Celsius): 25.00
Units of concentration: MOLAL
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
Maximum iterations: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

330	3.733E-03	-4.00
732	1.580E-03	-2.80
410	7.700E-05	-4.11
140	0.000E+00	-7.00
30	0.000E+00	-7.00

H2O has been inserted as a COMPONENT

3	1	
3301403	21.6600	-0.5300
5	1	
2003003	-8.7700	22.8000

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	1.000E-04	-4.000	3.733E-03
732	SO4-2	1.585E-03	-2.800	1.580E-03
410	K+1	7.762E-05	-4.110	7.700E-05
140	CO3-2	1.000E-07	-7.000	0.000E+00
30	Al+3	1.000E-07	-7.000	0.000E+00
2	H2O	1.000E+00	0.000	0.000E+00

Charge Balance: UNSPECIATED

Sum of CATIONS= 3.810E-03 Sum of ANIONS = 3.160E-03

PERCENT DIFFERENCE = 9.326E+00 (ANIONS - CATIONS)/(ANIONS + CATIONS)

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:
SO4-2 Log activity guess: -2.81
CO3-2 Log activity guess: -13.66

*** TITRATION: GIBBSITE (C)
*** Titration point 1 in the series of 3 ***
The series of titrant total concentrations (mol/L) are:
5.000E-04 1.000E-03 5.000E-03
*** The total concentration of titrant for this point is: 5.000E-04 mol/L

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
330	H+1	2.254E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	1.580E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.700E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
30	Al+3	5.000E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	4.072E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	1.049E-05	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 2.868E-03 Sum of ANIONS 2.218E-03

PERCENT DIFFERENCE = 1.278E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 3.899E-03

EQUILIBRIUM pH = 2.712

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17151639

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
3003000	al2o3	-11.831	[2.000] 30 [3.000] 2 [-6.000]330
2003000	al(oh)3 (am)	-6.889	[1.000] 30 [3.000] 2 [-3.000]330
6003000	alohso4	-1.389	[-1.000]330 [1.000] 30 [1.000]732 [1.000] 2
6003001	al4(oh)10so4	-15.587	[-10.000]330 [4.000] 30 [1.000]732 [10.000] 2
6041000	k-alum	-9.413	[1.000]410 [1.000] 30 [2.000]732 [12.000] 2
6041001	alunite	-21.635	[1.000]410 [3.000] 30 [2.000]732 [6.000] 2
2003001	boehmite	-4.667	[-3.000]330 [1.000] 30 [2.000] 2
2003002	diaspore	-2.962	[-3.000]330 [1.000] 30 [2.000] 2
2003003	gibbsite	-4.380	[1.000] 30 [3.000] 2 [-3.000]330

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:15:16

*** TITRATION: GIBBSITE (C)
*** Titration point 2 in the series of 3 ***
*** The total concentration of titrant for this point is: 1.000E-03 mol/L

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
330	H+1	7.540E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	1.580E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.700E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
30	Al+3	1.000E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	2.952E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	1.049E-05	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 2.287E-03 Sum of ANIONS 1.637E-03

PERCENT DIFFERENCE = 1.657E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 3.535E-03

EQUILIBRIUM pH = 3.186

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17151639

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
3003000	al2o3	-8.215	[2.000] 30 [3.000] 2 [-6.000]330
2003000	al(oh)3 (am)	-5.081	[1.000] 30 [3.000] 2 [-3.000]330
6003000	alohso4	-0.636	[-1.000]330 [1.000] 30 [1.000]732 [1.000] 2
6003001	al4(oh)10so4	-9.411	[-10.000]330 [4.000] 30 [1.000]732 [10.000] 2
6041000	k-alum	-9.239	[1.000]410 [1.000] 30 [2.000]732 [12.000] 2
6041001	alunite	-20.689	[1.000]410 [3.000] 30 [2.000]732 [6.000] 2
2003001	boehmite	-2.859	[-3.000]330 [1.000] 30 [2.000] 2
2003002	diaspore	-1.154	[-3.000]330 [1.000] 30 [2.000] 2
2003003	gibbsite	-2.572	[1.000] 30 [3.000] 2 [-3.000]330

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:15:16

*** TITRATION: GIBBSITE (C)
*** Titration point 3 in the series of 3 ***
*** The total concentration of titrant for this point is: 5.000E-03 mol/L

PART 5 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:15:16

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED		SORBED		PRECIPITATED	
		mol/L	percent	mol/L	percent	mol/L	percent
30	Al+3	1.140E-03	22.8	0.000E+00	0.0	3.860E-03	77.2
732	SO4-2	1.580E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.700E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	8.293E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	1.051E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	3.339E-04	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 2.145E-03 Sum of ANIONS 1.495E-03

PERCENT DIFFERENCE = 1.786E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 3.518E-03

EQUILIBRIUM pH = 3.545

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17151666

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
3003000	al2o3	-5.906	[2.000] 30 [3.000] 2 [-6.000]330
2003000	al(oh)3 (am)	-3.927	[1.000] 30 [3.000] 2 [-3.000]330
6003000	alohso4	-0.231	[-1.000]330 [1.000] 30 [1.000]732 [1.000] 2
6003001	al4(oh)10so4	-5.542	[-10.000]330 [4.000] 30 [1.000]732 [10.000] 2
6041000	k-alum	-9.224	[1.000]410 [1.000] 30 [2.000]732 [12.000] 2
6041001	alunite	-20.516	[1.000]410 [3.000] 30 [2.000]732 [6.000] 2
2003001	boehmite	-1.705	[-3.000]330 [1.000] 30 [2.000] 2
2003002	diaspore	0.000	[-3.000]330 [1.000] 30 [2.000] 2
2003003	gibbsite	-1.418	[1.000] 30 [3.000] 2 [-3.000]330

Test 5c.inp
4) CNLJB modified database
only parts 1, 5, and 6 of output

```
Like TEST1B, except titrate with 0.5 mmol, 1 mmol, 5 mmol gibbsite
rather that specifying 1 mmol as finite solid
25.00 MOLAL  0.000  0.00000E+00
0 0 1 1 0 2 0 0 1 1 2 0 0
 3 GIBBSITE (C)          TOTAL CONC mol/L
3 330  -3.000   30   1.000    2   3.000
  5.000E-04  1.000E-03  5.000E-03
0   0   0
    330  3.733E-03   -4.00                    /H+1
    732  1.580E-03   -2.80                    /SO4-2
    410  7.700E-05   -4.11                    /K+1
    140  0.000E+00   -7.00                    /CO3-2
     30  0.000E+00   -7.00                    /Al+3

  3   1
3301403    21.6600    -0.5300                 /CO2 (g)
  5   1
2003003    -8.7700    22.8000                 /GIBBSITE (C)
```

Test5c.out
Parts 1, 5, 6 of Output, all sweeps
4/CNLRA modified database

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:15:26

Like TEST1B, except titrate with 0.5 mmol, 1 mmol, 5 mmol gibbsite
rather that specifying 1 mmol as finite solid
Component file (COMP.DBS): comp.dbs COMP v4.02 02/12/2002
Thermodynamic file (THERMO.UNF): thermo.unf THERMO V4.02 02/05/2002
Gaussian DOM file (GAUSSIAN.DBS): gaussian.dbsGAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF): type6.unf TYPE6 V4.02 02/05/2002

Temperature (Celsius): 25.00
Units of concentration: MOLAL
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed for all solids in the thermodynamic database and
the print option for solids is set to: 1
Maximum iterations: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

---

330 3.733E-03 -4.00
732 1.580E-03 -2.80
410 7.700E-05 -4.11
140 0.000E+00 -7.00
30 0.000E+00 -7.00

H2O has been inserted as a COMPONENT
3 1
3301403 21.6600 -0.5300
5 1
2003003 -8.7700 22.8000

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	1.000E-04	-4.000	3.733E-03
732	SO4-2	1.585E-03	-2.800	1.580E-03
410	K+1	7.762E-05	-4.110	7.700E-05
140	CO3-2	1.000E-07	-7.000	0.000E+00
30	Al+3	1.000E-07	-7.000	0.000E+00
2	H2O	1.000E+00	0.000	0.000E+00

Charge Balance: UNSPECIATED

Sum of CATIONS= 3.810E-03 Sum of ANIONS = 3.160E-03

PERCENT DIFFERENCE = 9.326E+00 (ANIONS - CATIONS)/(ANIONS + CATIONS)

IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION:
SO4-2 Log activity guess: -2.81
CO3-2 Log activity guess: -13.66

*** TITRATION: GIBBSITE (C)
*** Titration point 1 in the series of 3 ***
The series of titrant total concentrations (mol/L) are:
5.000E-04 1.000E-03 5.000E-03
*** The total concentration of titrant for this point is: 5.000E-04 mol/L

PART 5 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:15:26

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
330	H+1	2.254E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	1.580E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.700E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
30	Al+3	5.000E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	4.072E-07	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	1.049E-05	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 2.868E-03 Sum of ANIONS 2.218E-03

PERCENT DIFFERENCE = 1.278E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 3.899E-03

EQUILIBRIUM pH = 2.712

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17152622

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
3003000	al2o3	-11.831	[2.000] 30 [3.000] 2 [-6.000]330
2003000	al(oh)3 (am)	-6.889	[1.000] 30 [3.000] 2 [-3.000]330
6003000	alohso4	-1.389	[-1.000]330 [1.000] 30 [1.000]732 [1.000] 2
6003001	al4(oh)10so4	-15.587	[-10.000]330 [4.000] 30 [1.000]732 [10.000] 2
6041000	k-alum	-9.413	[1.000]410 [1.000] 30 [2.000]732 [12.000] 2
6041001	alunite	-21.635	[1.000]410 [3.000] 30 [2.000]732 [6.000] 2
2003001	boehmite	-4.667	[-3.000]330 [1.000] 30 [2.000] 2
2003002	diaspore	-2.962	[-3.000]330 [1.000] 30 [2.000] 2
2003003	gibbsite	-4.380	[1.000] 30 [3.000] 2 [-3.000]330

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:15:26

*** TITRATION: GIBBSITE (C)
*** Titration point 2 in the series of 3 ***
*** The total concentration of titrant for this point is: 1.000E-03 mol/L

PART 5 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:15:26

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
330	H+1	7.540E-04	100.0	0.000E+00	0.0	0.000E+00	0.0
732	SO4-2	1.580E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.700E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
30	Al+3	1.000E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	2.952E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	1.049E-05	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 2.287E-03 Sum of ANIONS 1.637E-03

PERCENT DIFFERENCE = 1.657E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 3.535E-03

EQUILIBRIUM pH = 3.186

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17152628

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
3003000	al2o3	-8.215	[2.000] 30 [3.000] 2 [-6.000]330
2003000	al(oh)3 (am)	-5.081	[1.000] 30 [3.000] 2 [-3.000]330
6003000	alohso4	-0.636	[-1.000]330 [1.000] 30 [1.000]732 [1.000] 2
6003001	al4(oh)10so4	-9.411	[-10.000]330 [4.000] 30 [1.000]732 [10.000] 2
6041000	k-alum	-9.239	[1.000]410 [1.000] 30 [2.000]732 [12.000] 2
6041001	alunite	-20.689	[1.000]410 [3.000] 30 [2.000]732 [6.000] 2
2003001	boehmite	-2.859	[-3.000]330 [1.000] 30 [2.000] 2
2003002	diaspore	-1.154	[-3.000]330 [1.000] 30 [2.000] 2
2003003	gibbsite	-2.572	[1.000] 30 [3.000] 2 [-3.000]330

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:15:26

*** TITRATION: GIBBSITE (C)
*** Titration point 3 in the series of 3 ***
*** The total concentration of titrant for this point is: 5.000E-03 mol/L

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
30	Al+3	1.140E-03	22.8	0.000E+00	0.0	3.860E-03	77.2
732	SO4-2	1.580E-03	100.0	0.000E+00	0.0	0.000E+00	0.0
410	K+1	7.700E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	8.288E-06	100.0	0.000E+00	0.0	0.000E+00	0.0
140	CO3-2	1.051E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	3.339E-04	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 2.144E-03 Sum of ANIONS 1.494E-03

PERCENT DIFFERENCE = 1.787E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 3.492E-03

EQUILIBRIUM pH = 3.545

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17152633

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
3003000	al2o3	-5.906	[2.000] 30 [3.000] 2 [-6.000]330
2003000	al(oh)3 (am)	-3.927	[1.000] 30 [3.000] 2 [-3.000]330
6003000	alohso4	-0.231	[-1.000]330 [1.000] 30 [1.000]732 [1.000] 2
6003001	al4(oh)10so4	-5.542	[-10.000]330 [4.000] 30 [1.000]732 [10.000] 2
6041000	k-alum	-9.224	[1.000]410 [1.000] 30 [2.000]732 [12.000] 2
6041001	alunite	-20.515	[1.000]410 [3.000] 30 [2.000]732 [6.000] 2
2003001	boehmite	-1.705	[-3.000]330 [1.000] 30 [2.000] 2
2003002	diaspore	0.000	[-3.000]330 [1.000] 30 [2.000] 2
2003003	gibbsite	-1.418	[1.000] 30 [3.000] 2 [-3.000]330

~~Test6c~~ JBL 2/13/02

Test 6
4) modified CNUSA database
only Parts 1, 5, and 6 of output

```
Test file for Gaussian DOM model
DOC = 10 mg/L, Cd binding at pH 6.8

25.00 MOLAL  0.100  0.00000E+00
0 1 1 0 0 0 1 0 1 1 0 0 0
   10.00  0.000  0.000  0.000      0.00
0    0   0
    330  0.000E+00   -6.80 y                  /H+1
    144  0.000E+00   -6.00 y                  /DOM1
    160  3.000E-05   -4.52 y                  /Cd+2
    492  6.000E-05   -4.00 y                  /NO3-

  3   1
    330     6.8000     0.0000                 /H+1
```

Test6.out
Parts 1, 5, 6 of Output
w/ CNWRA modified database

PART 1 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:15:34

Test file for Gaussian DOM model
DOC = 10 mg/L, Cd binding at pH 6.8
Component file (COMP.DBS): comp.dbs COMP v4.02 02/12/2002
Thermodynamic file (THERMO.UNF): thermo.unf THERMO V4.02 02/05/2002
Gaussian DOM file (GAUSSIAN.DBS): gaussian.dbsGAUSSIAN V4.00 09/30/1999
Solids file (TYPE6.UNF): type6.unf TYPE6 V4.02 02/05/2002

Temperature (Celsius): 25.00
Units of concentration: MOLAL
Ionic strength: 0.100 molal; FIXED
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed only for those solids specified as ALLOWED
in the input file (if any).
Maximum iterations: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

---

330 0.000E+00 -6.80 y
144 0.000E+00 -6.00 y
160 3.000E-05 -4.52 y
492 6.000E-05 -4.00 y

H2O has been inserted as a COMPONENT
3 1
330 6.8000 0.0000

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	Name	ACTIVITY GUESS	log GUESS	ANAL TOTAL
330	H+1	1.585E-07	-6.800	0.000E+00
144	DOM1	1.000E-06	-6.000	0.000E+00
160	Cd+2	3.020E-05	-4.520	3.000E-05
492	NO3-1	1.000E-04	-4.000	6.000E-05
2	H2O	1.000E+00	0.000	0.000E+00

*** SPECIAL PARAMETERS for Dissolved Organic Matter:
DOC (mg/l): 10.00
Charge on DOM species are determined from fixed database values

** DOC COMPONENT 144:
Total Acidity (umol/mgC): 1.00
Total site concentration (mol/l): 1.000E-05

Charge Balance: UNSPECIATED

Sum of CATIONS= 6.000E-05 Sum of ANIONS = 8.800E-05

PERCENT DIFFERENCE = 1.892E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 5 of OUTPUT FILE

MINTEQA2 v4.02 DATE OF CALCULATIONS: 13-FEB-2002 TIME: 17:15:34

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	Name	DISSOLVED mol/L	DISSOLVED percent	SORBED mol/L	SORBED percent	PRECIPITATED mol/L	PRECIPITATED percent
492	NO3-1	6.000E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
144	DOM1	1.000E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
160	Cd+2	3.000E-05	100.0	0.000E+00	0.0	0.000E+00	0.0
2	H2O	8.836E-08	100.0	0.000E+00	0.0	0.000E+00	0.0
330	H+1	2.085E-07	100.0	0.000E+00	0.0	0.000E+00	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 5.838E-05 Sum of ANIONS 8.617E-05

PERCENT DIFFERENCE = 1.923E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 1.000E-01

EQUILIBRIUM pH = 6.800

DATE ID NUMBER: 20020213
TIME ID NUMBER: 17153473

Saturation indices and stoichiometry of all minerals

ID No	Name	SI	Composition by stoich. of components
2016000	cd(oh)2 (am)	-5.096	[-2.000]330 [1.000]160 [2.000] 2
2016001	cd(oh)2	-5.010	[1.000]160 [2.000] 2 [-2.000]330
2016002	monteponite	-6.469	[-2.000]330 [1.000]160 [1.000] 2

CONFIGURATION MANAGEMENT: MINTEQA2, Version 4.02

Prepared by

David R. Turner

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

1 TECHNICAL DESCRIPTION OF MINTEQA2, Version 4.02

MINTEQA2, Version 4.02 (June 2000 release; U.S. Environmental Protection Agency, 1999a,b) is an acquired geochemical speciation code, originally developed by the U.S. Environmental Protection Agency, National Exposure Research Laboratory, Ecosystems Research Division. The software is used by staff at the Center for Nuclear Waste Regulatory Analyses (CNWRA) in providing technical assistance to the U.S. Nuclear Regulatory Commission (NRC) in its high-level waste program. An earlier version, MINTEQA2, Version 3.11/3.12 is currently under configuration control in accordance with Technical Operating Procedure (TOP) 018.

MINTEQA2, Version 4.02 (released June 2000, U.S. Environmental Protection Agency, 1999a,b) is a geochemical equilibrium speciation code developed in FORTRAN 90 by the United States Environmental Protection Agency to model dilute aqueous systems. The code is PC-compatible, and is run in batch mode in the DOS-operating system. The original MINTEQ code was developed in the early 1980's at Pacific Northwest National Laboratory to combine the mathematical approach of the earlier MINEQL code with the extensive thermodynamic database of the United States Geological Survey code WATEQ3. The code was updated to MINTEQA2, Version 3.11/3.12 (released December 1991), and a preprocessing routine called PRODEFA2 was added to help construct the formatted input files used by the code. Since the original development, MINTEQA2 has become one of the more common codes used to simulate geochemical equilibria. For example, a standard aqueous geochemistry textbook (Langmuir, 1997), uses MINTEQA2 exclusively to set up and solve test problems in aqueous speciation.

1.1 Code Description

The documentation provided with the MINTEQA2, Version 4.02 file (downloaded from the EPA website at http://www.epa.gov/ceampubl/minteq.htm) includes a user's manual for MINTEQA2, version 3.0 (Allison et al., 1991) that describes the features and their implementation in the MINTEQA2 family of geochemical speciation codes. The download also includes two supplements that update the 1991 user's manual and summarize the changes and enhancements made in developing MINTEQA2, Version 4.02 file (U.S. Environmental Protection Agency, 1999a,b). Electronic and hard copies of these documents are included in this configuration control package for MINTEQA2, Version 4.02. In addition, the download from the EPA website includes several ASCII files that describe the code (READ.ME) and provide a listing of specific updates to the MINTEQA2, Version 4.02 code (UPDATE.TXT). A hard copy of READ.ME is included in Appendix A. Hard copy of UPDATE.TXT is included in Appendix B.

The entire compressed download file is included in this configuration management file, along with formatted thermodynamic databases prepared at the CNWRA.

1.1.1 Input

A MINTEQA2, Version 4.02 user typically has a problem relevant to a natural chemical system. This system is described in terms of the physical conditions such as temperature, and the concentrations of chemical components, species, solids and gases that are present. MINTEQA2 uses a formatted input file to identify the components of interest, read the concentrations, construct the chemical equilibrium model and solve for aqueous speciation and the distribution

construct the chemical equilibrium model and solve for aqueous speciation and the distribution of species between the solid, gas, and liquid phases. Input flags can be set to determine the level of output. The companion preprocessor PRODEFA2 has been developed and refined to help the user describe the geochemical problem and through a series of menus create the formatted input file necessary for a MINTEQA2 simulation. However, if the user is familiar with the formatting requirements, he or she can construct the input file without PRODEFA2, using an ASCII text editor.

The typical formatted input file for a MINTEQA2 problem is not very long , but contains a significant amount of information. During execution of a geochemical problem, the input file is read and the databases searched for the relevant component species and aqueous, gas, solid phases.

A key concept in the input file is the use of three-digit ID numbers for components, and seven-digit ID numbers for aqueous species, solids, redox couples, and gases. In addition, the first two digits of the ID number of solids contains information on the type of solid (e.g., oxide, sulfide, carbonate). These numbers are used by MINTEQA2 to identify components and species in the databases. Although there is a field for naming these items, it is for the benefit of the user in the output, and is not used in calculation by MINTEQA2. There are two constraints on the ID numbers: they must be unique and they must be contained in the appropriate databases. For the components and species entered in the database, these constraints have been met. However, since the ID numbers are not necessarily intuitive, it is unlikely that the user would know to associate the three-digit ID number 330 with the component H^+ or the seven-digit number 3300020 with OH^-. For this reason, while it is relatively easy to delete species, adding components, species, solids, or reactions requires reasonably sophisticated preprocessing to provide the user with what he/she can understand (e.g., names such as H^+, OH^-), and search the database for the appropriate ID numbers to provide the information necessary for a MINTEQA2 simulation.

1.1.2 Output

The results from the equilibrium geochemical speciation calculation are written to an output file specified by the user. MINTEQA2, Version 4.02 will overwrite previously existing files with the same name. In all cases, the output includes an echo of the input to verify that the input file was read correctly and a time stamp to verify the time of the run. Additional types of output include writing equilibrium mass distribution chemical component species (or aqueous species) to a comma delimited ASCII file that can be imported into commercial spreadsheets. The level of output varies and is set by the user in the input files. The equilibrium concentration of the element(s) of interest are reported in molality (moles contaminant/kg H_2O) as distributed between the dissolved, sorbed, and precipitated phases.

1.2 Hardware Requirements and Installation

MINTEQA2, Version 4.02 is designed for the IBM PC family of microcomputers or compatible systems running under version 3.30 or higher of the Microsoft or PC Disk Operating Systems (PC or MS DOS). Properly configured, MINTEQA2, Version 4.02 and its support files and programs can be executed under PC DOS, MS DOS 3.30 and later versions, DOS 4.0x, DOS 5.0x, or DOS 6.x; a DOS window or a DOS level system start up (i.e., boot) under Microsoft

Windows 3.1x, Microsoft Windows for WorkGroups, Windows 95, Windows 98, or NT operating systems. At the CNWRA, the software has been installed on a Pentium-based PC with a Microsoft Windows NT, Version 4.00 operating system.

To install MINTEQA2, Version 4.02 and/or related support files and programs on a hard disk, insert the first distribution diskette in a compatible diskette drive. At the DOS prompt, type:

A:\INSTALL or B:\INSTALL

at the DOS system prompt and press the <Enter> key. Then follow instructions and respond to the prompts presented on the monitor screen by the interactive installation program. This is a compressed, self-extracting, interactive installation program—with on-line, context sensitive help—that contains the MINTEQA2 model system (MINTEQA2, Version 4.02), dated June 2000.

If the MINTEQA2 model system is being installed from the MINTEQA2 installation file (INSTALMT.EXE) downloaded from the Internet, then the user types at the DOS prompt

INSTALMT

at the DOS system prompt and press the <Enter> key. This command assumes that the current default drive and sub-directory is the same drive and sub-directory that contain the file INSTALMT.EXE.

Running MINTEQA2, Version 4.02 requires that the code be installed in the same directory as the batch file MINRUN.BAT. The directory containing the MINTEQA2/PRODEFA2 executables also need each to contain each of the database files. The input and the database files are formatted using the format described in U.S. Environmental Protection Agency (1999a).

2 INSTALLATION CHECKS

The MINTEQA2, Version 4.02 software has been checked to ensure that it was installed correctly on the CNWRA PC platform (Pentium-based PC, Windows NT 4.00 operating system). Part of self-extracting installation package for MINTEQA2, Version 4.02 includes input and output of a set of 12 example problems developed to demonstrate the different capabilities of MINTEQA2, Version 4.02. The input files for these example problems were submitted in batch mode to MINTEQA2, Version 4.02 as installed, and the output compared against the files provided in the installation package. **With the exception of the time/date stamp, these files produced results identical to those provided by the MINTEQA2, Version 4.02 developers.** Both hard copy and electronic versions of these installation checks are provided in this configuration management package.

3 CONTENTS OF THIS CONFIGURATION MANAGEMENT PACKAGE

This configuration management includes the following information

Download file from the EPA website at http://www.epa.gov/ceampubl/minteq.htm (Electronic)

User's Manual for MINTEQA2, Version 3.0 and Supplements 1 and 2 for MINTEQA2, Version 4.02 (hard copy and electronic)

Software Summary Form TOP-4-1

Software Release Notice Form TOP-6

Installation check using 12 test problems with output as received, and output after installation on CNWRA PC platform (hard copy and electronic files)

Original databases as received (Electronic)

CNWRA-modified databases to include data for Am, Co, Cs, Eu, Np, Pu, Ra, Ru, Sn, Sr, Tc, Th, U, and Zr. This includes data from the Nuclear Energy Agency Thermodynamic Database for Am, Np, Pu, Tc, and Th. Data sources are also provided. (Electronic)

Source code for
- MINTEQA2, Version 4.02
- PRODEFA2 (the MINTEQA2, Version 4.02 preprocessor module)
- UNFORMAT (the code that converts the ASCII thermodynamic data to binary form

4 REFERENCES

The following documents are referenced or used in this configuration package for MINTEQA2, Version 4.02. Both electronic and hard copies of these documents are included in this configuration control package.

Allison, J.D., D.S. Brown, and K.J. Novo-Gradac. "MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems." Version 3.0 User's Manual. EPA/600/3–91/021. Athens, Georgia: U.S. Environmental Protection Agency. 1991.

Langmuir, D. *Aqueous Environmental Geochemistry.* Englewood Cliffs, New Jersey: Prentice-Hall, Inc. 1997.

U.S. Environmental Protection Agency. "MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems: User Manual Supplement for Version 4.0." Athens, Georgia: U.S. Environmental Protection Agency, National Exposure Research Laboratory, Ecosystems Research Division. 1999a.

U.S. Environmental Protection Agency. "Diffuse-Layer Sorption Reactions for use in MINTEQA2 for HWIR Metals and Metalloids." Athens, Georgia: U.S. Environmental Protection Agency, National Exposure Research Laboratory, Ecosystems Research Division. 1999b.

SOFTWARE SUMMARY FORM

01. Summary Date: 02/20/2002	02. Summary prepared by (Name and phone) David R. Turner (CNWRA): (201) 522-2139	03. Summary Action: REPLACEMENT (Replaces MINTEQA2, Version 3.11/3.12)
04. Software Date: 06/2000	05. Short Title:MINTEQA2/PRODEFA2, Version 4.02	
06. Software Title: MINTEQA2/PRODEFA2, Version 4.02: A Geochemical Assessment Model for Environmental Systems		07. Internal Software ID: None

08. Software Type: ☐ Automated Data System X Computer Program ☐ Subroutine/Module	09. Processing Mode: ☐ Interactive ☐ Batch X Combination	10. Application Area a. General: X Scientific/Engineering ☐ Auxiliary Analyses ☐ Total System PA ☐ Subsystem PA ☐ Other b. Specific: Acquired Geochemical Equilibrium Speciation Code. Developed by U.S. EPA.
11. Submitting Organization and Address: CNWRA/SwRI 6220 Culebra Road San Antonio, TX 78228		12. Technical Contact(s) and Phone: David R. Turner (210) 522-2139

13. Software Application: MINTEQA2, Version 4.02 is a DOS-based geochemical equilibrium speciation model for dilute aqueous species. MINTEQA2, Version 4.02 uses a thermodynamic database with formatted chemical reactions, equilibrium constants, and enthalpies of reaction to solve mass action and mass balance constraints in geochemical systems. The code is used to investigate geochemical processes such as aqueous speciation, precipitation/dissolution, gas partial pressures, redox behavior, sorption, and ion exchange. PRODEFA2 is an interactive pre-processor that uses menus to build the formatted input files for MINTEQA2.

14. Computer Platform PC/Pentium II	15. Computer Operating System: Windows NT, Version 4.00	16. Programming Language(s): Fortran 90	17. Number of Source Program Statements: Unknown
18. Computer Memory Requirements: 640 K RAM/1.4 Mb storage	19. Tape Drives: N/A	20. Disk Units: N/A	21. Graphics: N/A

22. Other Operational Requirements
ANSI.SYS device driver for PRODEFA2 menus

23. Software Availability: X Available ☐ Limited ☐ In-House ONLY	24. Documentation Availability: X Available ☐ Preliminary ☐ In-House ONLY

25. Acquired Code developed by U.S. Environmental Protection Agency

Software Developer: _____ Date: _____

CNWRA Form TOP-4-1 (05/98)

SOFTWARE RELEASE NOTICE

1. SRN Number:

2. Project Title: Radionuclide Transport Key Technical Issue | Project No. 20.01402.871

3. SRN Title: MINTEQA2/PRODEFA2, Version 4.02

4. Originator/Requestor: David R. Turner | Date: 02/20/2002

5. Summary of Actions

X Release of new software ☐ Change of access software

☐ Release of modified software: ☐ Software Retirement

☐ Enhancements made

☐ Corrections made

6. Validation Status

☐ Validated

☐ Limited Validation

X Not Validated Explain: Validation Plan Approved, to be implemented

7. Persons Authorized Access

Name	Read Only/Read-Write	Addition/Change/Delete
David R. Turner	Read-Write	
F. Paul Bertetti	Read-Write	

8. Element Manager Approval: Date:

9. Remarks:

NOTE: This acquired code was developed by the U.S. Environmental Protection Agency and supersedes/replaces MINTEQA2/PRODEFA2, Version 3.11/3.12 currently under configuration management.

CNWRA Form TOP-6 (09/01)

APPENDIX A

File: READ.ME

MINTEQA2
Metal Speciation Equilibrium Model for Surface and Ground Water

PRODEFA2
Problem Definition Program for MINTEQA2

Version 4.02

U.S. EPA Release, June 2000

Center for Exposure Assessment Modeling (CEAM)
National Exposure Research Lab - Ecosystems Research Division
Office of Research and Development (ORD)
U.S. Environmental Protection Agency (U.S. EPA)
960 College Station Road
Athens, Georgia 30605-2700

706/355-8400

CONTENTS

Introduction
Abstract
Year 2000 Compliance
Documentation
Distribution Diskettes
Selected File Names and Content
Development System
Routine Execution
Run Time and Performance
Modification
Technical Help Contact
Disclaimer

INTRODUCTION

MINTEQA2 is an equilibrium speciation model that can be used to calculate the equilibrium composition of dilute aqueous solutions in the laboratory or in natural aqueous systems. The model is useful for calculating the equilibrium mass distribution among dissolved species, absorbed species, and multiple solid phases under a variety of conditions including a gas phase with constant partial pressures.

PRODEFA2, the Problem Definition Program for MINTEQA2, is an interactive program that assists the user in developing and building an input data file for the MINTEQA2 model.

For a list of modifications to the MINTEQA2 model system since its last release (version 4.02, June 2000), refer to the files RELEASE.TXT and UPDATE.TXT.

> NOTE: For convenience, the terms "MINTEQA2 model system" and "MINTEQA2" will be used in this document to refer to the MINTEQA2 model and all associated support files and programs as a single unit. Therefore, the terms "MINTEQA2", and "MINTEQA2 model system" are synonymous for purposes of this document.

ABSTRACT

Refer to file ABSTRACT.TXT for an abstract of the MINTEQA2 model system.

YEAR 2000 COMPLIANCE

Refer to file YEAR2000.TXT for the MINTEQA2 model system year 2000 (Y2K) compliance statement.

DOCUMENTATION

It is recommended that the user obtain and reference the documents listed below to operate and apply the MINTEQA2 model system.

Copies of the following documents are included on the distribution diskettes and within the Internet distribution file INSTALMT.EXE.

Document Name(s)	File Name(s)
MINTEQA2 model system general execution and user support guide	READ.ME
MINTEQA2 Model System Release Notes	RELEASE.TXT
MINTEQA2 Model System Update Notes (Enhancements/updates/additions not covered in user manual file)	UPDATE.TXT
MINTEQA2 Model System Abstract	ABSTRACT.TXT

MINTEQA2 Model System Year 2000 (Y2K) Compliance Statement — YEAR2000.TXT

CEAM Software Product User Response Form — RESPONSE.TXT

MINTEQA2 User's Manual — USERMANU.PDF
"MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems: Version 3.0 User's Manual"

MINTEQA2 User's Manual Supplement 1 — SUPPLE1.PDF
"MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems: User Manual Supplement for Version 4.0"

MINTEQA2 User's Manual Supplement 2 — SUPPLE2.PDF
"Diffuse-Layer Sorption Reactions for use in MINTEQA2 for HWIR Metals and Metalloids".

NOTE: The files READ.ME and those ending in .TXT are ASCII text (non-binary) files. Files ending in PDF are Adobe(*) Acrobat(*) Portable Document Format (PDF) files. To view, print, and/or navigate a PDF document, a reader program must be installed on the users computer system. A free Adobe reader allows the user to view, navigate, and/or print PDF files across all major computing platforms. Acrobat Reader is a free viewing companion to Adobe Acrobat 3.0 and is available free from the Adobe world wide web (WWW) site at Uniform Resource Locator (URL) address: http://www.adobe.com.

To ensure that the user can view and/or print a PDF file in its entirety, the user must down load and install the most recent version/edition of the free Acrobat Reader. PDF files can be viewed across multiple platforms (Mac, Microcomputer, UNIX) using the appropriate reader for that platform.

These documents should be retained by the requester for reference.

DISTRIBUTION DISKETTES

NOTE: k=1,024; m=1,048,576; b=1 byte

Included are 2, 3.5 inch (1.44mb, DS/HD) DOS (Disk Operating System) formatted diskettes containing the Metal Speciation Equilibrium Model for Surface and Ground Water 2 (MINTEQA2,

version 4.02), U.S. EPA release, dated June 2000.

This model system is designed for the IBM PC family of microcomputers or compatible systems running under version 3.30 or higher of the Microsoft or PC Disk Operating Systems (PC or MS DOS--refer to DEVELOPMENT SYSTEM section). Properly configured, this model system and its support files and programs can be executed under PC DOS, MS DOS 3.30 and later versions, DOS 4.0x, DOS 5.0x, or DOS 6.x; a DOS window or a DOS level system start up (i.e., boot) under Microsoft Windows 3.1x, Microsoft Windows for WorkGroups, Windows 95, Windows 98, or NT operating systems.

To install the MINTEQA2 model system and/or related support files and programs on a hard disk, insert the first distribution diskette in a compatible diskette drive. Type

A:\INSTALL or B:\INSTALL

at the DOS system prompt and press the <Enter> key. Then follow instructions and respond to the prompts presented on the monitor screen by the interactive installation program. This is a compressed, self-extracting, interactive installation program--with on-line, context sensitive help--that contains the MINTEQA2 model system (MINTEQA2, version 4.02), dated June 2000.

> NOTE: If the MINTEQA2 model system is being installed from the MINTEQA2 installation file (INSTALMT.EXE) down loaded from the Internet, then the user should type
>
> INSTALMT
>
> at the DOS system prompt and press the <Enter> key. This command assumes that the current default drive and sub-directory is the same drive and sub-directory that contain the file INSTALMT.EXE. For further information and to access CEAM software products through the Internet, refer to the TECHNICAL HELP CONTACT section.
>
> NOTE: The content of the distribution diskettes can be copied to another set of "backup" diskettes using the DOS DISKCOPY command. Refer to the DOS Reference Manual or on-line help for command application and use. The "backup" diskettes must be the same size and storage density as the original source diskettes.

The following SELECTED FILE NAMES AND CONTENT section provides a brief functional description of selected MINTEQA2 model system files by name or file name extension type. Other sections in this document contain information about

- system development tools used to build the microcomputer release of the MINTEQA2 model system
- recommended hardware and software configuration for the execution of the model system and all support programs and files

- o program execution
- o sample run times
- o program modification
- o technical support

SELECTED FILE NAMES AND CONTENT

The self-extracting, interactive, installation executable program file exists in a compressed format to save disk space and file transfer time. This section contains a description of selected files that can be decompressed from the compressed distribution diskettes and/or file.

Follow the instructions shown on the interactive installation program screens and menus to install, decompress (extract), and restore file(s) to their original name and size in order to place the MINTEQA2 model system in a usable format on a hard or virtual disk. For comparison purposes, the original date and time of creation are also restored with each file.

> NOTE: Execution of the INSTALL or INSTALMT command can extract one or more MINTEQA2 model system files. These files are automatically stored into DOS sub-directories on the hard disk. The hard disk and sub-directory structure, under which the sub-directories shown below are stored, is selected by the user (e.g., C:\MINTEQA2) during execution of the INSTALL or INSTALMT program.
>
> The string "InstallationDirectory" will be used to denote the highest level default installation directory structure (e.g., C:\MINTEQA2) chosen by the user during execution of INSTALL or INSTALMT. Below the installation directory, all files are grouped and listed by the appropriate DOS sub-directory name into which they will be automatically stored.

** Sub-directory InstallationDirectory:

> NOTE: To execute a DOS batch command file (*.BAT)--and hence a model or program spawned (i.e., executed) buy a given batch command file--from any sub-directory located on a hard or virtual disk drive, try adding the MINTEQA2 installation sub-directory (e.g., C:\MINTEQA2) to the DOS search PATH and copy appropriate run time support files to the current default sub-directory. One way to accomplish this is to add or modify the PATH statement in the system start-up file, AUTOEXEC.BAT (located in the root directory on the start-up or boot drive). For example

PATH C:\;C:\DOS;C:\UTIL;C:\WP51;C:\MINTEQA2;

Refer to the DOS and/or Windows Reference Manual or on-line help for PATH command and AUTOEXEC.BAT file application and use.

MENU.BAT - DOS batch command file that displays the MINTEQA2 model system command menu on the monitor screen. To execute, type

MENU

at the DOS system prompt, press the <Enter> key, then follow the information screens and prompts displayed on the monitor screen.

FORMAT.BAT - DOS batch command file used to execute the FORMAT program. To execute, type

FORMAT

at the DOS system prompt, press the <Enter> key, then follow the information screens and prompts displayed on the monitor screen. For further information, refer to the ROUTINE EXECUTION section. This program can be used to individually convert the file THERMO.UNF or TYPE6.UNF from an unformatted (binary) to a formatted (ASCII, non-binary) text file format. If a file is stored in ASCII text format, it can be viewed and/or edited with an editor that can save files in ASCII text (non-binary) file format.

UNFORMAT.BAT - DOS batch command file used to execute the UNFORMAT program. To execute, type

UNFORMAT

at the DOS system prompt, press the <Enter> key, then follow the information screens and prompts displayed on the monitor screen. For further information, refer to the ROUTINE EXECUTION section. This program can be used to individually convert the file THERMO.DBS or TYPE6.DBS from a formatted (ASCII, non-binary) text file format to an unformatted (binary) format that can be read and processed by the MINTEQA2 model and/or PRODEFA2 program.

PRODEF.BAT - DOS batch command file used to execute the PRODEF program. To execute, type

PRODEF

at the DOS system prompt, press the <Enter> key,

then follow the information screens and prompts displayed on the monitor screen. For further information, refer to the ROUTINE EXECUTION section.

MINRUN.BAT - DOS batch command file used to execute the MINTEQA2 model. To execute, type

MINRUN

at the DOS system prompt, press the <Enter> key, then follow the information screens and prompts displayed on the monitor screen. For further information, refer to the ROUTINE EXECUTION section.

WARNING: Executable task image files (*.EXE) should only be executed using the corresponding DOS batch command file provided (FORMAT.BAT, UNFORMAT.BAT, PRODEF.BAT, MINRUN.BAT).

NOTE: Unless specified as a "binary" file (e.g., *.UNF) in their description herein, MINTEQA2 model input files are ASCII (non-binary) text files. ASCII text files can be viewed or edited using any editor program that can read and save a file to disk in ASCII text (non-binary) format.

NOTE: An input or output file name path specification and/or file name, as typed at a run time prompt, or as specified by the user within a MINTEQA2 model input prompt response file, must be a unique and valid DOS path and/or file name. An input data file name must also be a valid MINTEQA2 file name--either furnished with the distribution package or created, designated, and named by the user. A file name typed at a run time prompt or specified within a MINTEQA2 input prompt response file will be processed and executed in a given run of the model. Remember, a DOS file name can be from 1 to 8 characters and can have an optional 1 to 3 character file name extension.

NOTE: Refer to the explanation of the OUT_TEST*.OUT files for a procedure to compare the contents of an output file produced by the MINTEQA2 model on the users system, to an output file as provided within the distribution package (OUT_TEST*.OUT).

NOTE: Input prompt response files, for batch processing of the MINTEQA2 model, should only be created and/or modified using an editor program that can read and save a file to disk in ASCII text (non-binary) format. An input response file can be used to execute the MINTEQA2 model in batch mode and thus would contain valid responses to the interactive prompts

presented during the execution of the MINTEQA2 model. Using an input response file allows the program to run without user intervention or interruption, and may be set up for multiple response and/or data sets. This technique is useful if the user needs to execute the model repeatedly while changing, for example, one input parameter between model executions without having to enter or modify other parameters. A text editor that can read and save a file to disk in ASCII text (non-binary) format is needed to create and/or modify an input prompt response file.

NOTE: For further explanation, information, and/or listings of example input and output data and their associated files, refer to the user's manual.

THERMO.UNF
TYPE6.UNF - Chemical thermodynamic data base files that provide input to and will be read automatically by the MINTEQA2 model and PRODEFA2 program. These files are unformatted (binary), sequential files. Therefore, do NOT attempt to view, print, or edit these files.

THERMO.DBS
TYPE6.DBS - Formatted, sequential versions of the THERMO.UNF and TYPE6.UNF chemical thermodynamic data base files. These files are formatted ASCII text (non-binary), sequential files that can be viewed or edited using any editor program that can read and save a file to disk in ASCII text (non-binary) format.

*.INP - Eleven (11) test, input data files to test the installation and demonstrate application of the MINTEQA2 model. To test the installation, execute the MINTEQA2 model using each file as the name of the input file (refer to the ROUTINE EXECUTION section). The model interactively prompts the user for the input and output file names. These data are also furnished to provide instruction by example and can be used as templates for the preparation of a new or modified input sequence.

These sample input data files provide examples of input and exercise most sections and capabilities of the MINTEQA2 model. For further information on executing the MINTEQA2 model, refer to file MINRUN.BAT in this section or refer to the ROUTINE EXECUTION section.

** Sub-directory InstallationDirectory\OUT_TEST:

NOTE: The symbol "<Enter>" represents pressing the <Enter> or carriage return key. Responses and key strokes that can be typed by the user are underlined

with the hyphen character (-) and/or enclosed by the angle bracket characters (<>).

NOTE: Unless specified as a "binary" file, MINTEQA2 model output listing files are ASCII (non-binary) text files. ASCII text files can be viewed or edited using any editor program that can read and save a file to disk in ASCII text (non-binary) format.

.OUT - Sample output files produced by executing the model using the input files provided (.INP). These files were produced by execution of the MINTEQA2 model using each test input data file as described above (*.INP). To test the installation, execute the MINTEQA2 model using each input data file as provided with the distribution package.

After executing the MINTEQA2 model using each test input file provided (*.INP), compare the contents of the file so named by the user and produced (e.g., TEST1A.OUT) to the corresponding output file provided and stored within the sub-directory OUT_TEST (e.g., OUT_TEST\TEST1A.OUT).

To compare file contents, use the COMP (PC DOS) or FC (MS DOS) file compare command, or print both files then compare contents by hand.

For further information on executing the MINTEQA2 model, refer to file MINRUN.BAT in this section or the ROUTINE EXECUTION section.

Example MINTEQA2 execution and file comparison sequence:

Step	Description/Action

1) Set the default drive to the disk containing the model system sub-directory:

A:\> C:<Enter>
--

2) Change the DOS default sub-directory to the sub-directory designated by the user during the installation program as the installation sub-directory (e.g., MINTEQA2). Use the DOS CD (change directory) command at the DOS system prompt:

C:\> CD \MINTEQA2<Enter>
---

3) Execute the MINTEQA2 model:

C:\MINTEQA2> MINRUN<Enter>

~~~~~~
(Initial MINTEQA2 banner/registration screen displayed
here...press <Enter> key to clear screen and continue model
execution...)
~~~~~~
Follow and respond to the input and/or command prompts displayed on the monitor screen. MINTEQA2 4.02 run time diagnostic and information status screens and messages may be displayed while the model executes.
~~~~~~
When the MINTEQA2 model finishes executing, compare the output files supplied to those produced.

NOTE: Each MINTEQA2 model output file contains a unique date and time stamp value.

For example:

```
C:\MINTEQA2> COMP OUT_TEST\TEST1A.OUT TEST1A.OUT<Enter>
             ------------------------------------
```

or,

```
C:\MINTEQA2> FC OUT_TEST\TEST1A.OUT TEST1A.OUT<Enter>
             --------------------------------
```

DEVELOPMENT SYSTEM

The following list describes the language and program development tools used by the U.S. EPA Center for Exposure Assessment Modeling to build version 4.02 of the microcomputer implementation of the MINTEQA2 model system.

Also shown are the recommended minimum hardware and software configuration and the recommended \CONFIG.SYS configuration/environment file statements for the implementation and execution of this model system and all related support files and programs. Make sure that the IBM PC or compatible system has the statements listed below (refer to \CONFIG.SYS Statements) in the \CONFIG.SYS file, and re-boot the system to implement these changes before attempting to install or use the MINTEQA2 model system.

Development System:

Hardware System:	Fully IBM compatible 80386, 80486, or 80586
Language:	FORTRAN 90
Operating System:	DOS version 3.30 or higher. Properly configured, this model system should
~~~~~~

	also work on hardware platforms with PC DOS or MS DOS versions 4.0x, 5.0x, or 6.x., to include a DOS window, DOS box or boot under Windows 3.x, Windows for WorkGroups, Windows 95, Windows 98, or NT.
DOS Extender:	Phar Lap 386/DOS-extender; bound into application EXE file with automatic virtual memory management; distributed royalty free
Memory Manager:	Compatible with VDISK.SYS, QEMM386, HIMEM.SYS, RAMDRIVE.SYS, EMM386, CEMM, 386Max; compatible with DPMI, VCPI, and XMS standards
Compiler:	Lahey FORTRAN 90 version 3.50c and linker (386LINK, 8.0_Lahey2).
Link Editor:	Phar Lap 386LINK version 7.0
Overlay Structure:	None - linked as flat memory model and program
Storage Requirements:	(k=1,024; m=1,048,576)
Random Access Memory:	(approximate minimum free bytes needed to execute EXE file for optimum performance within extended, not expanded, memory (i.e., XMS))
	640k base (low end) memory, plus .38m bytes of free extended (XMS) memory and 1.0m bytes of free disk space; or, 1m byte of free extended (XMS) memory and 1.38m bytes disk space (non-optimized).
Diskette Drive:	Required for installation only.
Hard Disk Drive:	200m byte drive recommended (minimum) with 10.0m bytes free (minimum)
Installation Size:	Run Time: Approx. 5.0m bytes max.
Run time size:	After installation, up to approximately .5m bytes plus space for user input data or command files, output, and temporary files produced by model system (refer to MINIMUM FILE CONFIGURATION section).
Numerical Coprocessor:	Required.
\CONFIG.SYS Statements:	BREAK=ON BUFFERS=20 or BUFFERS=32 FILES=20

NOTE: Add the ANSI.SYS device driver for handling the display of the extended character set on the monitor screen.

For DOS or Windows 3.1x:
DEVICE=C:\DOS\ANSI.SYS
For Windows 95 or 98:
DEVICE=C:\WINDOWS\COMMAND\ANSI.SYS
For Windows NT:
DEVICE=C:\WINNT\SYSTEM32\ANSI.NT

DEVICE=extended memory manager

- and -

SHELL=C:\COMMAND.COM C:\ /e:512 /p

Printer: For *.PDF files only, HP LaserJet III PostScript or compatible printer (minimum).

Printer Software: For *.PDF files only, Adobe Acrobat reader version 3.0 or greater.

ROUTINE EXECUTION

NOTE: The symbol "<Enter>" represents pressing the <Enter> or carriage return key. Responses and key strokes that can be typed by the user are underlined with the hyphen character (-) and/or enclosed by the angle bracket characters (<>).

NOTE: It is possible that execution, not installation, of the MINTEQA2 model system could be incompatible with MS DOS and Windows software cache files SMARTDRV.SYS or SMARTDRV.EXE loaded from the system configuration files \CONFIG.SYS and/or \AUTOEXEC.BAT on the boot drive. If any portion of the MINTEQA2 model system prematurely halts, produces unusual results, and/or causes the host system to halt or hang, remove any SMARTDRV statements on the boot drive \CONFIG.SYS and/or \AUTOEXEC.BAT files, then re-boot the system to implement these changes before attempting to reuse any portion the MINTEQA2 model system.

Introduction
~~~~~~~~~~~~
Complete the installation process to make the full or any portion of the MINTEQA2 model system and related files resident on a hard (usually designated as "C:") or virtual disk drive. Then modify
~~~~~~~~~~~~

the \CONFIG.SYS system environment file and restart the microcomputer system. This needs to be completed only once for a given installation and/or execution of the MINTEQA2 model system.

DOS Storage Path
~~~~~~~~~~~~~~~~

Verify that the MINTEQA2 model system executable task image files (*.EXE), DOS batch command files (*.BAT), other run time support files (*.DBS, *.UNF, *.INI, *.SCR), and user defined input data and/or command file(s) are in the current default DOS sub-directory. It is convenient but not required to have these files in the same sub-directory.

> NOTE: To execute a DOS batch command file (*.BAT)--and hence a model or program spawned (i.e., executed) buy a given batch command file--from any sub-directory located on a hard or virtual disk drive, add the MINTEQA2 installation sub-directory (e.g., C:\MINTEQA2) to the DOS search PATH and copy other appropriate run time support files to the current default sub-directory. One way to accomplish this is to add or modify the PATH statement in the system start-up file, AUTOEXEC.BAT (located in the root directory on the start-up or boot drive). For example
>
> PATH C:\;C:\DOS;C:\UTIL;C:\WP51;C:\MINTEQA2
>
> If any portion of the MINTEQA2 model system prematurely halts, produces unusual results, and/or causes the host system to halt or hang, copy all DOS batch and other run time support files from the MINTEQA2 model system installation sub-directory to the current default sub-directory from where the MINTEQA2 model system will be executed via the DOS search PATH statement.
>
> Refer to the DOS Reference Manual or on-line help for PATH command and AUTOEXEC.BAT file application and use.

Routine Execution Steps
~~~~~~~~~~~~~~~~~~~~~~~

Step Description/Action
~~~~ ~~~~~~

1) Set the default drive to the disk containing the MINTEQA2 model system sub-directory. For example:

   A:\> C:<Enter>
        --

2) Change the DOS default sub-directory to the sub-directory designated by the user during the installation program as the installation sub-directory (e.g., MINTEQA2). Use the DOS CD (change directory) command at the DOS system prompt:

   C:\> CD \MINTEQA2<Enter>

~~~~

NOTE: A common problem is for a DOS executable or batch command file (*.EXE, *.BAT) to be unable to locate a file because it assumes the file is on the default drive and/or sub-directory when it is not. If input and/or other run time support file(s) are not on the default drive and sub-directory, the user can type a drive and/or path name ahead of the file name. For further information, refer to the "File Name and Path Specifications" sub-section later in this document or the DOS Reference Manual.

NOTE: The MINTEQA2 model system is a DOS, not Windows, application. All executable files and programs should be executed from a DOS command line prompt from a system booted from the DOS level or a DOS window from within Microsoft Windows (95/98/NT).

3) To execute the PRODEF program, type:

```
C:\MINTEQA2> PRODEF<Enter>
             ------
```

After an opening banner/registration screen is displayed on the monitor, press the <Enter> key to clear the screen and begin execution. The program will prompt the user for information needed for this run of the program. Follow and respond to the menu, prompts, and parameter options presented on the monitor screen.

4) To execute the MINTEQA2 model, type:

```
C:\MINTEQA2> MINRUN<Enter>
             ------
```

NOTE: The normal sequence of execution is to execute the PRODEFA2 program (to create or modify a MINTEQA2 model input file), then execute the MINTEQA2 model.

After an opening banner/registration screen is displayed on the monitor, press the <Enter> key to clear the screen and begin model execution. The model will prompt the user for an input data file, an output data file, and/or information needed for this run of the model. After the input and output file names have been typed by the user and validated by the MINTEQA2 model, the MINTEQA2 model will begin execution.

IMPORTANT NOTE: The file name MININ.DAT is a reserved file name within the MINTEQA2 model system. Therefore, if the file MININ.DAT
a) already exists in the directory where the MINTEQA2 model is being executed (e.g., \MINTEQA2), and
b) is a properly formatted and parameterized MINTEQA2 model input data file and command set, the MINTEQA2 model will automatically read and process this file as

the input data file. The MINTEQA2 model will therefore not prompt the user for the name of either an input or output file as described above. Under this condition, the results from the execution of the model will automatically be placed in the output file MINOUT.OUT.

Viewing Output Results

After executing a MINTEQA2 model system executable task image file, exiting MINTEQA2, and returning to the DOS prompt, the user can view an output file (e.g., TEST1A.OUT), if any, produced by the execution of a program or model if and only if that file is in ASCII text (non-binary) format. Results can be viewed by scrolling through the output file that was (1) a result of model or program execution and/or (2) named by the user at a run time prompt. A word processor or text editor is convenient for this purpose, or the command

```
TYPE filename | MORE
```

can be used where "filename" is the name of the output file.

However, the TYPE command is awkward for a file that exceeds the 80-column screen width. Alternatively, the output file can be printed. A compressed print mode (132 column) should be used to avoid awkward--wrapped around--output from lines that exceed 80 columns. The DOS MODE command can be used for this purpose. For a parallel printer assigned to LPT1, the DOS command

```
MODE LPT1: 132
```

will cause most printers to print in compressed mode. For further information, refer to the DOS Reference Manual.

File Name and Path Specifications

A file name, path specification, and/or the parameter file name argument "filename" must be a unique and valid DOS path and/or file name. The user response "filename" must also be a valid MINTEQA2 model system command, input, or output file name--either furnished with the distribution package (refer to SELECTED FILE NAMES AND CONTENT section) or created, designated, and named by the user. A file name used as input data for a program or model in the MINTEQA2 model system will be processed and executed in that run of the program or model.

In general, file names used for input data, command, and/or output listing files (except for the test input and example output cases provided) are arbitrary, but must follow the rules for DOS file names. A file name should assist the user with identifying the contents or purpose of a file (e.g., INPUT.DAT, OUTPUT.LST).

Any DOS file name can be from 1 to 8 characters and can have an optional 0 to 3 character file name extension. Any characters beyond 8 in the file name or beyond 3 in the file name extension will be truncated and ignored by the DOS operating system. Refer to the DOS Reference Manual for further information on file names and disk file input/output procedures, rules, and commands.

RUN TIME AND PERFORMANCE

The following run times (approximate) were observed using the test input data files as furnished with the distribution version of the MINTEQA2 model system. Remember that these times were obtained using input test data that may not be representative of a "real world" problem and/or data. The test data have been furnished for testing the installation of the MINTEQA2 model system and for instruction by example.

In general, these input test data were not intended to be representative of full scale model simulations. They were developed to test the installation of significant sections of model code.

The run times listed in the table below were produced on a Dell OptiPlex Gn+ 200 megahertz class microcomputer running under a DOS window, under Windows 95, and using 640k bytes of random access (low end) memory (RAM) with 32 megabytes of extended memory. Significantly slower run times are possible on a computer system with less memory, slower central processing unit (CPU), and less disk space.

** MINTEQA2 Model System Test Runs

Input Data File	Approx. Run Time (min:sec)
TEST1A.INP	0:01
TEST1B.INP	0:01
TEST2A.INP	0:01
TEST2B.INP	0:01
TEST2C.INP	0:01
TEST3.INP	0:01
TEST4.INP	0:01
TEST5A.INP	0:01
TEST5B.INP	0:01

Remember, program run time and performance can be affected by many microcomputer system and program parameters including

- o available disk space
- o available memory
- o processor/CPU classification
- o CONFIG.SYS and AUTOEXEC.BAT file options and parameter

values
- o disk and/or file storage and/or fragmentation

MODIFICATION

Included with the distribution release are

- o executable task image files for the MINTEQA2 model system
- o MINTEQA2 model FORTRAN source code files for IBM PC and compatible microcomputer systems (refer to DEVELOPMENT SYSTEM section).

A FORTRAN compiler and link editor are NOT required to execute any portion of the MINTEQA2 model system. If the user wishes to modify any portion of the MINTEQA2 model system, it will be up to the user to supply and/or obtain

- o an appropriate text editor that saves files in ASCII text (non-binary) format
- o FORTRAN program development tools to recompile and link edit the MINTEQA2 model system executable files (*.EXE)

The U.S. EPA CEAM cannot support, maintain, and/or be responsible for modifications that change the function of any executable task image file (*.EXE) or DOS batch command file (*.BAT) supplied with this model package.

TECHNICAL HELP CONTACT

NOTE: This section assumes that the user has successfully completed the installation process to make the full or any portion of the MINTEQA2 model system and related files resident and fully operational on a hard (usually designated as "C:") or virtual disk drive. For further information on installation and execution, refer to the DISTRIBUTION DISKETTES and ROUTINE EXECUTION sections.

For questions and/or information concerning

- o installation and/or testing of the MINTEQA2 model system and/or support programs or files, call 706/355-8400 for assistance or send mail via Internet to ceam@epamail.epa.gov
- o MINTEQA2 model and/or program content, application, and/or theory, contact Mr. Frank Stancil, U.S. EPA CEAM Manager for assistance at the address shown below

- use of the CEAM Internet node, or Listserver mailing list system, contact the Web Master at 706/355-8400
- CEAM software and distribution Quality Assurance and Control, call 706/355-8400
- other environmental software products and documentation distributed through CEAM, contact the Model Distribution Coordinator at 706/355-8400
- other support available through CEAM, contact Mr. Frank Stancil, U.S. EPA CEAM Manager

  - by mail at the following address

    Center for Exposure Assessment Modeling (CEAM)
    National Exposure Research Laboratory - Ecosystems Research Division
    U.S. Environmental Protection Agency (U.S. EPA)
    960 College Station Road
    Athens, Georgia 30605-2700

  - by telephone at 706/355-8000
  - by fax at 706/355-8104
  - by E-mail or Internet at ceam@epamail.epa.gov

To help technical staff provide better assistance, write down a response to the following topics before calling or writing. If calling, be at the computer, with the computer on, and in the proper sub-directory (e.g., C:\MINTEQA2) when the call is placed.

- program information:

  - describe the problem, including the exact wording of any error and/or warning message(s)
  - list the exact steps, command(s), and/or keyboard key sequence that will reproduce the problem

- machine information:

  - list computer brand and model
  - list available RAM (as reported by DOS CHKDSK or MEM command)
  - list extended memory present and free (XMS)
  - list name and version of extended memory (XMS) manager (i.e., HIMEM, VDISK, RAMDRIVE, etc.)
  - list available hard disk space (as reported by DOS CHKDSK command)
  - list the brand and version of DOS (as reported by DOS VER command)
  - list the name of any memory resident (TSR) program(s) installed
  - printer brand and model
  - monitor brand and model

NOTE: If contacting CEAM by mail or fax, include responses to the above information within correspondence.

CEAM operates a UNIX Listserver mailing list system. The name of the list is CEAM-USERS. Listserver is an automated mailing list system. A user can add him/her-self to a selected mailing list, post messages, and/or review/read messages. Lists can be moderated (owner decides which messages are made public) or un-moderated (all incoming messages are posted). Listserver is best suited for e-mail discussion groups. It is not a file service such as for the distribution of CEAM software products.

This listserver broadcasts up-to-date information concerning CEAM software products, activities, and events. This includes announcements for CEAM and/or non-CEAM supported workshops and training sessions; software product version release, updates, and documentation information; hints on software installation, operation, application, problems, and/or enhancements; and the exchange of information quickly among users, and between users and CEAM support personnel.

NOTE: The CEAM-USERS list is not moderated.

To subscribe, execute a mail service to send the following information:

NOTE: The symbol "<Enter>" represents pressing the <Enter> or carriage return key. Responses and key strokes that can be typed by the user are underlined with the hyphen character (-) and/or enclosed by the angle bracket characters (<>).

```
mail listserver@unixmail.rtpnc.epa.gov<Enter>
-------------------------------------
Subject:<Enter> (i.e., leave subject line blank)
subscribe CEAM-USERS yourfirstname yourlastname<Enter>
-------------------------------------------------
```

The user can also check the status of this model system or any other CEAM software product through the U.S. EPA public access server

mountain.epa.gov

CEAM software products and their status are available through the World Wide Web (WWW). If the user has access to the World Wide Web through a web browser, selected CEAM software products, including MINTEQA2, can be accessed and their release status checked at the following Uniform Resource Locator (URL):

http://www.epa.gov/ceampubl

DISCLAIMER

Mention of trade names or use of commercial products does not

constitute endorsement or recommendation for use by the United States Environmental Protection Agency.

Execution of any portion of the MINTEQA2 model system, and modification to the DOS system configuration files (i.e., \CONFIG.SYS and \AUTOEXEC.BAT) must be used and/or made at the user's own risk. Neither the U.S. EPA nor the program author(s) can assume responsibility for model and/or program modification, content, output, interpretation, or usage.

The MINTEQA2 program and files have been extensively tested and verified. However, as for all complex software products, the programs herein may not be completely free of errors and may not be applicable for all cases. In no event will the U.S. EPA be liable for direct, indirect, special, incidental, or consequential damages arising out of the use of the programs and/or associated documentation.

CEAM software products are built using FORTRAN-77, FORTRAN-90, assembler, other third and/or forth generation symbolic reference languages, and operating system interface command languages. The code structure and logic of these products is designed for single-user, single-tasking, non-LAN environment and operating platform for microcomputer installations (i.e., single user on dedicated system).

> NOTE: FORTRAN source code files are NOT required to document, execute, and/or test any model, program, or associated run time support file as provided on the distribution diskettes or the Internet installation file.

MINTEQA2 is a large-scale complex model system. The model source code relies on multiple interdependencies. Modification and recompilation of FORTRAN source code files should be attempted only by experienced research personnel with substantial expertise in FORTRAN development tools and the MINTEQA2 modeling system. Their application is mostly for additional research and development, including comparison to field or laboratory data, other theories, and further enhancements, such as graphical interfaces. THE SEPARATE USE OF THE FORTRAN SOURCE CODE OUTSIDE THE MINTEQA2 SHELL IS NOT RECOMMENDED BY THE U.S. EPA FOR ROUTINE APPLICATIONS OR ENVIRONMENTAL IMPACT STATEMENTS.

A user will be on their own if he/she attempts to install a CEAM product on a multi-user, multi-tasking, and/or LAN based system (i.e., Windows, DESQview, any LAN). CEAM cannot provide installation, operation, and/or general user support under any combination of these configurations. Instructions and conditions for proper installation and testing are provided with the product in a READ.ME file. While multiuser/multitasking/LAN installations could work, none of the CEAM products have been thoroughly tested under all possible conditions. CEAM can provide selected and/or limited scientific and/or application support for selected products if the user proves that a given

product is installed and working correctly using the test input data files provided with the distribution release.

- o WordPerfect is a registered trademark of WordPerfect Corporation
- o Microway and Number Smasher are registered trademarks of Microway, Inc.
- o Intel, 386, 486, and 860 are registered trademarks of Intel Corporation.
- o F77L is a registered trademark of Lahey Computer Systems, Inc. All other Lahey products are trademarks of Lahey Computer Systems, Inc.
- o IBM, Personal Computer/XT (PC/XT), Personal Computer/AT (PC/AT), PC DOS, VDISK, and Personal System/2 (PS/2) are registered trademarks of International Business Machines Corporation
- o PKZIP, PKUNZIP, and PKSFX are registered trademarks and/or trademarks of PKWARE, Incorporated.
- o DESQview is a trademark of Quarterdeck Office Systems, Inc.
- o Sun and SunOS are registered trademarks of Sun Microsystems, Inc.
- o SPARC is a registered trademark of SPARC International, Inc.
- o UNIX is a registered trademark of American Telephone and Telegraph
- o SVS FORTRAN-77 is a trademark of Silicon Valley Software
- o PRIME and PRIMOS are trademarks of Prime Computers, Inc.
- o Microsoft, RAMDRIVE, HIMEM, MS, and MS-DOS are registered trademarks of Microsoft Corporation
- o Windows, Windows95, Windows98, NT are trademarks of Microsoft Corporation
- o RM/FORTRAN is a trademark of Language Processors, Inc.
- o DEC, VAX, VMS, and DCL are trademarks of Digital Equipment Corporation
- o US Robotics is a registered trademark and Courier HST is a trademark of U.S. Robotics, Inc.
- o VP-Expert is a registered trade mark of WordTech Systems, Inc.

##########

DWD/dwd - June 2000 - C:\MINTEQA2\README\READ.ME

APPENDIX B

File: UPDATE.TXT

MINTEQA2 Model System Update Notes

Center for Exposure Assessment Modeling (CEAM)
National Exposure Research Laboratory - Ecosystems Research Division
Office of Research and Development (ORD)
U.S. Environmental Protection Agency (U.S. EPA)
960 College Station Road
Athens, Georgia 30605-2700

706/355-8400

The following are explanations of scientific, application, and/or operational changes and/or addendums, undocumented or otherwise, in the MINTEQA2 modeling system user manual file and other support documentation since the publication of the user manual file for version 3.11.

A brief explanation and/or example may be given for each change/enhancement.

Changes Version 4.01

Date: Wednesday, 1 December 1999. Time: 11:54:25.

For a summary of changes, refer to the file ABSTRACT.TXT. For a detail description of changes to the MINTEQA2 model system and its support documentation, refer to the files SUPPLE1.PDF and SUPPLE2.PDF.

All MINTEQA2 user manuals are available as Adobe(*) Acrobat(*) Portable Document Format (PDF) files (*.PDF) within the DOCUMENT sub-directory if the user chose to install the user's manuals from the INSTALMT.EXE program install menu. To view, print, and/or navigate a PDF document, a reader program must be installed on the users computer system. A free Adobe reader allows the user to view, navigate, and/or print PDF files across all major computing platforms. Acrobat Reader is a free viewing companion to Adobe Acrobat 3.0 and is available free from the Adobe world wide web (WWW) site at Uniform Resource Locator (URL) address: http://www.adobe.com.

To ensure that the user can view and/or print a PDF file in its entirety, the user must down load and install the most recent version/edition of the free Acrobat Reader. PDF files can be viewed across multiple platforms (Mac, Microcomputer, UNIX) using the appropriate reader for that platform.

Changes Version 4.02
~~~~~~~~~~~~~~~~~~~~
Date: Monday, 5 June 2000. Time: 08:48:35.
~~~~~~
For a summary of changes, refer to the file ABSTRACT.TXT. For a detail description of changes to the MINTEQA2 model system, versions 4.xx, and its support documentation, refer to the files SUPPLE1.PDF and SUPPLE2.PDF.

I. Problem with FRMT program for MINTEQ.

CEAM examined a problem with the FRMT program output. CEAM discovered three types of differences between the THERMO.DBS and TYPE6.DBS files generated by using FRMT and the original THERMO.DBS and TYPE6.DBS files supplied with version 4.01. These are listed and explained below within paragraphs labeled A), B), and C).

A) There are occurrences of null spaces in the FRMT-generated files where hard blank spaces appear in the original files. These are always due to extraneous, unnecessary spaces in the original that fall outside the formatted region of the file. An example is on the very first line in file THERMO.DBS where there are some trailing blanks after the version and date in the original that are ignored by FRMT. There are other instances of this, always at the end of legitimate data fields. This type of difference will show up in a file comparison using FC, but is of no concern.

B) There are instances where the original file contained blank entries in positions where floating point values are read. These will be read as zero by any program reading the file. The FRMT program output will show actual zero values in the format appropriate to the format descriptor used (e.g., 0.000 rather than blanks). Conversely, there are instances where integer component ID numbers (3-digits) appear in the original with leading zeroes shown (e.g., 002). The FRMT program will ignore the leading zeros, and its output will show blanks in these leading positions (e.g., bb2, where b represents a blank). Though they will be found by a file comparison using FC (DOS File Compare), these types of differences are of no concern.

C) The last line of each set of lines representing a species (usually three lines per species) has been prematurely truncated so that the ionic strength and temperature that pertain to the originally cited log K value for the species do not appear in the FRMT-generated files. These values appear in the original files in columns 72 - 80, but only for those species whose original cited ionic strength and temperature could be determined. The premature truncation means that null spaces appear in these positions in the FRMT-generated files. This problem needs to be corrected, but users should be aware that these values are not used in PRODEFA2 or MINTEQA2. They appear in the data base only to give the user some feel for the quality of the log K value. The idea is that a log K value that was originally measured at 0.5 M ionic strength (and has necessarily been corrected to zero ionic strength) might be less reliable than a value measured at 0.01 ionic strength. The information is presented to the user to help in making value judgments about the data. The important point is that the values are not used in calculations.

The problem was corrected by changing the length of the character variable "source" from 60 to 70 in both UNFRMT.FOR and FRMT.FOR. The format descriptor was changed from A60 to A70 for format statement 9082 in both programs. The revised files are attached are included with version 4.02.

II. Error in MINTEQ Model Version 4.01

An error in the MINTEQA2 model system, version 4.01, as distributed through the CEAM web external/public access server site, was discovered. The error was corrected in version 4.02 as explained below.

The error occurs in version 4.01 and will not result in erroneous results, but will result in an error being reported to the user. The error occurs in unusual circumstances as described below. The error condition is reported to the user through Lahey FORTRAN 90 (LF90) bounds checking for array indices in subroutine SOLID. The circumstances that cause the error are:

1. If the user has specified several constraints (fixed pH, Eh, redox reactions, etc), and;
2. The precipitation option is turned on, and;
3. A solid phase with many components (five or six) appears as an equilibrium constraint (infinite solid) or precipitates during the calculations. Examples include certain apatite minerals or clay minerals.

The error occurs due to inadequate dimension of certain temporary variables in subroutine SOLID. Logic in SOLID determines which component should be eliminated when a species is established by the user as an equilibrium constraint and when a solid precipitates during calculations. The methodology used in making the best choice involves counting the total number of candidate components. Candidate components are those that make-up the fixed or precipitated species that have not yet been fixed. The ID numbers of these candidate components are stored in temporary arrays in subroutine SOLID. The number of elements (dimensions) of these arrays is hard-coded as 12. In choosing 12, the total number of candidates that could be present in a model run were under estimated. The presence of solid species with many components can cause the number of candidate components to exceed 12. When this happens, the -chk compiler option invoked in the distribution version will detect an array element outside the bounds specified in the declaration statement.

The offending code occurs on lines 102-103 in subroutine SOLID, version 4.01:

```
      integer idtyp34(20),ncomp(20),idcomp(20,8),idfree(12),nspcf34(12),
     *        nspcf12(12)
```

EPA CEAM changed the code (dimension of arrays) as follows in version 4.02:

```
      integer idtyp34(nxdim),ncomp(nxdim),idcomp(nxdim,8),idfree(nxdim),
     *        nspcf34(nxdim), nspcf12(nxdim)
```

Listed below is an input file listing (TEST30.INP) that produces the error in version 4.01. Version 4.02 corrects this problem, therefore this example input file, as listed, will not produce this error in version 4.02.

```
Test30 for error in subroutine SOLID, version 4.01. March 2000.

25.00 MG/L   0.000  0.00000E+00
0 1 1 1 1 0 0 0 1 1 0 0 0
   33.00    0.0   0.00  0.000      0.00
0   0   0
    330  0.000E+00   -7.52 y                    /H+1
      1  0.000E+00   -1.21 y                    /E- (ENTERED AS EH)
    490  1.360E+01   -4.96 y                    /NH4+1
    140  6.383E+02   -2.69 y                    /CO3-2
    180  1.170E+04   -1.65 y                    /Cl-1
    270  1.100E-00   -4.98 y                    /F-1
    492  4.500E+01   -4.25 y                    /NO3-1
    491  2.000E-02   -5.98 y                    /NO2-1
    580  2.910E-00   -5.55 y                    /PO4-3
    732  2.180E+03   -2.59 y                    /SO4-2
    730  1.030E-01  -28.00 y                    /HS-1
    144  0.000E+00   -6.00 y                    /DOM1
    100  3.700E-01   -6.27 y                    /Ba+2
    150  8.540E+02   -2.29 y                    /Ca+2
    280  2.000E-02   -6.32 y                    /Fe+2
    460  8.120E+02   -2.62 y                    /Mg+2
    470  1.000E-00   -5.34 y                    /Mn+2
    410  4.480E+01   -3.36 y                    /K+1
    500  6.680E+03   -1.86 y                    /Na+1
    281  9.800E-01  -11.75 y                    /Fe+3

  3   2
    330     6.9100     0.0000                   /H+1
2802810    13.0320   -42.7000                   /Fe+2/Fe+3

                    ##########################
```

SOFTWARE VALIDATION TEST PLAN FOR MINTEQA2, VERSION 4.02

Prepared for

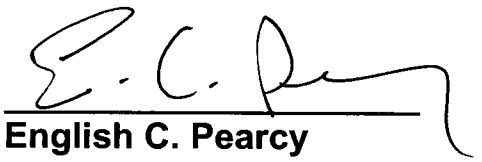
U.S. Nuclear Regulatory Commission
Contract NRC–02–97–009

Prepared by

David R. Turner

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

Approved by:



English C. Pearcy
Manager, Geohydrology and Geochemistry

11/8/2001
Date

CONTENTS

Section			Page
1	SCOPE OF THE VALIDATION		1
2	REFERENCES		1
3	ENVIRONMENT		3
	3.1	Software—Introduction	3
	3.2	Code Description	3
		3.2.1 Input	3
		3.2.2 Output	4
	3.3	Hardware Requirements and Installation	4
4	PREREQUISITES		9
5	ASSUMPTIONS AND CONSTRAINTS		9
6	TEST CASES		11
	6.1	Installation Check	11
	6.2	Aqueous Speciation	11
	6.3	Mineral Solubility	12
	6.4	Gas Chemistry	13
	6.5	Sorption—Surface Complexation Modeling	13
	6.6	Redox Conditions	13
	6.7	Temperature Effects	14
	6.8	Modified Database	14
7	TEST INPUTS		15
8	TEST PROCEDURES		15
	8.1	Installation Check	15

CONTENTS (Continued)

Section		Page
8.2	Comparison With Hand Calculations	15
8.3	Comparison with PHREEQC, Version 2.4.2 Simulations	15

FIGURES

Figure Page

3-1 Example MINTEQA2 Input File 5

TABLES

Table		Page
3-1	Line-by-Line Description of a Typical MINTEQA2 Input File	6
3-2	Formatting Requirements for the Different Lines in a Typical MINTEQA2 Input File	8

1 SCOPE OF THE VALIDATION

This document establishes the Software Validation Test Plan for validating the installation and functionality of the geochemical equilibrium speciation code MINTEQA2, Version 4.02 (December 1999 release; U.S. Environmental Protection Agency, 1999a,b). MINTEQA2, Version 4.02 is an acquired code, originally developed by the U.S. Environmental Protection Agency, National Exposure Research Laboratory, Ecosystems Research Division. The software is used by staff at the Center for Nuclear Waste Regulatory Analyses (CNWRA) is providing technical assistance to the U.S. Nuclear Regulatory Commission (NRC) in its high-level waste program.

This Software Validation Test Plan applies to MINTEQA2, Version 4.02, and is intended to validate the software for use in modeling geochemical equilibrium reactions as identified in the test cases described in Section 6. An earlier version, MINTEQA2, Version 3.11/3.12 is currently under configuration control in accordance with Technical Operating Procedure (TOP) 018. As necessary, this validation plan identifies differences from the earlier MINTEQA2, Version 3.11/12 MINTEQA2 Version 4.02 will be placed under TOP-018 configuration control prior to performing the validation activities outlined in Sections 6 and 7 (Allison et al., 1991), and describes how they will be evaluated in the software validation.

MINTEQA2, Version 4.02 includes a number of capabilities that are not planned for use in CNWRA applications and will therefore not be tested at this time:

- Ion Exchange
- Freundlich Isotherm
- Langmuir Isotherm
- Triple-Layer Model
- Constant Capacitance Model
- Composite Organic Liquid Model

If a decision is made to use these code capabilities, this software validation test plan will be modified as necessary.

2 REFERENCES

The following documents are referenced or used as the basis for this Software Validation Test Plan.

Allison, J.D., D.S. Brown, and K.J. Novo-Gradac. "MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems." Version 3.0 User's Manual. EPA/600/3–91/021. Athens, Georgia: U.S. Environmental Protection Agency. 1991.

CNWRA. "Technical Operating Procedure (TOP-18): Development and Control of Scientific and Engineering Software, Revision 8, Change 0 (October 5, 2001)." San Antonio, Texas: Center for Nuclear Waste Regulatory Analyses. 2001.

Dzombak, D.A. and Morel, F.M.M. *Surface Complexation Modeling: Hydrous Ferric Oxide.* New York: John Wiley and Sons. 1990.

Grenthe, I., J. Fuger, R Konings, R.J. Lemire, A.B. Muller, C. Nguyen-Trung, and H. Wanner. *Chemical Thermodynamics Series, Volume 1: Chemical Thermodynamics of Uranium.* Nuclear Energy Agency, Organization for Economic Cooperation and Development. New York: Elsevier. 1992.

Langmuir, D. *Aqueous Environmental Geochemistry.* Englewood Cliffs, New Jersey: Prentice-Hall, Inc. 1997.

Lemire, R.J., J. Fuger, H. Nitsche, P. Potter, M.H. Rand, J. Rydberg, K. Spahiu, J.C. Sullivan, W.J. Ullman, P. Vitorge, and H. Wanner. *Chemical Thermodynamics Series, Volume 4: Chemical Thermodynamics of Neptunium and Plutonium.* Nuclear Energy Agency, Organization for Economic Cooperation and Development. New York: Elsevier. 2001.

Parkhurst, D.L. and C.A.J. Appelo. "User's Guide to PHREEQC (Version 2)—A Computer Program for Speciation, Batch-reaction, One-dimensional Transport, And Inverse Geochemical Calculations." Water-Resources Investigations Report 99–4259. Denver, Colorado: U.S. Geological Survey. 1999.

Rard, J.A., M.H. Rand, G. Anderegg, and H. Wanner. *Chemical Thermodynamics Series, Volume 3: Chemical Thermodynamics of Technetium.* Nuclear Energy Agency, Organization for Economic Cooperation and Development. New York: Elsevier. 1999.

Richardson, S.M. and H.Y. McSween, Jr. *Geochemistry: Pathways and Processes.* Englewood Cliffs, New Jersey: Prentice-Hall, Inc. 1989.

Silva, R.J., G. Bidoglio, M.H. Rand, P.B. Robouch, H. Wanner, and I. Puigdomenich. *Chemical Thermodynamics Series, Volume 2: Chemical Thermodynamics of Americium.* Nuclear Energy Agency, Organization for Economic Cooperation and Development. New York: Elsevier. 1995.

Stumm, W. and J.J. Morgan. *Aquatic Chemistry: Chemical Equilibria and Rates in Natural Waters.* 3rd Edition. New York, New York: Wiley-Interscience. 1996.

Turner, D.R., T. Griffin, and T.B. Dietrich. "Radionuclide Sorption Modeling Using the MINTEQA2 Speciation Code." Scientific Basis for Nuclear Waste Management—XVI. C. Interrante and R. Pabalan, eds. Symposium Proceedings. Pittsburgh, Pennsylvania: Material Research Society. pp. 783–789. 1993.

Turner, D.R. "Mechanistic Approaches to Radionuclide Sorption Modeling." CNWRA 93-019. San Antonio, Texas: CNWRA. 1993.

U.S. Environmental Protection Agency. "MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems: User Manual Supplement for Version 4.0." Athens, Georgia: U.S. Environmental Protection Agency, National Exposure Research Laboratory, Ecosystems Research Division. 1999a.

U.S. Environmental Protection Agency. "Diffuse-Layer Sorption Reactions for use in MINTEQA2 for HWIR Metals and Metalloids." Athens, Georgia: U.S. Environmental Protection Agency, National Exposure Research Laboratory, Ecosystems Research Division. 1999b.

Wolery, T.J. "EQ3/6, A Computer Program for Geochemical Aqueous Speciation-Solubility Calculations: Theoretical Manual, User's Guide, and Related Documentation (Version 7.0)." UCRL–MA–11066 Pt III. Livermore, California: Lawrence Livermore National Laboratory. 1992.

3 ENVIRONMENT

3.1 Software—Introduction

MINTEQA2, Version 4.02 (released December 1999, U.S. Environmental Protection Agency, 1999a,b) is a geochemical equilibrium speciation code developed in FORTRAN 90 by the United States Environmental Protection Agency to model dilute aqueous systems. The code is PC-compatible, and is run in batch mode in the DOS-operating system (see Section 3.2 of this Software Validation Test Plan). The original MINTEQ code was developed at Pacific Northwest National Laboratory to combine the mathematical approach of the earlier MINEQL code with the extensive thermodynamic database of the United States Geological Survey code WATEQ3. The code was updated to MINTEQA2, Version 3.11/3.12 (released December 1991), and a preprocessing routine called PRODEFA2 was added to help construct the formatted input files used by the code. Since the original development, MINTEQA2 has become one of the more common codes used to simulate geochemical equilibria (e.g., Langmuir, 1997).

3.2 Code Description

The following description of MINTEQA2 is based on the source code and on the user's manual (Allison et al., 1991) provided with the MINTEQA2, Version 4.02 file (downloaded from the EPA website at http://www.epa.gov/ceampubl/minteq.htm).

3.2.1 Input

A MINTEQA2, Version 4.02 user typically has a problem relevant to a natural chemical system. This system is described in terms of the physical conditions such as temperature, and the concentrations of chemical components, species, solids and gases that are present. MINTEQA2 uses a formatted input file to identify the components of interest, read the concentrations, construct the chemical equilibrium model and solve for aqueous speciation and the distribution of species between the solid, gas, and liquid phases. Input flags can be set to determine the level of output. The companion preprocessor PRODEFA2 has been developed and refined to help the user describe the geochemical problem and through a series of menus create the formatted input file necessary for a MINTEQA2 simulation. However, if the user is

familiar with the formatting requirements, he or she can construct the input file without PRODEFA2, using an ASCII text editor.

The typical formatted input file for a MINTEQA2 problem is not very long (Figure 3-1), but contains a significant amount of information. The line by line description of the input file (Figure 3-1) is given in Table 3-1. The format of the input file is listed in Table 3-2. The input file is read and the databases searched in the Subroutine INPUT; the reader is referred to the source code for more detail on the structure of the input file.

A key concept in the input file is the use of three-digit ID numbers for components, and seven-digit ID numbers for aqueous species, solids, redox couples, and gases. In addition, the first two digits of the ID number of solids contains information on the type of solid (e.g., oxide, sulfide, carbonate). These numbers are used by MINTEQA2 to identify components and species in the databases. Although there is a field for naming these items, it is for the benefit of the user in the output, and is not used in calculation by MINTEQA2. There are two constraints on the ID numbers: they must be unique and they must be contained in the appropriate databases. For the components and species entered in the database, these constraints have been met. However, since the ID numbers are not necessarily intuitive, it is unlikely that the user would know to associate the three-digit ID number 330 with the component H^+ or the seven-digit number 3300020 with OH^-. For this reason, while it is relatively easy to delete species, adding components, species, solids, or reactions requires reasonably sophisticated preprocessing to provide the user with what he/she can understand (e.g., names such as H^+, OH^-), and search the database for the appropriate ID numbers to provide the information necessary for a MINTEQA2 simulation.

3.2.2 Output

The results from the equilibrium geochemical speciation calculation are written to an output file specified by the user. MINTEQA2, Version 4.02 will overwrite previously existing files with the same name. In all cases, the output includes an echo of the input to verify that the input file was read correctly and a time stamp to verify the time of the run. Additional types of output include writing equilibrium mass distribution chemical component species (or aqueous species) to a comma delimited ASCII file that can be imported into commercial spreadsheets. The level of output varies and is set by the user in the input files. The equilibrium concentration of the element(s) of interest are reported in molality (moles contaminant/kg H_2O) as distributed between the dissolved, sorbed, and precipitated phases.

3.3 Hardware Requirements and Installation

MINTEQA2, Version 4.02 is designed for the IBM PC family of microcomputers or compatible systems running under version 3.30 or higher of the Microsoft or PC Disk Operating Systems (PC or MS DOS). Properly configured, MINTEQA2, Version 4.02 and its support files and programs can be executed under PC DOS, MS DOS 3.30 and later versions, DOS 4.0x, DOS 5.0x, or DOS 6.x; a DOS window or a DOS level system start up (i.e., boot) under Microsoft Windows 3.1x, Microsoft Windows for WorkGroups, Windows 95, Windows 98, or NT operating systems.

```
Line 1            Deep non-saline groundwater (Table 7-4 in KBS-3/II Geology)
Line 2            Uranium solubility (pH=7); Soddyite control; oxidizing
Line 3            25.00 MG/L   0.000  0.00000E-01
Line 4            0 0 1 0 3 0 0 0 1 2 0 0 0
Line 9            0   0   0
Line 11a              330  0.000E-01   -7.00 y                    /H+1
Line 11b              732  9.600E+00   -4.00 y                    /SO4-2
    |                 580  2.000E-01   -5.68 y                    /PO4-3
    |                 492  5.000E-01   -5.09 y                    /NO3-1
    |                 270  5.000E+00   -3.58 y                    /F-1
    |                 180  7.000E+01   -2.70 y                    /Cl-1
    |                 730  5.000E-01   -4.82 y                    /HS-1
    |                 150  1.800E+01   -3.35 y                    /Ca+2
    |                 460  4.300E+00   -3.75 y                    /Mg+2
    |                 500  6.500E+01   -2.55 y                    /Na+1
    |                 410  3.900E+00   -4.00 y                    /K+1
    |                 280  5.000E+00   -4.05 y                    /Fe+2
    |                 470  5.000E-01   -5.04 y                    /Mn+2
    |                  30  2.000E-02   -6.13 y                    /Al+3
    |                 490  2.000E-01   -4.96 y                    /NH4+1
    |                 770  1.100E+01   -3.94 y                    /H4SiO4
    |                 891  0.000E-01  -21.00 y                    /U+4
    |                 140  1.210E+02   -3.00 y                    /CO3-2
    |                 893  0.000E-01  -21.43 y                    /UO2+2
    |                 281  0.000E-01  -20.75                      /Fe+3
Line 11n                1  0.000E-01   -4.23                      /E- (ENTERED AS EH)
BLANK LINE
Line 12 (Type 3)    3   4
Line 13a          8918930     9.0644   -34.3840                   /U+4/UO2+2
    |             2802810    13.0320   -10.0000                   /Fe+2/Fe+3
    |                   1     4.2258     0.0000                   /E- (ENTERED AS EH)
Line 13n            330     7.0000     0.0000                     /H+1
Line 12 (Type 4)    4   1
Line 13a          8089304    -0.5123     0.0000   5.000E-02       /Soddyite
BLANK LINE
```

Figure 3-1. Example MINTEQA2 input file

Table 3-1. Line-by-Line Description of a Typical MINTEQA2 Input File				
Line No.	**Description**		**Variable Name**	**Type**
1	Problem Title		DESC	Character*75
2	Problem Title		CARRY	Character*75
3	(i)	Temperature in °C	TEMP	Real*8
	(ii)	Concentration Units	FLAG	Character*5
	(iii)	Fixed ionic strength [see line 4, flag (vii) ISOPT]	FIONS	Real*8
4	(i)	Flag—Alkalinity (0 = Total carbonate specified; 1=alkalinity)	ICORALK	Integer*4
	(ii)	Flag—	IDEBUG	Integer*4
	(iii)	Flag—Terminate if Charge Imbalance exceeds 30% (0=Yes; 1=No)	ICHARGE	Integer*4
	(iv)	Flag—Print options for solids (0=Ppt only allowed solids; 1=	IPRINT	Integer*4
	(v)	Flag—Maximum number of iterations (0=40; 1=10; 2=100; 3=200; 4=500)	NITER	Integer*4
	vi)	Flag—	IPARM	Integer*4
	(vii)	Flag—Ionic strength option (0=computed; 1=fixed)	ISOPT	Integer*4
	(viii)	Flag—	IPRDCT	Integer*4
	(ix)	Flag—Activity coefficient option (0=Debye Huckel; 1=Davies Equation)	KKDAV	Integer*4
	(x)	Flag—Output options (0=Full; 1=Intermediate; 2=Abbreviated)	KKTHR	Integer*4
	(xi)	Flag—Sweep Options [0=No sweep; 1=Yes(-log c); 2=Yes(conc)]	ISWEEP	Integer*4
	(xii)	Flag—Number components for spreadsheet (0 to 6)	N123	Integer*4
	(xiii)	Flag—type of output to spreadsheet [0=No file; 1=Equil mass %; 2=Equil mass conc (molal); 3=Equil conc(molal)]	NTYP123	Integer*4
5	No line entry if no sweep option (ISWEEP = 0)		—	—
6	No line entry if no sweep option (ISWEEP = 0)		—	—
7	No line entry if no output to spreadsheet (N123 and NTYP123 = 0)		—	—
8	No line entry if no output to spreadsheet (N123 and NTYP123 = 0)		—	—

Table 3-1. Line-by-Line Description of a Typical MINTEQA2 Input File (Continued)				
Line No.	**Description**		**Variable Name**	**Type**
9	(i)	Flag—Model Sorption? (0=No sorption; 1-4 Check for model specific parameters)	IADS	Integer*4
	(ii)	Number of sorption surfaces (0=No sorption; 1-5maximum)	NUMADS	Integer*4
	(iii)	FlagSorption model (0= No sorption; 1-7 for specific models)	IABQ	Integer
10	No line entry if no sorption model		—	—
11	(i)	Water chemistry—Component ID# (must be in COMP.DBS)	IDXT	Integer
	(ii)	Total dissolved concentration	TT	Real*8
	(iii)	log free activity guess	GXT	Real*8
	(iv)	Flag—Adjust/Improve guess (N=No; Not N (e.g., blank, Y)=Yes)	RGT	Character*1
	REPEAT (i-iv) FOR N COMPONENTS		—	—
	BLANK LINE			
12	(i)	Types (3-6)	LTYPE	Integer
	(ii)	Number of Type (3-6)	NTYPE	Integer
13	(i)	Species/Component ID (Must be in THERMO.DBS/COMP.DBS)	IDYT/IDXT	Integer
	(ii)	Equilibrium constant (Log K from THERMO.DBS)	GKT	Real*8
	(iii)	Enthalpy of reaction (From THERMO.DBS)	DHT	Real*8
	(v)	If Type 4, concentration of finite solid	CONC	Real*8
	REPEAT LINES 12-13 for Types (3-6) Type 3 = Fixed activity Type 4 = Finite solids Type 5 = Possible solids Type 6 = Excluded species (e.g., non specified redox couples, infinite solids)		—	—
	BLANK LINE			

Table 3-2. Formatting Requirements for the Different Lines in a Typical MINTEQA2 Input File	
Line Number	**Format**
Line 1 (DESC)	(a75)
Line 2 (CARRY)	(a75)
Line 3 (TEMP, FLAG, FIONS)	(f5.2, 1x, a5, 1x, f6.3, 1x, f7.4)
Line 4 (ICORALK, IDEBUG, ICHARG, IPRINT, NITER, IPARM, ISOPT, IPRDCT, KKDAV, KKTHR, ISWEEP, N123, NTYPE123)	(13(i1, 1x))
Line 5 (No line entry if no sweep)	—
Line 6 (No line entry if no sweep)	—
Line 7 (No line entry if no spreadsheet output)	—
Line 8 (No line entry if no spreadsheet output)	—
Line 9 (IADS, NUMADS, IABQ)	(i1, 3x, i1, 3x, i1)
Line 10 (No line entry if no sorption models)	—
Line 11 (IDXT, TT, GXT, RGT)	(i7, 1x, e10.3, 1x, f7.2, 1x, a1)
BLANK LINE	
Line 12 (LTYPE, NTYPE)	(i3, 1x, i3)
Line 13 (No Type 4)	(i7, 2(2x, f9.4))
Line 13 (Type 4 only)	(i7, 2(2x, f9.4), 2x, e10.3)
BLANK LINE	

To install MINTEQA2, Version 4.02 and/or related support files and programs on a hard disk, insert the first distribution diskette in a compatible diskette drive. Type

A:\INSTALL or B:\INSTALL

at the DOS system prompt and press the <Enter> key. Then follow instructions and respond to the prompts presented on the monitor screen by the interactive installation program. This is a compressed, self-extracting, interactive installation program—with on-line, context sensitive help—that contains the MINTEQA2 model system (MINTEQA2, Version 4.02), dated June 2000.

If the MINTEQA2 model system is being installed from the MINTEQA2 installation file (INSTALMT.EXE) downloaded from the Internet, then the user should type

INSTALMT

at the DOS system prompt and press the <Enter> key. This command assumes that the current default drive and sub-directory is the same drive and sub-directory that contain the file INSTALMT.EXE.

4 PREREQUISITES

Running MINTEQA2, Version 4.02 requires that the code be installed in the same directory as the batch file MINRUN.BAT. The directory containing the MINTEQA2/PRODEFA2 executables also need each to contain each of the database files described below in Section 5.0 The input and the database files are must be formatted using the format described in Appendix B of U.S. Environmental Protection Agency (1999a).

5 ASSUMPTIONS AND CONSTRAINTS

The results from geochemical equilibrium speciation codes are dependent on the type and quality of the data used in the simulation. These are typically contained in databases that are searched and read by the code based on the input provided by the user. While these databases can be modified by the user to incorporate additional species or different thermodynamic data, they are considered separately from the input file that defines the geochemical problem, and should not be modified in the context of running the simulation. MINTEQA2, Version 4.02 uses a total of 10 databases to construct and execute a geochemical equilibrium model. All of these databases must be present in the working directory for the code to run. All of these databases are in formatted ASCII and may be modified outside of a given run. Formatting details can be found in Appendix B of the supplement to the user's manual (U.S. Environmental Protection Agency, 1999a). Smaller databases can be searched more quickly by the program, resulting in faster run-time. A larger database is more inclusive, but comes at the cost of computational speed. THERMO.DBS and TYPE6.DBS (see below) can be modified in formatted ASCII, but MINTEQA2 actually looks for and reads the binary files THERMO.UNF and TYPE6.UNF. If THERMO.DBS and TYPE6.DBS are modified, the *.UNF files must be regenerated using the program UNFRMT provided with the code.

COMP.DBS — This database contains the set of components from which the user can select those relative to the problem of interest. Components are the basic chemical units from which all species in the different thermodynamic databases can be constructed. These generally, but not always, correspond to the cation or anionic state of the element in solution (e.g. Ca^{2+}, Cs^{+}, Cl^{-}, CO_3^{2-}). Different oxidation/reduction states are accounted for by adding an additional component (e.g., both U^{4+} and UO_2^{2+} are included as components). The components are identified by a three digit ID number which is how they recognized from the input file for inclusion in the MINTEQA2 calculations. If the component is not present in COMP.DBS, then the user cannot consider it in the geochemical problem. While, it is a relatively simple matter to modify COMP.DBS to include additional components, additional data must be added to the other databases for aqueous complexation, redox, and solid precipitation reactions for the addition to be of practical value.

THERMO.DBS — This is the main database and contains the thermodynamic data for all species formatted to be considered in a MINTEQA2 simulation. Identified to MINTEQA2 by a unique seven digit number, the data include the reaction stoichiometry for the formation of the species, gas, solid, or redox couple and an equilibrium constant for the reaction at 25 °C. The

reaction is defined in terms of MINTEQA2 components identified by the three digit number provided in the input file. Additional data include enthalpies of reaction for correction to temperatures other than 25 °C, Debye-Hückel parameters for calculating activity coefficients, and gram formula weights. MINTEQA2, Version 4.02 also includes a block for identifying thermodynamic data sources.

TYPE6.DBS — This database is a subset of the data included in THERMO.DBS for the formation of solids. The formatting of the data is the same and the included data are identical.

REDOX.DBS — Like TYPE6.DBS, this database is a subset of the data included in THERMO.DBS for the half reactions forming redox couples such as Fe^{2+}/Fe^{3+} and U^{4+}/UO_2^{2+}. The formatting of the data is the same and the included data are identical.

GASES.DBS — Like TYPE6.DBS and REDOX.DBS, this database is a subset of the data included in THERMO.DBS for the formation of gases from the component species. The Log K value is the equilibrium constant of the reaction corrected for the partial pressure of the gas in atmospheres. MINTEQA2 requires that the partial pressures of all gases be fixed for a given problem.

ERROR.DBS — This database contains the error codes and messages for MINTEQA2 runs.

ALK.DBS — Rather than measuring dissolved carbonate in the aqueous system water analyses commonly report alkalinity (capacity of the system to neutralize acid). ALK.DBS includes the component ID number and the alkalinity factor of the principal components at the CO_2 equivalence point. This can be modified by the user, and is only called if the flag in the input file specifies that alkalinity is to be used to specify inorganic carbon.

FEO-DLM.DBS — This database contains sorption binding constants for a number of toxic elements such as Cd, Zn, Pb, and SeO_4^{2-}. These binding constants are taken from the work of Dzombak and Morel (1990) who studied sorption of these elements on hydrous ferric oxide (HFO) using the diffuse layer model. This database is called by the user in the input file if he/she is studying sorption on HFO and is not otherwise used.

ANALYT.DBS — This database contains the coefficients necessary to modify the equilibrium constant for the effects of temperature according to the relationship:

$$\text{Log } K_T = A + BT + C/T + D \text{ Log}(T) + ET^2 + F/T^2 + GT^{0.5}$$

where T is temperature in Kelvin. The appropriate coefficients have been determined for only a few of the species included in THERMO.DBS, and temperature corrections are generally made using the Van't Hoff relation and the enthalpy of reaction (ΔDH_r°). Because the Van't Hoff

relation assumes a constant enthalpy of formation over the temperature of interest, it is limited to fairly low temperatures of less than 100 °C. The user wishes to use a temperature other than 25 °C, he/she should be aware of this limitation.

COMPLIG.DBS — The latest version of MINTEQA2 (Version 4.02) includes binding constants for trace metals with organic ligands. A database of trace metal reactions with Suwannee River dissolved organic matter and their mean log K values is included in the file COMPLIG.DBS. The incorporation of these reactions in standard equilibria calculations is accomplished by including a separate subroutine (COMPOSIT). The user's manual describes how additional ligands can be added to the database if desired by the user.

Historically, the original MINTEQA2 databases have been modified to include extensive thermodynamic data for toxic elements such as Cd, Zn, Pb, As, Hg, and Cu as well as organic ligands such as EDTA, Citrate, and Acetate. Additional modifications at the Center for Nuclear Waste Regulatory Analyses (CNWRA) have included the addition of thermodynamic data (ΔDH_r° and log K) for almost 600 aqueous species and solids involving 14 potentially important radioelements, including U, Pu, Th, Np, Am, Sr, Cs, Ra, Sn, Zr, Tc, Ru, Eu, and Co (Turner, 1993; Turner et al., 1993). Thermodynamic data for U, Pu, Np, Am, and Tc are from the Nuclear Energy Agency Thermodynamic Database Project (Grenthe et al., 1992; Silva et al., 1995, Rard et al., 1999, and Lemire et al., 2001). The source for other data is the EQ3/6 database (Release Gembochs.v2-eq8-data0.alt.r2, 02Aug95).

6 TEST CASES

Although geochemical equilibrium modeling can be performed using hand calculations (Richardson and McSween, 1989), the large number of chemical component species present in natural systems can make for extremely complex calculations. Validation of MINTEQA2, Version 4.02 model results against hand calculations for simple systems can exercise basic code functions, but a more rigorous testing of the code and its databases is beyond a hand check.

In addition to testing basic code functions against simplified problems, one way to address the issue of complexity in code validation and build confidence in model results is to test MINTEQA2, Version 4.02 against results from another geochemical speciation code such as PHREEQC, Version 2.4.2 Parkhurst and Appelo, 1999) or EQ3/6 (Wolery, 1992). This approach is followed in the test cases outlined below. Simple worked problems from standard geochemistry textbooks (e.g., Richardson and McSween, 1989; Stumm and Morgan, 1996; Langmuir, 1997) and test problems in the user's manual for PHREEQC, Version 2.4.2 will be selected to test different geochemical processes such as speciation and solubility calculations, and adapted to MINTEQA2, Version 4.02 input requirements. To test MINTEQA2, Version 4.02 the same intensive properties (temperature, pressure) will be used and all chemical reactions are written in terms of the appropriate component species for MINTEQA2, Version 4.02. Some differences in how PHREEQC, Version 2.4.2 and MINTEQA2, Version 4.02 compute ionic strength corrections (extended Debye-Hückel versus Davies equation) may lead to differences in speciation that will be examined and resolved as necessary. For simple systems of a few components the same thermodynamic data (e.g., log K at 298K) will be used to ensure

consistency between calculational results. For more complicated systems involving seawater, the problems will be run using the overall databases. Resulting differences will be evaluated and resolved as necessary. It is anticipated that MINTEQA2, Version 4.02 test results will agree with hand calculations and PHREEQC, Version 2.4.2 calculations within a few percent.

6.1 Installation Check

The first validation test will be to ensure that the MINTEQA2, Version 4.02 software is installed correctly on the PC platform. Following instructions outlined in section 3.2 of this test plan will open the self-extracting installation package for MINTEQA2, Version 4.02. Part of this package includes input and output of a set of 12 example problems developed to demonstrate the different capabilities of MINTEQA2, Version 4.02. The input files for these example problems will be submitted to MINTEQA2, Version 4.02 as installed, and the output will be compared against the files provided in the installation package. With the exception of the time/date stamp, these files should produce results identical to those provided by the MINTEQA2, Version 4.02 developers.

6.2 Aqueous Speciation

Parkhurst and Appelo (1999) provide an example to calculate the distribution of aqueous species in seawater and the saturation state of seawater relative to a set of minerals. To demonstrate how to expand the model to new elements, uranium is added to the aqueous model defined by the PHREEQC, Version 2.4.2 database.

Output to be compared includes, but is not limited to:

- Percent of different aqueous species such as CO_3^{-2}, $Ca(OH)_2$ (aq), etc.
- Solubility indices [log (Ion Activity Product) - log K] for minerals such as halite, calcite, and SiO_2

6.3 Mineral Solubility

Richardson and McSween (1989) present two worked problems to investigate the solubility of barite at 298 K in pure water (Worked Problem 3-6), and in a 0.2 m NaCl solution (Worked Problem 3-8). The results of the problems are expressed in terms of $m_{Ba^{++}}$.

Output to be compared includes, but is not limited to:

- Molality of Ba^{++}
- Solubility indices [log (Ion Activity Product)—log K_{eq}] with respect to Ba^{++}

6.4 Gas Chemistry

Stumm and Morgan (1996) present several aqueous carbonate speciation problems. Included is Example 7.8, equilibrating calcite ($CaCO_3$) in sea water at 25 °C, and open to atmosphere (fixed $P_{CO_2} = 3.55 \times 10^{-4}$ atm). This problem can be used to test the gas chemistry subroutines of MINTEQA2, Version 4.02.

Output to be compared includes, but is not limited to:

- Total carbonate species (e.g., HCO_3^-, CO_3^{-2})
- pH
- alkalinity

6.5 Sorption—Surface Complexation Modeling

Parkhurst and Appelo (1999) provide an example to use PHREEQC, Version 2.4.2 to calculate Zn^{++} sorption on ferrihydrite (HFO) using the diffuse-layer surface complexation model and parameters described in Dzombak and Morel (1990). Sorption at 298 K is investigated for two Zn^{++} concentrations (10^{-4} and 10^{-7} molal), and the results are presented in terms of dissolved and sorbed Zn^{++} molality as a function of pH.

Output to be compared includes, but is not limited to:

- Total dissolved Zn^{++} as a function of pH
- Total sorbed Zn^{++} as a function of pH

6.6 Redox Conditions

Stumm and Morgan (1996) present a number of relatively simple calculations to determine redox equilibrium. These include calculating electron activity (pe) for Fe and Mn systems open to atmosphere (Example 8.2) and equilibrium distribution in the SO_4^{2-}–HS^- system (Example 8.4). These calculations will provide a good check of redox equilibrium in MINTEQA2, Version 4.02 which uses pe as a master variable to control redox potential.

Output to be compared includes, but is not limited to:

- Calculated equilibrium pe for the three solutions presented in Example 8.2 (Stumm and Morgan, 1996)
- Equilibrium distributions of sulfur compounds as a function of pe for the conditions presented in Example 8.4 (Stumm and Morgan, 1996)

6.7 Temperature Effects

Parkhurst and Appelo (1999) provide an example to use PHREEQC, Version 2.4.2 to calculate the solubility of gypsum and anhydrite in pure water, over a range in temperature from 298 K to 373 K. This provides an opportunity to independently check the ability of MINTEQA2, Version 4.02 to both calculate solubility (see section 6.3 of this test plan) and the correction of equilibrium for the effects of temperature. Only the pH and temperature are used to define a pure water solution. Gypsum and anhydrite are allowed to react to equilibrium (saturation index equal to 0.0), and the initial phase assemblage has 1 mol of each mineral. Each mineral will react either to equilibrium or until it is exhausted in the assemblage. Temperature is swept through 1° intervals from 25 °C (298 K) through 75 °C (373 K).

Both MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 use the Van't Hoff relationship and enthalpies of reaction ($\Delta H_r°$) to correct equilibrium constants for the effects of temperature. If the same thermodynamic data are used, both codes should produce the same results.

Output to be compared includes, but is not limited to:

- gypsum and anhydrite solubility as a function of temperature from 25 °C (298 K) through 75 °C (373 K).

6.8 Modified Database

The main code function to be checked in this section of the test plan is to ensure that the MINTEQA2, Version 4.02 database modified to include NEA radionuclide thermodynamic data is correct and produces reasonable results. If thermodynamic data are the same, different geochemical equilibrium speciation codes should produce similar results. The most straightforward way to test this is to compare aqueous speciation results from several different codes. This approach has been used before (Turner, 1993; Turner et al., 1993) to examine the modified MINTEQA2, Version 3.11/3.12 database.

Speciation checks for uranium and neptunium will be performed using results from MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2. Identical thermodynamic data for neptunium and uranium will be used to examine speciation as a function of pH, both under CO_2-free and atmospheric CO_2 conditions. Temperature will be fixed at 25 °C (298 K). Low concentrations will be used to avoid the complications of precipitation of pure phases. The focus of the check is the CNWRA-modifications to the MINTEQA2, Version 4.02 database, and very simple solutions will be used to minimize the effects of major ions such as Ca^{2+}, Mg^{++}. Although both MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 are reported to use the WATEQ data compilations, small differences are likely to persist in thermodynamic data for many of the chemical component systems that are beyond the intended scope of this validation test plan.

Output to be compared includes, but is not limited to:

- Percent of different uranium and neptunium aqueous species as a function of pH

7 TEST INPUTS

In all test cases, the test inputs will consist of a batch input file formatted for MINTEQA2, Version 4.02 (see Figure 3-1). This formatted input file can be prepared using either the preprocessor PRODEFA2 included with MINTEQA2, Version 4.02, or with an ASCII text editor. Chemical conditions in the MINTEQA2, Version 4.02 input file such as temperature, component concentration, and gas pressure will be set at values consistent with the problems described in Section 6 of this software validation test plan. For simple test problem systems, identical thermodynamic data will be used to facilitate comparison of results. For complex test problem systems such as those involving seawater, the problem will be run using the MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 thermodynamic databases. Differences will be evaluated and resolved as necessary.

8 TEST PROCEDURES

In all test cases, the formatted input file described in Section 7.0 will be submitted for batch run in MINTEQA2, Version 4.02. Results from MINTEQA2, Version 4.02 the output file created by each run will be evaluated as summarized in the following sections.

8.1 Installation Check

The input files test problems provided with the MINTEQA2, Version 4.02 installation package will be run. The results of these batch runs will be compared to the output files provided with the MINTEQA2, Version 4.02 installation package.

8.2 Comparison with Hand Calculations

The test problems described in Sections 6.3 (Mineral Solubility) and 6.4 (Gas Chemistry) involve comparison of MINTEQA2, Version 4.02 results against the results of hand calculations. The results, including component concentration and mineral saturation, will be compared in tabular form.

8.3 Comparison with PHREEQC, Version 2.4.2 Simulations

For test problems involving comparison against PHREEQC, Version 2.4.2 simulations, output from the two computer programs will be compared in several ways:

- Comparison of component concentrations—This will be done in tabular form for a limited suite of dominant aqueous species.
- Comparison of mineral saturation indices—This will be done in tabular form for a limited set of dominant minerals.
- Graphic comparison of aqueous speciation—This is an effective means of comparing model results for speciation and sorption as a function of independent variables such as pH, Eh, and P_{CO2}.

It is anticipated that results from the two codes will agree within a few percent, although there may be differences due to disparities between the thermodynamic databases used in the code. Any differences resulting from these comparisons will be documented, evaluated, and resolved as necessary. It is important to remember that it is beyond the scope of this validation test plan to resolve all differences in between the MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 thermodynamic databases.

SOFTWARE VALIDATION REPORT FOR MINTEQA2, VERSION 4.02

Prepared for

U.S. Nuclear Regulatory Commission
Contract NRC–02–97–009

Prepared by

David R. Turner

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

Approved by:

English C. Pearcy
Manager, Geohydrology and Geochemistry

5/8/2002
Date

TABLE OF CONTENTS

Section Page

TABLE OF CONTENTS ii
FIGURES iii
TABLES iv

1 SCOPE OF THE VALIDATION 1

2 THERMODYNAMIC DATA USED IN TESTING 1

3 TEST CASES 1

3.1 Installation Check—Results 2

3.2 Validation Check—Results 2
3.2.1 Aqueous Speciation 2
3.2.2 Mineral Solubility 6
3.2.3 Aqueous and Gas Phase Carbonate Chemistry 6
3.2.4 Sorption—Surface Complexation Modeling 8
3.2.5 Redox Equilibria 9
3.2.6 Temperature Effects 13
3.2.7 Modified Database 17

4 SUMMARY AND CONCLUSIONS 23

5 REFERENCES 23

APPENDIX A

FIGURES

Figure		Page
3-1	Comparison of Aqueous Speciation of Seawater from MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2	4
3-2	Comparison of Zn-ferrihydrite Sorption Results for MINTEQA2, Version 4.02 (circles) and PHREEQC, Version 2.4.2 (triangles)	10
3-3	Calculated $HS^- - SO_4^{2-}$ Speciation as a Function of Electron Activity (pe) for Example 8.4.	14
3-4	Comparison of Saturation Indexes (SI) Calculated by MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 for Anhydrite and Gypsum and a Function of Temperature	16
3-5	Aqueous Speciation Predicted by MINTEQA2, Version 4.02 (solid line, filled circles) and PHREEQC, Version 2.4.2 (dotted line, open triangles) as a Function of pH.	18

TABLES

Table		Page
3-1	Comparison of MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 Calculated Concentrations of Selected Component Species, Carbonate Species, and Redox Sensitive Species T = 25 °C, $P_{O2} = 10^{-0.66}$ atm	3
3-2	Comparison of Barite Solubility Results for Richardson and McSween (1989) and MINTEQA2, Version 4.02	7
3-3	Representative Seawater Composition	7
3-4	Seawater in Equilibrium with Calcite at 25 °C, and Open to Atmosphere	8
3-5	Fresh Water in Equilibrium with Calcite at 25 °C, and variable P_{CO2}	8
3-6	Comparison of MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 Results for Zn Sorption on Ferrihydrite (Percent Sorbed).	9
3-7	Calculated Electron Activity (pe) for Example 8.2	11
3-8	Calculated $HS^- - SO_4^{2-}$ Speciation as a Function of Electron Activity (pe) for Example 8.4	11
3-9	Comparison of Saturation Indexes (SI) Calculated by MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 for Anhydrite and Gypsum as a Function of Temperature	15
3-10	Comparison of pe Calculated by MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 Results as a Function of pH.	19
3-11	Comparison of MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 Results for Neptunium Speciation as a Function of pH.	20
3-12	Comparison of MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 Results for Uranium Speciation as a Function of pH.	22

1 SCOPE OF THE VALIDATION

The purpose of this document is to report the results of the validation testing for the geochemical equilibrium speciation code MINTEQA2, Version 4.02 (December 1999 release; U.S. Environmental Protection Agency, 1999a,b) performed under the Software Validation Test Plan (Turner, 2001). MINTEQA2, Version 4.02 is an acquired code, originally developed by the U.S. Environmental Protection Agency, National Exposure Research Laboratory, Ecosystems Research Division. The software is used by staff at the Center for Nuclear Waste Regulatory Analyses (CNWRA) in providing technical assistance to the U.S. Nuclear Regulatory Commission (NRC) in its high-level nuclear waste program.

As stated in Technical Operating Procedures (TOP)-018 (CNWRA, 2001), one purpose of software validation is to develop confidence that the software is correctly implementing numerical algorithms intended to represent the theory that is the basis for the code. One means of developing this confidence is benchmarking the software against hand calculations and similar software packages. This type of benchmarking is one of the major methods used in the validation results reported here, and as described in the approved software validation test plan for MINTEQA2, Version 4.02 (Turner, 2001).

MINTEQA2, Version 4.02 includes a number of capabilities that are not planned for use in CNWRA applications and were not tested at this time

- Ion Exchange
- Freundlich Isotherm
- Langmuir Isotherm
- Triple-Layer Model
- Constant Capacitance Model
- Composite Organic Liquid Model

If a decision is made to use these code capabilities, the software validation test plan will be modified as necessary and the report supplemented.

2 THERMODYNAMIC DATA USED IN TESTING

Historically, the original MINTEQA2 databases have been modified to include extensive thermodynamic data for toxic elements such as Cd, Zn, Pb, As, Hg, and Cu as well as organic ligands such as EDTA, Citrate, and Acetate. Additional modifications at the CNWRA have included the addition of thermodynamic data (ΔH_r° and log K) for almost 600 aqueous species and solids involving 14 potentially important radioelements, including U, Pu, Th, Np, Am, Sr, Cs, Ra, Sn, Zr, Tc, Ru, Eu, and Co (Turner, 1993; Turner, et al., 1993). Thermodynamic data for U, Pu, Np, Am, and Tc are from the Nuclear Energy Agency Thermodynamic Database Project (Grenthe, et al., 1992; Silva, et al., 1995; Rard, et al., 1999; Lemire, et al., 2001). The source for other data is the EQ3/6 database (Release Gembochs.v2-eq8-data0.alt.r2, 02Aug95).

3 TEST CASES

The test cases to be used in the validation testing have been identified previously (Turner, 2001). The following sections are intended to report the results of the testing. For

simple systems of a few components the same thermodynamic data (e.g., log K at 298K) were used to ensure consistency between calculational results. For more complicated systems with a large number of components, the problems were run using the overall databases. When using the same data, we anticipated that differences between MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 would be small. In most cases, this was true, but in some cases, differences were larger than expected. Possible reasons for the differences are discussed. The MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 input files are included in Appendix A. Key model results are summarized in tables or figures for each of the test cases. Output files for MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 are quite extensive, and are included in electronic form on the compact disc accompanying this report.

3.1 Installation Check—Results

The installation of MINTEQA2, Version 4.02 software was checked as part of bringing the code into configuration management under Technical Operating Procedure (TOP)-018 for the CNWRA (2001). The results indicate that the code was installed correctly on the personal computer platform and produced the correct results for 12 different example problems provided with MINTEQA2, Version 4.02. The results are documented in the configuration management package for MINTEQA2, Version 4.02 stored in the CNWRA quality assurance records room.

3.2 Validation Check—Results

Benchmarking is the major method that has been used in validating the MINTEQA2, Version 4.02 geochemical speciation code. MINTEQA2, Version 4.02 results are tested against hand calculations for simple systems reported in geochemical text books (Richardson and McSween, 1989; Stumm and Morgan, 1996; Langmuir, 1997), and against computer simulations of more complicated geochemical systems using the geochemical speciation code PHREEQC, Version 2.4.2 (Parkhurst and Appelo, 1999). PHREEQC, Version 2.4.2 is currently under CNWRA Technical Operating Procedures (TOP)-018 configuration management. The PHREEQC family of geochemical codes have been developed by the U.S. Geological Survey separately from MINTEQA2, Version 4.02 and similar results from the two codes provides confidence that MINTEQA2, Version 4.02 is correctly implementing the thermodynamics for solving geochemical problems.

3.2.1 Aqueous Speciation

Parkhurst and Appelo (1999) provide an example to calculate the distribution of aqueous species in seawater and the saturation state of seawater at 25 °C relative to a set of minerals. Representative calculated speciation results are reported in Table 3-1. Additional speciation checks are reported in Section 3.8 of this report.

As originally posed in the PHREEQC, Version 2.4.2 user's manual (Parkhurst and Appelo, 1999), the speciation problem specified thermodynamic equilibrium constants for the uranium aqueous speciation in the input file. With the update to both MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 to include data from the Nuclear Energy Agency thermodynamic databases (Grenthe, et al., 1992; Silva, et al., 1995; Rard, et al., 1999; Lemire, et al., 2001), we used the values from the databases for uranium speciation, rather than specifying thermodynamic data in the input files. The original formulation of Example 1 in the PHREEQC,

Table 3-1. Comparison of MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 Calculated Concentrations of Selected Component Species, Carbonate Species, and Redox Sensitive Species T = 25 °C, $P_{O_2} = 10^{-0.66}$ atm.		
Species	Aqueous Concentration (molal) MINTEQA2, Version 4.02	Aqueous Concentration (molal) PHREEQC, Version 2.4.2
Non-Redox/Non-Carbonate Species		
K^+	1.033×10^{-2}	1.040×10^{-2}
Na^+	4.766×10^{-1}	4.786×10^{-1}
Cl^-	5.656×10^{-1}	5.657×10^{-1}
Carbonate Species		
CO_3^{2-}	3.024×10^{-5}	3.728×10^{-5}
HCO_3^-	1.613×10^{-3}	1.480×10^{-3}
$Na\,HCO_3$	2.058×10^{-4}	1.626×10^{-4}
UO_2CO_3	1.242×10^{-12}	1.668×10^{-13}
Redox-Sensitive Species		
$U(IV)_{total}$	1.419×10^{-37}	6.233×10^{-38}
$U(V)_{total}$	5.437×10^{-28}	4.660×10^{-29}
$U(VI)_{total}$	1.267×10^{-8}	1.437×10^{-8}
$U^{V}O_2(CO_3)_3^{5-}$	1.071×10^{-21}	7.159×10^{-32}
$U^{VI}O_2(CO_3)_3^{4-}$	1.180×10^{-8}	1.422×10^{-8}
Saturation Indices (SI) with respect to solid phases		
Anhydrite	-0.68	-0.85
Calcite	0.88	0.79
Halite	-2.43	-2.51
Schoepite	-4.88	-5.86
Uraninite	-27.37	-28.38

Version 2.4.2 user's manual (Parkhurst and Appelo, 1999) also used the NO_3^-/NH_4^+ redox couple to control the oxidation state of uranium, while controlling the distribution of the other redox sensitive elements (Fe, Mn) by the overall redox equilibrium with atmospheric oxygen. MINTEQA2, Version 4.02 does not allow the user to specify separate redox controls, so the entire problem was formulated to control all redox reactions, including uranium speciation, only by atmospheric oxygen. Because of the large number of aqueous species in a multicomponent solution like seawater, only a few representative species concentrations are included in

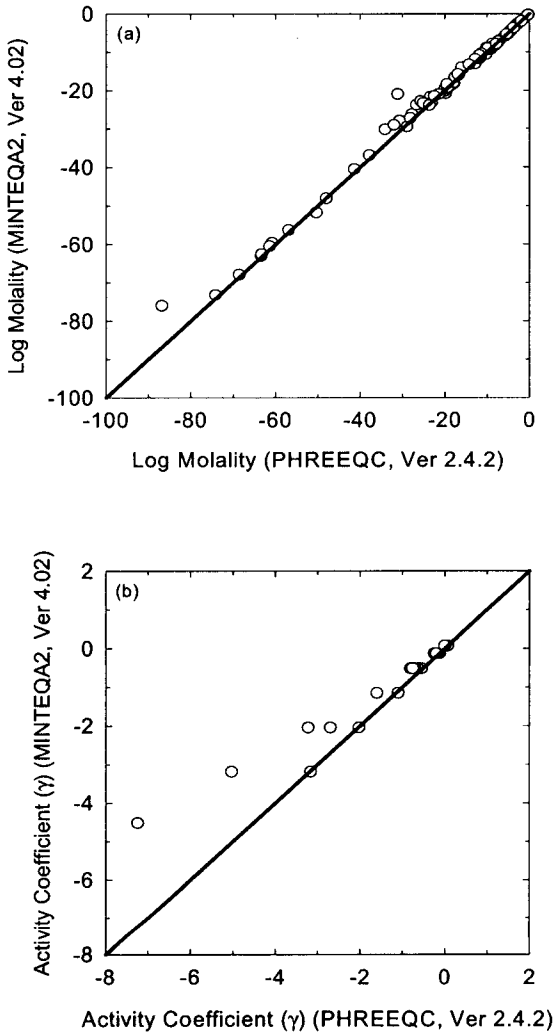


Figure 3-1. Comparison of Aqueous Speciation of Seawater from MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2. (a) Comparison of Concentration (log molality) of Aqueous Species; (b) Comparison of the Calculated Activity Coefficients (γ) Used by the Two Computer Codes. The Solid Line Indicates a One–To–One Perfect Correlation Between Model Results.

Table 3-1. A graphical comparison of the calculated concentration of more than 100 aqueous species (Figure 3-1a) shows a reasonable, although not perfect correlation among the results. Although there are some order of magnitude differences between calculated concentrations of several species (e.g., $UO_2(CO_3)_3^{5-}$ and UO_2CO_3), most calculated values agree within a factor of two. Calculated mineral saturations (Table 3-1) also show reasonable agreement, and MINTEQA2 results are consistent with PHREEQC predictions of saturation and undersaturation. The discrepancies between the two codes appear to be due to two principal factors, differences in the thermodynamic databases and slight differences in activity coefficients.

The aqueous species included in the two thermodynamic databases are not identical. For example, MINTEQA2, Version 4.02 includes the nitrate species $CaNO_3^+$, $MnNO_3^+$, and $FeNO_3^+$ that are not part of the PHREEQC, Version 2.4.2 database, while PHREEQC, Version 2.4.2 includes KOH (aq) and the carbonate species $FeCO_3$ (aq) and $MnCO_3$ (aq) that are not in the MINTEQA2 database. Most of these species are present in small amounts and do not have a large effect on the overall speciation, but may still account for part of the observed differences in speciation. Also, although the modifications made at the CNWRA have resulted in identical thermodynamic data for the uranium species, there are slight differences in the thermodynamic data for a number of common aqueous species. For example, for the following reaction included in both thermodynamic databases:

$$CO_3^{2-} + H^+ = HCO_3^- \qquad (3\text{-}1)$$

the equilbrium constant (Log K) for the reaction in Equation (3-1) is 10.329 in MINTEQA2, Version 4.02, while in PHREEQC, Version 2.4.2 the value is 10.29. Although the differences are small, there are a large number of species in the problem, and the cumulative effect of such differences may be amplified. Although both MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 are reported to use the WATEQ data compilations, these types of small differences persist in thermodynamic data for many of the chemical component systems that are beyond the intended scope of this validation test plan.

A second cause of the differences in the results from the two computer codes is likely to be due to differences in how activity coefficient, (γ) are calculated for aqueous species. Comparing the results from the two codes (Figure 3-1b) indicates that there are differences in calculated values for γ. Typically, MINTEQA2, Version 4.02 calculates a higher activity coefficient than PHREEQC, Version 2.4.2. The close agreement with the one-to-one correspondence line in Figure 3-1b indicates that the differences are generally small, but there are a few cases where the different formulations result in calculated values for γ that differ by a factor of two or more. The codes use slightly different equations for activity coefficients. In PHREEQC, Version 2.4.2, the **b** term in the Davies equation is -0.3*(I.S.), compared with -0.24*(I.S.) in MINTEQA2, Version 4.02 (Parkhurst and Appelo, 1999; Allison, et al., 1991). The differences in calculated γ become significant at the elevated ionic strength of seawater (0.6 to 0.7 molal). Also, because of the z^2 term in the Davies equation, the differences in activity coefficient formulations between the two codes is more pronounced for highly charged aqueous species. For example, for $UO_2(CO_3)_3^{4-}$, the dominant uranium species in the simulation, $\gamma = 9.0 \times 10^{-3}$ for MINTEQA2, Version 4.02 compared to $\gamma = 6.0 \times 10^{-3}$ calculated using PHREEQC,

Version 2.4.2. This effect is also compounded by slight differences in calculated ionic strengths for the two solutions (0.6653 for MINTEQA2, Version 4.02, versus 0.6745 for PHREEQC, Version 2.4.2). The iterative scheme used by both codes employs mass balance and mass action constraints to adjust γ, and ionic strength and converge on species concentrations.

3.2.2 Mineral Solubility

Richardson and McSween (1989) present two worked problems to investigate the solubility of barite ($BaSO_4$) at 298 K in pure water (Worked Problem 3-7), and in a 0.2 m NaCl solution (Worked Problem 3-8). Using an iterative solution of the congruent barite dissolution reaction, Richardson and McSween (1989) demonstrated that barite solubility increases with ionic strength. The results for barite solubility reported in Richardson and McSween (1989) differ slightly from the results calculated by MINTEQA2, Version 4.02 (Table 3-2). The results differ by less than 2 percent, and are likely due to slight differences in the activity coefficient formulation, and a more complete handling of the geochemical system in MINTEQA2, Version 4.02. For example, the extended Debye-Hückel is used in MINTEQA2 (Allison, et al., 1991), versus the Debye-Hückel formulation used in Richardson and McSween (1989). MINTEQA2, Version 4.02 also includes the dissociation products of water (H^+ and OH^-) in the geochemical system, resulting in small changes in calculated ionic strength. Reevaluating the Richardson and McSween (1989) calculations using the activity coefficients calculated by MINTEQA2, Version 4.02 shows excellent agreement between the two sets of results (Table 3-2). Both the MINTEQA2, Version 4.02 and Richardson and McSween (1989) solubility calculations are in good agreement with the experimental data of Blount (1977) as reported in Richardson and McSween (1989).

3.2.3 Aqueous and Gas Phase Carbonate Chemistry

Stumm and Morgan (1996) present several hand calculations of aqueous carbonate speciation. Included is Example 7.8, equilibrating calcite ($CaCO_3$) in sea water at 25 °C, and open to atmosphere (fixed $P_{CO_2} = 3.55 \times 10^{-4}$ atm). The seawater composition is not specified in the example problem, but a representative composition is provided in Table 15.2 of Stumm and Morgan (1996) and reproduced in Table 3-3 of this report.

As indicated in the problem formulation, initial Ca^{2+}, HCO_3^-, and B were omitted. Results from Stumm and Morgan (1996) and MINTEQA2, Version 4.02 are compared in Table 3-4.

The model results agree very well for pH, and $H_2CO_3(aq)$, and agree within less than a factor of two for Ca^{2+}, HCO_3^-, and CO_3^{2-} concentrations. The differences in HCO_3^- and CO_3^{2-} are likely due to uncertainty in starting composition and slight differences in thermodynamic data for the aqueous carbonate system; Stumm and Morgan (1996) do not indicate the precise starting composition of the seawater used in their calculations. As noted previously, there are also likely to be differences due to the thermodynamic data for aqueous speciation, and different activity coefficient models. Because the details of the model inputs are not presented in Stumm and Morgan (1996), it is not possible to evaluate these differences in more detail.

Alternatively, Langmuir (1997) presents results for calcite solubility in fresh water at 25 °C, and under variable fixed P_{CO_2}. These results are easier to interpret due to the simpler geochemical system.

Table 3-2. Comparison of Barite Solubility Results for Richardson and McSween (1989) and MINTEQA2, Version 4.02				
	m_{Ba2+} (molal)	m_{SO42-} (molal)	γ_{Ba2+} (D-H)	γ_{SO42-} (D-H)
Problem 3-7 (pure H_2O)				
MINTEQA2, Version 4.02	1.055×10^{-5}	1.055×10^{-5}	0.97018	0.97011
Richardson and McSween (1989)	1.051×10^{-5}	1.051×10^{-5}	0.9704	0.9704
Richardson & McSween calculations with MINTEQA2 activity coefficients	1.055×10^{-5}	1.055×10^{-5}	0.97018	0.97011
Blount (1977)	1.06×10^{-5}	1.06×10^{-5}	N/R	N/R
Problem 3-8 (0.2 m NaCl)				
MINTEQA2, Version 4.02	3.675×10^{-5}	3.675×10^{-5}	0.29726	0.26082
Richardson and McSween (1989)	3.611×10^{-5}	3.611×10^{-5}	0.2987	0.2671
Richardson & McSween calculations with MINTEQA2 activity coefficients	3.675×10^{-5}	3.675×10^{-5}	0.29726	0.26082
Blount (1977)	3.7×10^{-5}	3.7×10^{-5}	N/R	N/R
N/R not reported				

Table 3-3. Representative Seawater Composition (Stumm and Morgan, 1996; Table 15.2).	
Constituent	**Concentration (mg/L)**
Na^+	10770
Mg^{2+}	1290
Ca^{2+}	412.1
K^+	399
Sr^{2+}	7.9
Cl^-	19354
SO_4^{2-}	2712
HCO_3^-	142.4
Br^-	67.3
F^-	1.3
B	4.5

Table 3-4. Seawater in Equilibrium with Calcite at 25 °C, and Open to Atmosphere (fixed $P_{CO_2} = 3.55 \times 10^{-4}$ atm). All Concentrations in Molarity.					
	pH	Ca^{2+} (total)	HCO_3^- (total)	CO_3^{2-} (total)	H_2CO_3(aq) (total)
Problem 7.8					
MINTEQA2, Version 4.02	8.32	1.234×10^{-3}	1.93×10^{-3}	2.63×10^{-4}	1.03×10^{-5}
Stumm and Morgan (1996)	8.34	1.51×10^{-3}	2.77×10^{-3}	3.80×10^{-4}	1.05×10^{-5}

Again, there are slight differences (Table 3-5) due to thermodynamic data or different activity coefficient models, [Langmuir (1997) does not provide this information in Table 6.3], but at all three P_{CO_2} values covering two orders of magnitude, the agreement is within one percent (Table 3-5). The overall excellent agreement indicates that MINTEQA2, Version 4.02 is correctly implementing carbonate equilibria in aqueous speciation calculations.

Table 3-5. Fresh Water in Equilibrium with Calcite at 25 °C, and Variable P_{CO_2}			
	pH	Ca^{2+} (mg/L)	HCO_3^- (mg/L)
$P_{CO_2} = 10^{-3.5}$ bar = $10^{-3.51}$ atm			
MINTEQA2, Version 4.02	8.284	19.8	58.1
Langmuir (1997); Table 6.3	8.29	20	58
$P_{CO_2} = 10^{-2.5}$ bar = $10^{-2.51}$ atm			
MINTEQA2, Version 4.02	7.628	43.8	131.1
Langmuir (1997); Table 6.3	7.62	44	131
$P_{CO_2} = 10^{-1.5}$ bar = $10^{-1.51}$ atm			
MINTEQA2, Version 4.02	6.976	100.5	300.0
Langmuir (1997); Table 6.3	6.97	100	298

3.2.4 Sorption—Surface Complexation Modeling

Parkhurst and Appelo (1999) provide an example of the use of PHREEQC, Version 2.4.2 to calculate Zn^{2+} sorption on ferrihydrite (HFO) using the diffuse-layer surface complexation model and parameters described in Dzombak and Morel (1990). Sorption at 25 °C (298 K) is investigated for two Zn^{2+} concentrations (10^{-4} and 10^{-7} molal), and the results are presented in terms of dissolved and sorbed Zn^{2+} molality as a function of pH. For more direct comparison of model results, the input file for MINTEQA2, Version 4.02 (Appendix A) includes modified equilibrium constants for $Zn(OH)^+$, $Zn(OH)_2$(aq), $Zn(OH)_3^-$, and $Zn(OH)_4^{2-}$ that match those in the PHREEQC, Version 2.4.2 database. In addition, the species $ZnNO_3^+$ and $Zn(NO_3)_2$(aq) are excluded from the MINTEQA2, Version 4.02 run since they are not included in the

PHREEQC, Version 2.4.2 database. Model results are given in Table 3-6 (percent sorbed) and shown in Figure 3-2 (surface complex concentration).

The results from MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 show excellent agreement, indicating that the surface complexation modeling subroutines are performing as expected. The minor variations are likely due to differences in how the two codes sweep through a range in pH. In PHREEQC, Version 2.4.2, pH is fixed based on titration with 1.0 m NaOH, in contrast to MINTEQA2, Version 4.02, where pH is fixed externally by adjusting H^+ activity. This leads to differences in both Na^+ concentrations and ionic strength.

3.2.5 Redox Equilibria

Stumm and Morgan (1996) present a number of relatively simple calculations to determine redox equilibrium and equilibrium distribution in the SO_4^{2-}–HS^- system (Example 8.4). MINTEQA2, Version 4.02 uses electron activity (pe) as a master variable to control redox potential. Comparison of redox equilibria results are provided in Tables 3-7 and 3-8.

Table 3-6. Comparison of MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 Results for Zn Sorption on Ferrihydrite (Percent Sorbed). DLM Constants from Dzombak and Morel (1990).

	$Zn_T = 1 \times 10^{-4}$ molal		$Zn_T = 1 \times 10^{-7}$ molal	
pH	MINTEQA2 (% sorbed)	PHREEQC (% sorbed)	MINTEQA2 (% sorbed)	PHREEQC (% sorbed)
5.00	0.3	0.3	0.3	0.3
5.25	0.8	0.8	0.9	0.9
5.50	1.7	1.7	2.4	2.4
5.75	3.0	3.0	6.2	6.3
6.00	4.5	4.5	15.3	15.5
6.25	6.2	6.3	33.0	33.2
6.50	9.2	9.3	57.3	57.6
6.75	15.1	15.2	78.7	78.9
7.00	24.8	25.0	91.1	91.2
7.25	37.4	37.6	96.6	96.7
7.50	50.4	50.6	98.8	98.8
7.75	62.4	62.5	99.6	99.6
8.00	72.3	72.4	99.8	99.8

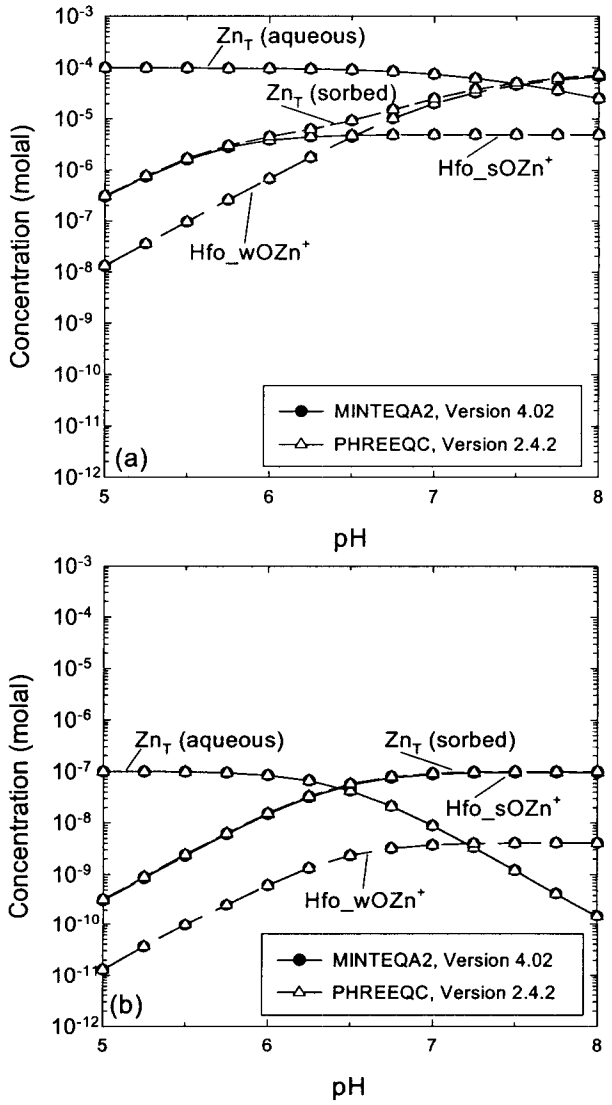


Figure 3-2. Comparison of Zn-ferrihydrite Sorption Results for MINTEQA2, Version 4.02 (circles) and PHREEQC, Version 2.4.2 (triangles). MINTEQA2, Version 4.02 Thermodynamic Data Have Been Modified to Match the PHREEQC, Version 2.4.2 Database.

Table 3-7. Calculated Electron Activity (pe) for Example 8.2 in Stumm and Morgan (1996).			
	pe calculated		
Geochemical System	MINTEQA2, Version 4.02	Hand Calculation ($\gamma = 1.0$)	Hand Calculation (γ from Davies equation)
$\{Fe^{2+}\} = 10^{-3}$ M $\{Fe^{3+}\} = 10^{-5}$ M	10.891	11.01	10.89
pH = 7.5 P_{O2} = 0.22 atm	13.106	12.94	13.106
$\{Mn^{2+}\} = 10^{-5}$ M Equilibrium with γ–MnO_2	6.925	6.92	6.925

Table 3-8. Calculated HS^-–SO_4^{2-} Speciation as a Function of Electron Activity (pe) for Example 8.4 in Stumm and Morgan (1996).						
	MINTEQA2, Version 4.02		Hand Calculation ($\gamma = 1.0$)		Hand Calculation (γ from Davies equation)	
pe	mHS^-(molal)	mSO_4^{2-}(molal)	mHS^-(molal)	mSO_4^{2-}(molal)	mHS^-(molal)	mSO_4^{2-}(molal)
-9.0	1.00×10^{-4}	9.89×10^{-21}	1.00×10^{-4}	9.55×10^{-21}	1.00×10^{-4}	9.89×10^{-21}
-8.8	1.00×10^{-4}	3.94×10^{-19}	1.00×10^{-4}	3.80×10^{-19}	1.00×10^{-4}	3.94×10^{-19}
-8.6	1.00×10^{-4}	1.57×10^{-17}	1.00×10^{-4}	1.51×10^{-17}	1.00×10^{-4}	1.57×10^{-17}
-8.4	1.00×10^{-4}	6.24×10^{-16}	1.00×10^{-4}	6.03×10^{-16}	1.00×10^{-4}	6.24×10^{-16}
-8.2	1.00×10^{-4}	2.48×10^{-14}	1.00×10^{-4}	2.40×10^{-14}	1.00×10^{-4}	2.48×10^{-14}
-8.0	1.00×10^{-4}	9.89×10^{-13}	1.00×10^{-4}	9.55×10^{-13}	1.00×10^{-4}	9.89×10^{-13}
-7.8	1.00×10^{-4}	3.94×10^{-11}	1.00×10^{-4}	3.80×10^{-11}	1.00×10^{-4}	3.94×10^{-11}
-7.6	1.00×10^{-4}	1.57×10^{-9}	1.00×10^{-4}	1.51×10^{-9}	1.00×10^{-4}	1.57×10^{-9}
-7.4	9.99×10^{-4}	6.24×10^{-8}	9.99×10^{-4}	6.02×10^{-8}	9.99×10^{-4}	6.24×10^{-8}
-7.2	9.76×10^{-5}	2.43×10^{-6}	9.77×10^{-5}	2.34×10^{-6}	9.76×10^{-5}	2.43×10^{-6}
-7.0	5.00×10^{-5}	5.00×10^{-5}	5.12×10^{-5}	4.88×10^{-5}	5.00×10^{-5}	5.00×10^{-5}
-6.8	2.43×10^{-6}	9.76×10^{-5}	2.56×10^{-6}	9.74×10^{-5}	2.43×10^{-6}	9.76×10^{-5}
-6.6	6.25×10^{-8}	9.99×10^{-5}	6.60×10^{-8}	9.99×10^{-5}	6.25×10^{-8}	9.99×10^{-5}
-6.4	1.57×10^{-9}	1.00×10^{-4}	1.66×10^{-9}	1.00×10^{-4}	1.57×10^{-9}	1.00×10^{-4}
-6.2	3.95×10^{-11}	1.00×10^{-4}	4.17×10^{-11}	1.00×10^{-4}	$3.95E \times 10^{-11}$	1.00×10^{-4}
-6.0	9.91×10^{-13}	1.00×10^{-4}	1.05×10^{-12}	1.00×10^{-4}	9.91×10^{-13}	1.00×10^{-4}

Table 3-8. Calculated HS^-–SO_4^{2-} Speciation as a Function of Electron Activity (pe) for Example 8.4 in Stumm and Morgan (1996) (continued).						
	MINTEQA2, Version 4.02		Hand Calculation ($\gamma = 1.0$)		Hand Calculation (γ from Davies equation)	
pe	mHS^-(molal)	mSO_4^{2-}(molal)	mHS^-(molal)	mSO_4^{2-}(molal)	mHS^-(molal)	mSO_4^{2-}(molal)
-5.4	1.57×10^{-17}	1.00×10^{-4}	1.66×10^{-17}	1.00×10^{-4}	1.57×10^{-17}	1.00×10^{-4}
-5.2	3.95×10^{-17}	1.00×10^{-4}	4.17×10^{-17}	1.00×10^{-4}	3.95×10^{-17}	1.00×10^{-4}
-5.0	9.91×10^{-21}	1.00×10^{-4}	1.05×10^{-20}	1.00×10^{-4}	9.91×10^{-21}	1.00×10^{-4}

Example 8.2 presents three different geochemical problems to calculate electron activity (pe) for Fe and Mn systems open to atmosphere. Simple thermodynamic calculations can be used to calculate pe.

Example 8.2(a). An acid solution with $\{Fe^{3+}\} = 10^{-5}$ M; $\{Fe^{2+}\} = 10^{-3}$ M

$$pe = \log K + \log \frac{\{Fe^{3+}\}}{\{Fe^{2+}\}} \tag{3-2}$$

Example 8.2(b). Natural water with pH = 7.5 in equilibrium with atmosphere ($P_{O2} = 0.22$ atm)

$$pe = \frac{1}{2}\log K + \frac{1}{4}\log P_{O2} - pH \tag{3-3}$$

Example 8.2(c). Natural water with pH = 8 in equilibrium with γ–MnO_2

$$pe = \frac{1}{2}\log K - 2pH - \frac{1}{2}\log \{Mn^{2+}\} \tag{3-4}$$

Equilibrium constants (log K) were modified in the MINTEQA2, Version 4.02 input files to match the values provided in Stumm and Morgan (1996). Formation of ferric- and ferrous-hydroxy species was suppressed in the MINTEQA2, Version 4.02 simulation of Example 8.2(a) to match the geochemical equilibrium model used in Stumm and Morgan (1996). Also, a dilute NaCl (10^{-3} M) solution was added to the natural water in Example 8.2(b) to avoid problems with creating a singular matrix in the MINTEQA2, Version 4.02 simulation. Comparison of model results in Table 3-7 show that there are slight differences in calculated pe values. In Stumm and Morgan (1996), the assumption is that the activity coefficients for all of the components are unity (γ = 1.0), while MINTEQA2, Version 4.02 uses the Davies equation to correct for ionic strength effects. Incorporating activity coefficients calculated with the Davies equation improves the agreement significantly.

Example 8.4 (Stumm and Morgan, 1996) calls for a simple calculation of the speciation of HS^- and SO_4^{2-} as a function of pe, with pH = 10, and $\{HS^-\} + \{SO_4^{2-}\} = 10^{-4}$ M. Aqueous speciation

log K values for the reaction in Equation (3-5) were modified in the MINTEQA2, Version 4.02 input file to match the values (log K = 34.02) provided in Stumm and Morgan (1996). Based on the redox equilibrium reaction

$$SO_4^{2-} + 9H^+ + 8e^- = HS^- + 4H_2O \quad (3\text{-}5)$$

pe can be expressed in terms of pH and component activity

$$pe = \frac{1}{8}\left(\log K + pH + \log [SO_4^{2-}] + \log [HS^-]\right) \quad (3\text{-}6)$$

The results from MINTEQA2, Version 4.02 are compared with hand calculations using Equation (3-6)

Comparison of the results in Table 3-8 show that there is very good agreement. MINTEQA2, Version 4.02 correctly predicts the crossover point (pe = -7.0) where the concentrations of HS^- and SO_4^{2-} are equal. There is a slight discrepancy when unity activity coefficients (γ = 1) were assumed for the hand calculations. Performing the hand calculations with the activity coefficients derived for each pe value by MINTEQA2, Version 4.02 using the Davies equation results in a match to the HS^- and SO_4^{2-} concentrations predicted by MINTEQA2, Version 4.02 to at least three significant figures (Table 3-8). Concentration-pe plots comparing MINTEQA2, Version 4.02 and hand calculation results (Figure 3-3) demonstrate the excellent agreement, indicating that MINTEQA2, Version 4.02 correctly implements redox equilibria reactions.

3.2.6 Temperature Effects

Parkhurst and Appelo (1999) provide an example of the use of PHREEQC, Version 2.4.2 to calculate the solubility of gypsum and anhydrite in pure water, over a range in temperature from 25 °C (298 K) to 75 °C (373 K). Only the pH and temperature are used to define a pure water solution. Gypsum and anhydrite are allowed to react to equilibrium, and the initial phase assemblage has 1 mol of each mineral. Each mineral will react either to equilibrium or until it is exhausted in the assemblage. For both MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2, the degree of saturation with respect to a given mineral is indicated by the saturation index (SI), such that

$$SI = \log \frac{IAP}{K} \quad (3\text{-}7)$$

where IAP is the ion activity product, and K is the equilibrium constant. When a solution is undersaturated with respect to a given mineral, SI < 0. Under supersaturated conditions, SI > 0, and SI = 0 at equilibrium.

As a default, both MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 use the Van't Hoff relationship and enthalpies of reaction ($\Delta H_r°$) to correct equilibrium constants for the effects of temperature. If data are available, both MINTEQA2, Version 4.02 and PHREEQC,

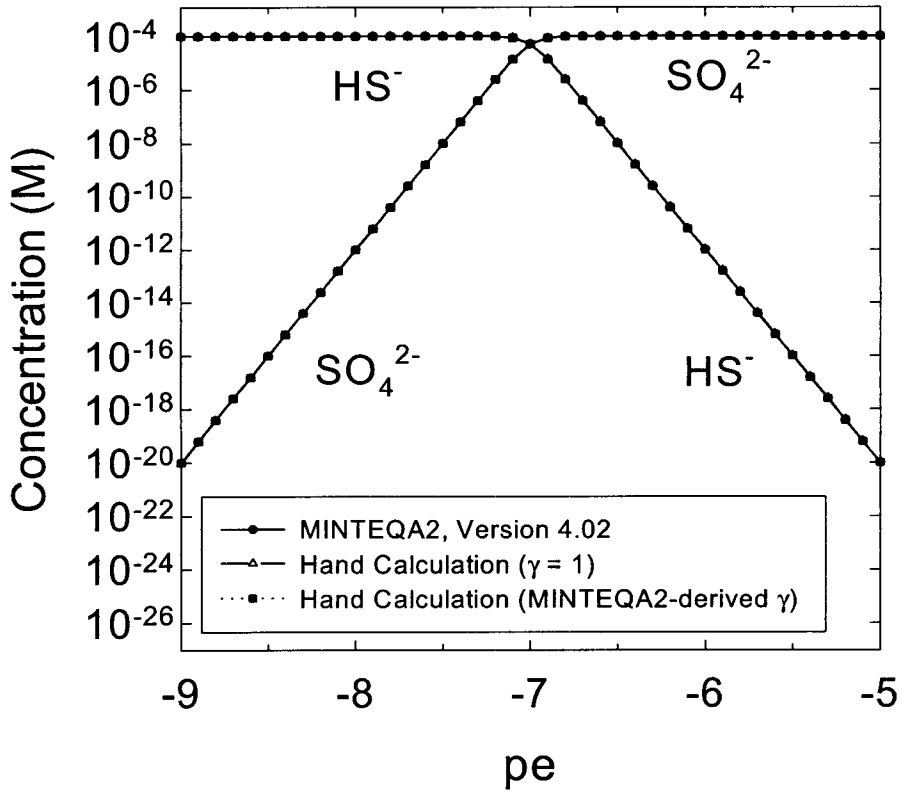


Figure 3-3. Calculated $HS^- - SO_4^{2-}$ Speciation as a Function of Electron Activity (pe) for Example 8.4 in Stumm and Morgan (1996).

Version 2.4.2 will employ a polynomial expression to correct equilibrium constants for the effects of temperature:

$$\text{Log } K_T = A_1 + A_2T + \frac{A_3}{T} + A_4\text{Log}(T) + A_5T^2 + \frac{A_6}{T2} + A_7\sqrt{T} \qquad (3\text{-}8)$$

where K_T is the equilibrium constant at a given temperature T in Kelvin.

If the same thermodynamic data and polynomial expressions are used, both codes should produce similar results. PHREEQC, Version 2.4.2 provides a polynomial expression in the phreeqc.dat database for both anhydrite and gypsum. In conducting this validation exercise, the same thermodynamic constants and polynomial expressions were used for anhydrite and gypsum (Appendix A).

Comparing the results in Table 3-9 and Figure 3-4(a) shows a slight discrepancy between the SI values calculated by MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2. This discrepancy is likely due to differences in the aqueous speciation and differences in how the two codes calculate the activity of water. The PHREEQC, Version 2.4.2 database includes the aqueous species $CaHSO_4^+$, which is not included in the MINTEQA2, Version 4.02 database. In addition, there are slight differences in the equilibrium constants and analytic temperature effect corrections for the aqueous species $CaSO_4(aq)$, HSO_4^-, and $CaOH^+$. In calculating the concentrations of individual ionic species to correct the activity of water, MINTEQA2, Version 4.02 includes the concentrations of the two minerals anhydrite and gypsum (1.0 mole of each). This gives a larger correction to unit activity (a_{H2O} = 0.949) , and results in a constant variation in the calculated SI values. If, however, gypsum or anhydrite is assigned to be present in an infinite amount in the MINTEQA2, Version 4.02 input file, then the activity correction for water does not include the minerals, and is much smaller. Runs under this condition show a much closer agreement with the SI values calculated by PHREEQC, Version 2.4.2 (Figure 3-4b).

Table 3-9. Comparison of Saturation Indexes (SI) Calculated by MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 for Anhydrite and Gypsum as a Function of Temperature.

	MINTEQA2, Version 4.02			PHREEQC, Version 2.4.2		
T(°C)	pH	SI(Anhy)	SI(Gyp)	pH	SI(Anhy)	SI(Gyp)
25	7.08	-0.175	0.000	7.07	-0.220	0.000
30	7.01	-0.153	0.000	7.00	-0.200	0.000
35	6.94	-0.126	0.000	6.94	-0.171	0.000
40	6.88	-0.096	0.000	6.88	-0.141	0.000
45	6.82	-0.061	0.000	6.82	-0.106	0.000
50	6.76	-0.023	0.000	6.77	-0.068	0.000
55	6.70	0.000	-0.019	6.72	-0.026	0.000
60	6.65	0.000	-0.064	6.67	0.000	-0.019
65	6.59	0.000	-0.112	6.62	0.000	-0.067
70	6.54	0.000	-0.162	6.57	0.000	-0.117
75	6.49	0.000	-0.216	6.53	0.000	-0.170

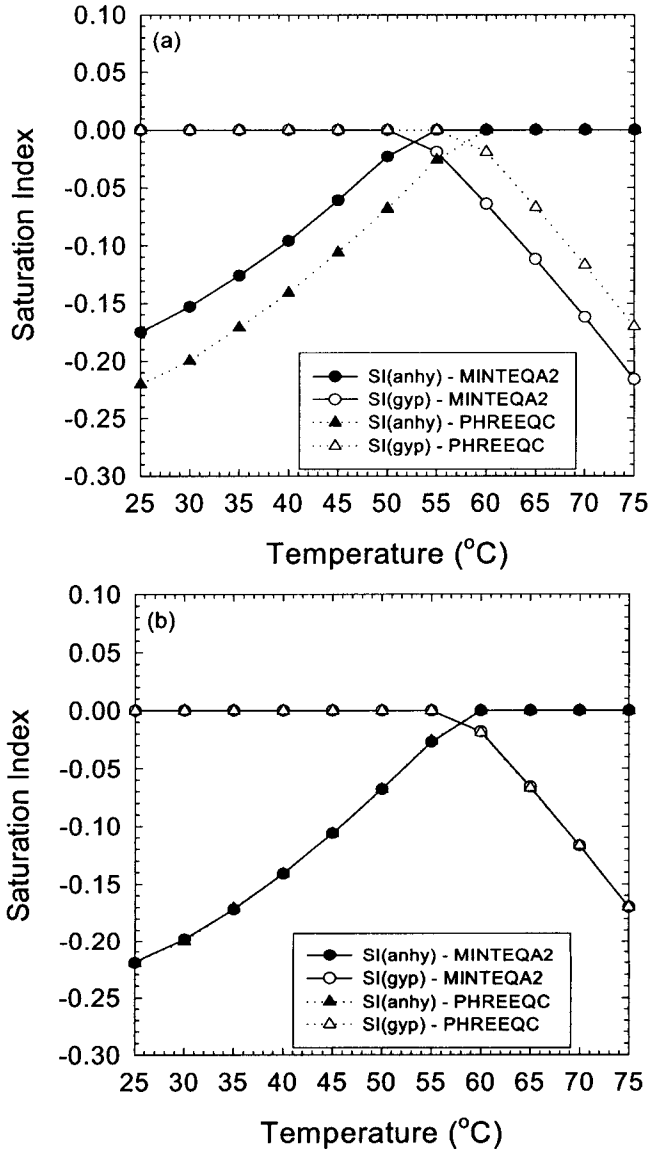


Figure 3-4. Comparison of Saturation Indexes (SI) Calculated by MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 for Anhydrite and Gypsum as a Function of Temperature. (a) 1.0 mole anhydrite + 1.0 mole gypsum; (b) Infinite Gypsum (25° to 55°C), Infinite Anhydrite (60° to 75 °C).

3.2.7 Modified Database

The main code function to be checked in this section of the test plan is to ensure that the MINTEQA2, Version 4.02 database modified to include Nuclear Energy Agency radionuclide thermodynamic data is correct and produces reasonable results. If thermodynamic data are the same, different geochemical equilibrium speciation codes should produce similar results. The most straightforward way to test this is to compare aqueous speciation results from several different codes. This approach has been used before (Turner, 1993; Turner, et al., 1993) to examine the modified MINTEQA2, Version 3.11/3.12 database.

Speciation checks for uranium and neptunium were performed using MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2. Identical thermodynamic data from the Nuclear Energy Agency thermodynamic database for neptunium and uranium (Grenthe, et al., 1992; Lemire, et al., 2001) were used to examine speciation as a function of pH under atmospheric CO_2 ($10^{-3.5}$ atm) and O_2 ($10^{-0.66}$ atm) conditions. Temperature was fixed at 25 °C (298 K). Low concentrations were used to avoid the complications of precipitation of pure phases, and the redox couples were allowed to establish the distribution among the different oxidation states of Np and U. The focus of the check is the CNWRA-modifications to the MINTEQA2, Version 4.02 database, and very simple solutions of 0.1 M $NaNO_3$ were used to minimize the effects of major ions such as Ca^{2+}, Mg^{2+}.

Comparison of the predicted speciation indicates good agreement between PHREEQC, Version 2.4.2 and MINTEQA2, Version 4.02 for Np and U (Figure 3-5). With atmospheric oxygen ($P_{O2} = 10^{-0.66}$ atm), both codes calculate similar pe values for the system over the pH range (Table 3-10). Not only is there good agreement for aqueous speciation as a function of pH, but there is also good agreement between the two codes in simulating the changing dominance of different oxidation states for redox sensitive elements like Np and U (Tables 3-11 and 3-12). For example, both codes predict a change from Np(V)-dominance at pH < 8 to Np(VI)-dominance of $NpO_2(CO_3)_2^{2-}$ and $NpO_2(CO_3)_3^{2-}$ at pH > 8. There are minor differences that are most likely due to activity coefficient calculation, as discussed previously in Section 3.2. Also, there are slight differences in calculated ionic strength due to differences in how pH is determined. Finally, there are differences in how the two codes handle the activity of the neutral species $UO_2(OH)_2(aq)$ and $UO_2CO_3(aq)$. While PHREEQC, Version 2.4.2 assigns unity activity coefficients (i.e., $\gamma = 1$) to neutral species, MINTEQA2, Version 4.02 corrects for ionic strength effects using the relationship

$$\log \gamma = 0.1(\text{I.S.}) \tag{3-9}$$

where I.S. is the ionic strength of the solution. For the ionic strength used in the simulation (0.1 m $NaNO_3$), the activity coefficient for $UO_2(OH)_2(aq)$ and $UO_2CO_3(aq)$ is 1.02.

Despite these small differences, the agreement is excellent for a system open to atmosphere over the range in pH, even for very complicated redox-sensitive aqueous systems such as neptunium and uranium. This indicates that the databases are correctly formatted for both MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2, both codes are correctly reading the modified databases, and both codes are calculating aqueous speciation in a similar fashion.

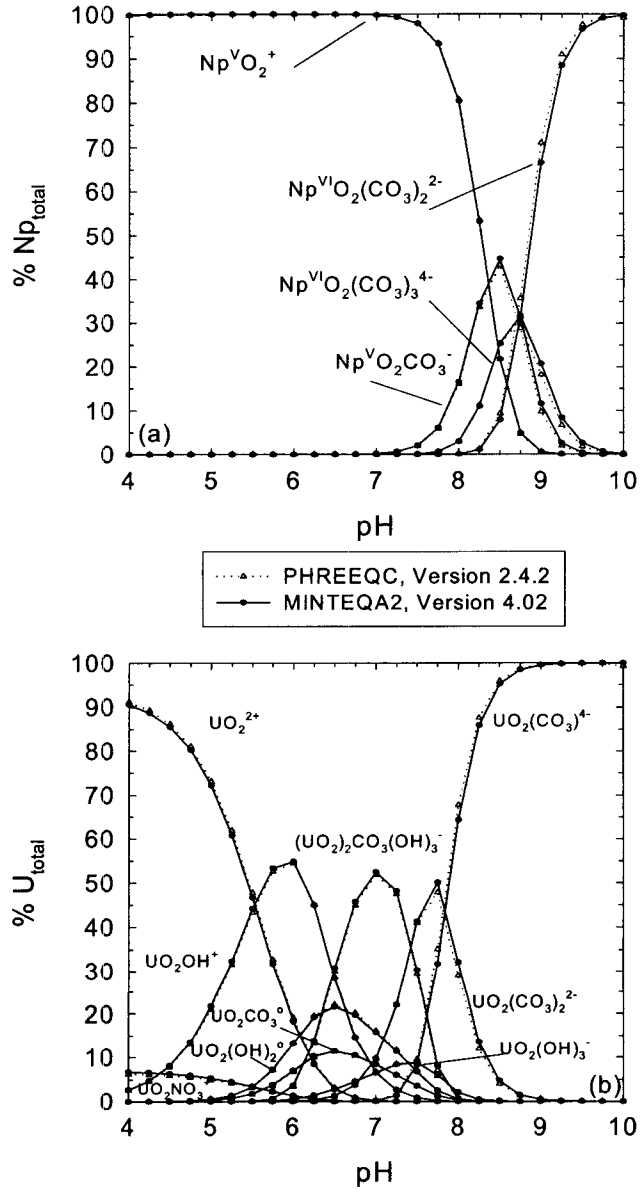


Figure 3-5. Aqueous Speciation Predicted by MINTEQA2, Version 4.02 (solid line, filled circles) and PHREEQC, Version 2.4.2 (dotted line, open triangles) as a Function of pH. T = 25 °C, $P_{CO2} = 10^{-3.5}$ atm $P_{CO2} = 10^{-0.66}$ atm, (a) Neptunium Speciation with $Np_{TOTAL} = 10^{-7}$ m. Neptunium Oxidation States Change with pH and Both Np(V)-Species and Np(VI)-Species Are Shown; (b) Uranium Speciation with $U_{TOTAL} = 10^{-7}$ m. Uranium Speciation is Dominated by U(VI) Over Entire pH Range, and Only U(VI) Species Are Shown.

Table 3-10. Comparison of pe Calculated by MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 Results as a Function of pH. Background Electrolyte Is 0.1 M $NaNO_3$, T = 25 °C, $P_{CO_2} = 10^{-3.5}$ atm, $P_{O_2} = 10^{-0.66}$ atm.		
pH	pe MINTEQA2, Version 4.02	pe PHREEQC, Version 2.4.2
4.00	16.61	16.62
4.50	16.11	16.12
5.00	15.61	15.62
5.50	15.11	15.12
6.00	14.61	14.62
6.50	14.11	14.12
7.00	13.61	13.62
7.50	13.11	13.12
8.00	12.61	12.62
8.50	12.11	12.12
9.00	11.61	11.62
9.50	11.11	11.12
10.00	10.61	10.64

Table 3-11. Comparison of MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 Results for Neptunium Speciation as a Function of pH. $Np_{total} = 10^{-7}$ M, 0.1 M $NaNO_3$, T = 25 °C, $P_{CO2} = 10^{-3.5}$ atm, $P_{O2} = 10^{-0.66}$ atm. Both Np(V) and Np(VI) Are Present, as Indicated.

	Percent (%) of Total Neptunium							
pH	$Np^{V}O_2^+$ MINTEQA2	$Np^{V}O_2^+$ PHREEQC	$Np^{V}O_2CO_3^-$ MINTEQA2	$Np^{V}O_2CO_3^-$ PHREEQC	$Np^{VI}O_2(CO_3)_2^{2-}$ MINTEQA2	$Np^{VI}O_2(CO_3)_2^{2-}$ PHREEQC	$Np^{VI}O_2(CO_3)_3^{4-}$ MINTEQA2	$Np^{VI}O_2(CO_3)_3^{4-}$ PHREEQC
4.00	99.77	99.77	0.00	0.00	0.00	0.00	0.00	0.00
4.25	99.87	99.87	0.00	0.00	0.00	0.00	0.00	0.00
4.50	99.92	99.92	0.00	0.00	0.00	0.00	0.00	0.00
4.75	99.95	99.95	0.00	0.00	0.00	0.00	0.00	0.00
5.00	99.97	99.97	0.00	0.00	0.00	0.00	0.00	0.00
5.25	99.98	99.98	0.00	0.00	0.00	0.00	0.00	0.00
5.50	99.98	99.98	0.00	0.00	0.00	0.00	0.00	0.00
5.75	99.99	99.99	0.00	0.00	0.00	0.00	0.00	0.00
6.00	99.99	99.99	0.00	0.00	0.00	0.00	0.00	0.00
6.25	99.98	99.98	0.01	0.01	0.00	0.00	0.00	0.00
6.50	99.97	99.97	0.02	0.02	0.00	0.00	0.00	0.00
6.75	99.92	99.92	0.06	0.06	0.00	0.00	0.00	0.00
7.00	99.78	99.78	0.20	0.20	0.00	0.00	0.00	0.00
7.25	99.31	99.33	0.64	0.62	0.02	0.02	0.00	0.00
7.50	97.85	97.91	2.01	1.95	0.11	0.11	0.00	0.00
7.75	93.29	93.46	6.05	5.88	0.61	0.61	0.01	0.01
8.00	80.41	80.78	16.47	16.06	2.95	2.97	0.09	0.11
8.25	53.27	53.70	34.52	33.77	10.99	11.11	1.08	1.27

Table 3-11. Comparison of MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 Results for Neptunium Speciation as a Function of pH. $Np_{total} = 10^{-7}$ M, 0.1 M $NaNO_3$, T = 25 °C, $P_{CO2} = 10^{-3.5}$ atm, $P_{O2} = 10^{-0.66}$ atm. Both Np(V) and Np(VI) Are Present, as Indicated. (continued)

	Percent (%) of Total Neptunium							
pH	$Np^{V}O_2^+$ MINTEQA2	$Np^{V}O_2^+$ PHREEQC	$Np^{V}O_2CO_3^-$ MINTEQA2	$Np^{V}O_2CO_3^-$ PHREEQC	$Np^{VI}O_2(CO_3)_2^{2-}$ MINTEQA2	$Np^{VI}O_2(CO_3)_2^{2-}$ PHREEQC	$Np^{VI}O_2(CO_3)_3^{4-}$ MINTEQA2	$Np^{VI}O_2(CO_3)_3^{4-}$ PHREEQC
8.50	21.80	21.75	44.66	43.25	25.31	25.36	7.90	9.29
8.75	4.84	4.58	31.35	28.82	31.66	30.21	31.53	35.75
9.00	0.56	0.48	11.50	9.64	20.74	18.17	66.49	71.02
9.25	0.04	0.03	2.59	1.94	8.38	6.67	88.47	90.88
9.50	0.00	0.00	0.45	0.28	2.63	1.80	96.62	97.65
9.75	0.00	0.00	0.06	0.02	0.68	0.32	99.10	99.44
10.00	0.00	0.00	0.01	0.00	0.15	0.02	99.75	99.16

Table 3-12. Comparison of MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 Results for Uranium Speciation as a Function of pH. $U_{total} = 10^{-7}$ M, 0.1 M $NaNO_3$, T = 25 °C, $P_{CO2} = 10^{-3.5}$ atm, $P_{O2} = 10^{-0.66}$ atm. All Uranium Species are U(VI), the Dominant Uranium Species Over the Entire pH Range.

	Percent (%) of Total Uranium											
pH	UO_2^{2+} MINTEQA2	UO_2^{2+} PHREEQC	$UO_2(CO_3)_2^{-2}$ MINTEQA2	$UO_2(CO_3)_2^{2-}$ PHREEQC	$UO_2(CO_3)_3^{4-}$ MINTEQA2	$UO_2(CO_3)_3^{4-}$ PHREEQC	$(UO_2)_2CO_3(OH)_3^-$ MINTEQA2	$(UO_2)_2CO_3(OH)_3^-$ PHREEQC	UO_2OH^+ MINTEQA2	UO_2OH^+ PHREEQC	$UO_2(OH)_2(aq)$ MINTEQA2	$UO_2(OH)_2(aq)$ PHREEQC
4.00	90.56	91.13	0.00	0.00	0.00	0.00	0.00	0.00	2.71	2.61	0.01	0.01
4.25	88.67	89.30	0.00	0.00	0.00	0.00	0.00	0.00	4.72	4.55	0.02	0.02
4.50	85.46	86.18	0.00	0.00	0.00	0.00	0.00	0.00	8.09	7.81	0.06	0.06
4.75	80.22	81.08	0.00	0.00	0.00	0.00	0.00	0.00	13.51	13.06	0.18	0.18
5.00	72.15	73.16	0.00	0.00	0.00	0.00	0.00	0.00	21.60	20.96	0.52	0.51
5.25	60.78	61.93	0.00	0.00	0.00	0.00	0.01	0.01	32.36	31.55	1.38	1.36
5.50	46.67	47.84	0.00	0.00	0.00	0.00	0.07	0.07	44.19	43.34	3.36	3.32
5.75	31.72	32.73	0.01	0.01	0.00	0.00	0.62	0.57	53.41	52.74	7.22	7.19
6.00	18.33	19.06	0.08	0.08	0.00	0.00	3.65	3.46	54.89	54.60	13.20	13.24
6.25	8.44	8.85	0.37	0.37	0.00	0.00	13.78	13.25	44.96	45.08	19.23	19.44
6.50	2.99	3.16	1.32	1.31	0.00	0.00	30.76	30.01	28.32	28.61	21.54	21.94
6.75	0.86	0.92	3.80	3.80	0.02	0.03	45.72	45.01	14.56	14.78	19.70	20.15
7.00	0.22	0.23	9.66	9.67	0.19	0.22	52.50	51.88	6.58	6.69	15.83	16.22
7.25	0.05	0.05	21.95	21.95	1.39	1.61	48.18	47.55	2.66	2.70	11.37	11.65
7.50	0.01	0.01	41.31	40.94	8.26	9.49	30.34	29.38	0.89	0.90	6.77	6.86
7.75	0.00	0.00	50.14	47.86	31.72	35.13	7.95	7.14	0.19	0.19	2.60	2.54
8.00	0.00	0.00	32.11	29.08	64.31	67.70	0.58	0.47	0.02	0.02	0.53	0.49
8.25	0.00	0.00	13.52	11.83	85.84	87.60	0.02	0.01	0.00	0.00	0.07	0.06
8.50	0.00	0.00	4.72	4.05	95.17	95.85	0.00	0.00	0.00	0.00	0.01	0.01
8.75	0.00	0.00	1.53	1.29	98.45	98.69	0.00	0.00	0.00	0.00	0.00	0.00
9.00	0.00	0.00	0.48	0.39	99.52	99.60	0.00	0.00	0.00	0.00	0.00	0.00
9.25	0.00	0.00	0.15	0.11	99.85	99.88	0.00	0.00	0.00	0.00	0.00	0.00
9.50	0.00	0.00	0.04	0.03	99.96	99.95	0.00	0.00	0.00	0.00	0.00	0.00
9.75	0.00	0.00	0.01	0.01	99.99	99.91	0.00	0.00	0.00	0.00	0.00	0.00
10.00	0.00	0.00	0.00	0.00	100.00	99.30	0.00	0.00	0.00	0.00	0.00	0.00

4 SUMMARY AND CONCLUSIONS

Comparisons for a variety of geochemical problems (solubility, gas chemistry, redox, sorption) show that MINTEQA2, Version 4.02 produces results that are consistent with those produced by other methods such as hand calculations, experiments, and other computer codes. For the simplest systems, the MINTEQA2, Version 4.02 results agree well with those calculated by other methods. For more complicated systems, however, there are differences in how the problems are formulated in the different codes, especially activity coefficient corrections, that lead to differences in the results. Typically, when combined with slight differences in the thermodynamic databases used by the two codes, these differences have a relatively small effect, but some can lead to large variance between the calculational results produced by the two codes, particularly for highly-charged aqueous species.

Overall, the agreement of trends and results between MINTEQA2, Version 4.02 and the various calculational methods used in the model validation exercise indicates that the code is correctly and consistently applying mass action and mass balance constraints to calculating geochemical equilibrium. As has been demonstrated for the geochemical systems, considered in this validation exercise, the observed differences in calculational results are generally small, but in some cases they can be larger than might otherwise be expected. For the purposes of this validation, the differences in results do not seem to represent errors in the formulation of MINTEQA2, Version 4.02, but instead reflect different approaches to geochemical equilibrium calculations used by different calculation methods (hand calculations and computer code simulations), differences in computational approach, and minor differences in thermodynamic databases that are beyond the scope of this model validation to address. These types of variations are often observed among geochemical speciation codes (Morrey, et al., 1986; Emren, et al., 1999), however, and indicate that the code user should pay careful attention to interpreting the results of any geochemical speciation calculations.

5 REFERENCES

Allison, J.D., D.S. Brown, and K.J. Novo-Gradac. "MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems. Version 3.0 User's Manual." EPA/600/3–91/021. Athens, Georgia: U.S. Environmental Protection Agency. 1991.

Blount, C.W. "Barite solubilities and thermodynamic quantities up to 300 °C and 1400 bars." *American Mineralogist* Vol. 272: pp. 438–475. 1977.

CNWRA. "Technical Operating Procedure (TOP)-18: Development and Control of Scientific and Engineering Software, Revision 8, Change 0 (October 5, 2001)." San Antonio, Texas: Center for Nuclear Waste Regulatory Analyses. 2001.

Dzombak, D.A. and Morel, F.M.M. "Surface Complexation Modeling: Hydrous Ferric Oxide." New York: John Wiley and Sons. 1990.

Emren, A.T., R. Arthur, P.D. Glynn, and J. McMurry. "The modeler's influence on calculated solubilities for performance assessments at the Äspö hard-rock laboratory. *Scientific Basis for Nuclear Waste Management—XXII*. D. Wronkiewicz and J.H. Lee, eds. Symposium Proceedings. Pittsburgh, Pennsylvania: Material Research Society. pp. 559–566. 1999.

Grenthe, I., J. Fuger, R. Konings, R.J. Lemire, A.B. Muller, C. Nguyen-Trung, and H. Wanner. "Chemical Thermodynamics Series, Volume 1: Chemical Thermodynamics of Uranium." Nuclear Energy Agency, Organization for Economic Cooperation and Development. New York: Elsevier. 1992.

Langmuir, D. *Aqueous Environmental Geochemistry*. Englewood Cliffs, New Jersey: Prentice-Hall, Inc. 1997.

Lemire, R.J., J. Fuger, H. Nitsche, P. Potter, M.H. Rand, J. Rydberg, K. Spahiu, J.C. Sullivan, W.J. Ullman, P. Vitorge, and H. Wanner. "Chemical Thermodynamics Series, Volume 4: Chemical Thermodynamics of Neptunium and Plutonium." Nuclear Energy Agency, Organization for Economic Cooperation and Development. New York: Elsevier. 2001.

Morrey, J.R., C.T. Kincaid, C.J. Hostetler, S.B. Yabusaki, and L.W. Vail. "Geohydrochemical Models for Solute Migration. Volume 3: Evaluation of Selected Computer Codes." EPRI–EA–3417. Palo Alto, California: Electric Power Research Institute. 1986.

Parkhurst, D.L. and C.A.J. Appelo. "User's Guide to PHREEQC (Version 2)—A Computer Program for Speciation, Batch-reaction, One-dimensional Transport, And Inverse Geochemical Calculations." Water-Resources Investigations Report 99–4259. Denver, Colorado: U.S. Geological Survey. 1999.

Rard, J.A., M.H. Rand, G. Anderegg, and H. Wanner. "Chemical Thermodynamics Series, Volume 3: Chemical Thermodynamics of Technetium." Nuclear Energy Agency, Organization for Economic Cooperation and Development. New York: Elsevier. 1999.

Richardson, S.M. and H.Y. McSween, Jr. *Geochemistry: Pathways and Processes.* Englewood Cliffs, New Jersey: Prentice-Hall, Inc. 1989.

Silva, R.J., G. Bidoglio, M.H. R, P.B. Robouch, H. Wanner, and I. Puigdomenich. "Chemical Thermodynamics Series, Volume 2: Chemical Thermodynamics of Americium." Nuclear Energy Agency, Organization for Economic Cooperation and Development. New York: Elsevier. 1995.

Stumm, W. and J.J. Morgan. *Aquatic Chemistry: Chemical Equilibria and Rates in Natural Waters.* 3rd Edition. New York, New York: Wiley-Interscience. 1996.

Turner, D.R. "Mechanistic Approaches to Radionuclide Sorption Modeling." CNWRA 93-019. San Antonio, Texas: Center for Nuclear Waste Regulatory Analyses. 1993.

Turner, D.R. "Software Validation Test Plan for MINTEQA2, Version 4.02." San Antonio, Texas: Center for Nuclear Waste Regulatory Analyses. 2001.

Turner, D.R., T. Griffin, and T.B. Dietrich. Radionuclide sorption modeling using the MINTEQA2 speciation code. *Scientific Basis for Nuclear Waste Management—XVI.* C. Interrante and R. Pabalan, eds. Symposium Proceedings. Pittsburgh, Pennsylvania: Material Research Society. pp. 783–789. 1993.

U.S. Environmental Protection Agency. "MINTEQA2/PRODEFA2, A Geochemical Assessment Model for Environmental Systems: User Manual Supplement for Version 4.0." Athens, Georgia:

U.S. Environmental Protection Agency, National Exposure Research Laboratory, Ecosystems Research Division. 1999a.

U.S. Environmental Protection Agency. "Diffuse-Layer Sorption Reactions for use in MINTEQA2 for HWIR Metals and Metalloids." Athens, Georgia: U.S. Environmental Protection Agency, National Exposure Research Laboratory, Ecosystems Research Division. 1999b.

APPENDIX A

MINTEQA2, Version 4.02 and PHREEQC, Version 2.4.2 input files

Validation Test Case 1.

The installation of MINTEQA2, Version 4.02 software was checked as part of bringing the code into configuration management under Technical Operating Procedure (TOP)-018 for the CNWRA. The results indicate that the code was installed correctly on the PC platform and produced the correct results for 12 different example problems provided with MINTEQA2, Version 4.02. The results are documented in the configuration management package for MINTEQA2, Version 4.02 stored in the CNWRA QA Records Room.

Validation Test Case 2a—Aqueous Speciation. PHREEQC, Version 2.4.2 input file for seawater speciation check (from Parkhurst and Appelo, 1999)

```
TITLE Modified Example 1.--Add uranium and speciate seawater.
SOLUTION 1  SEAWATER FROM NORDSTROM ET AL.  (1979)
        units   ppm
        pH      8.22
        pe      8.451
        density 1.000
        temp    25.0
        redox   O(0)/O(-2)
        Ca              412.3
        Mg              1291.8
        Na              10768.0
        K               399.1
        Fe              0.002
        Mn              0.0002
        Si              4.28
        Cl              19353.0
        C(4)            141.682 as HCO3
        S(6)            2712.0
        N(5)            0.29    gfw   62.0
        N(-3)           0.03    as    NH4
        U               3.3     ppb
        O(0)            1.0     O2(g) -0.66
END
```

Validation Test Case 2b—Aqueous Speciation. MINTEQA2, Version 4.02 input file for seawater speciation check (from Parkhurst and Appelo, 1999)

```
Add U and speciate seawater (Nordstrom et al., 1979)
Modified PHREEQC 2.4.2 Ex.  1 (Parkhurst and Appelo, 1999)
25.00 PPM    0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -8.22 y                    /H+1
    150  4.123E+02   -1.99 y                    /Ca+2
    460  1.292E+03   -1.27 y                    /Mg+2
    500  1.077E+04   -0.33 y                    /Na+1
    410  3.991E+02   -1.99 y                    /K+1
    280  0.000E+00  -11.75                      /Fe+2
    281  2.000E-03   -7.45 y                    /Fe+3
    470  2.000E-04   -8.44 y                    /Mn+2
    471  0.000E+00  -11.74 y                    /Mn+3
    770  4.280E+00   -3.82 y                    /H4SiO4
    180  1.935E+04   -0.26 y                    /Cl-1
    140  1.393E+02   -2.63 y                    /CO3-2
    732  2.712E+03   -1.55 y                    /SO4-2
    492  2.900E-01   -5.33 y                    /NO3-1
    490  3.000E-02   -5.78 y                    /NH4+1
    891  0.000E+00  -12.43 y                    /U+4
    892  0.000E+00  -12.43 y                    /UO2+1
    893  3.300E-03   -7.86 y                    /UO2+2
      1  0.000E+00   -7.00 y                    /E-1

  3   6
3300021   -82.4318   571.6600                  /O2 (g)
2802810    13.0320   -42.7000                  /fe+2/fe+3
4704710    25.3500  -107.8000                  /mn+2/mn+3
8918930     9.0400  -143.8600                  /u+4/uo2+2
8928930     1.4800    -6.1300                  /uo2+/uo2+2
    330     8.2200     0.0000                  /H+1
  6   1
      1     0.0000     0.0000                  /E-1
```

Validation Test Case 3a—Mineral Solubility. MINTEQA2, Version 4.02 input file. Barite Solubility in pure H2O comparison to Richardson and McSween (1989) (Worked Problem 3-7):

```
Validation for Barite (BaSO4) solubility
Solubility comparison to Richardson & McSween (1989)
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 0 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    100  0.000E+00   -7.00 y                    /Ba+2
    732  0.000E+00   -7.00 y                    /SO4-2

  3   1
6010000     9.9800   -23.0000                   /barite(baso4)
  6   2
3307320     1.9900    22.0000                   /hso4-
1003300   -13.3570    60.8100                   /baoh+
```

Note: HSO_4^- and $BaOH^+$ are aqueous species included in the MINTEQA2, Version 4.02 database, but excluded in this calculation for direct comparison to the results of Richardson and McSween (1989). Also, although the Davies equation is the MINTEQA2, Version 4.02 default, a flag is set to use extended Debye-Hückel approach to calculate activity coefficients as a more direct comparison to Richardson and McSween (1989).

Validation Test Case 3b—Mineral Solubility. MINTEQA2, Version 4.02 input file. Barite Solubility in 0.2 m NaCl comparison to Richardson and McSween (1989) (Worked Problem 3-8):

```
Validation for Barite solubility in 0.2m NaCl solution
Solubility comparison to Richardson & McSween (1989)
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 0 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    100  0.000E+00   -7.00 y                    /Ba+2
    732  0.000E+00   -7.00 y                    /SO4-2
    500  2.000E-01   -0.70                      /Na+1
    180  2.000E-01   -0.70 y                    /Cl-1

  3   1
6010000     9.9800   -23.0000                   /barite(baso4)
  6   3
3307320     1.9900    22.0000                   /hso4-
1003300   -13.3570    60.8100                   /baoh+
5007320     0.7300     1.0000                   /naso4-
```

Note: HSO_4^-, $BaOH^+$, and $NaOH^+$ are aqueous species included in the MINTEQA2, Version 4.02 database, but excluded in this calculation for direct comparison to the results of Richardson and McSween (1989). Also, although the Davies equation is the MINTEQA2, Version 4.02 default, a flag is set to use extended Debye-Huckel approach to calculate activity coefficients as a more direct comparison to Richardson and McSween (1989).

Validation Test Case 4a—Gas Chemistry. MINTEQA2, Version 4.02 input file. Aqueous speciation of seawater in equilibrium with calcite at 25 °C, and open to atmosphere (fixed P_{CO_2} = 3.55 × 10^{-4} atm) (Stumm and Morgan, 1996; Example 7.8).

```
Calcite-Seawater with PCO2 = 1E-3.5 atm
Example 7.8; Stumm&Morgan(1996); Seawater from Table 15.2
25.00 PPM    0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    500  1.077E+04   -0.33 y                    /Na+1
    460  1.290E+03   -1.28 y                    /Mg+2
    410  3.990E+02   -1.99 y                    /K+1
    800  7.900E+00   -4.04 y                    /Sr+2
    180  1.935E+04   -0.26 y                    /Cl-1
    732  2.712E+03   -1.55 y                    /SO4-2
    270  1.300E+00   -4.16 y                    /F-1
    130  6.730E+01   -3.07 y                    /Br-1
    150  0.000E+00  -11.60                      /Ca+2
    140  0.000E+00   -7.00 y                    /CO3-2

  3   2
5015001     8.4800     8.0000                  /calcite
3301403    21.5968    -4.0600                  /CO2 (g)
```

Note: The data from Table 15.2 in Stumm and Morgan (1996) are reported in g/L. These values are converted to molality by MINTEQA2, assuming that the density of water ~1 g/mL. This assumption is slightly inaccurate for seawater, where the density of water is slightly > 1g/mL.

Validation Test Case 4b—Gas Chemistry. MINTEQA2, Version 4.02 input file. Aqueous speciation of fresh water in equilibrium with calcite at 25 °C, and variable P_{CO_2} (Langmuir, 1997; Table 6.3).

```
Calcite solubility in fresh water, 25C with PCO2=1e-3.5 bar
Langumuir (1997), Calculated values in Table 6.3
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 4 3
ccsol.csv        140     150 3301400 3301401
0   0   0
    150  0.000E+00  -11.60 y                    /Ca+2
    140  0.000E+00   -7.00 y                    /CO3-2
    330  0.000E+00   -7.00 y                    /H+1

  3   2
5015001     8.4800     8.0000                  /calcite
3301403    21.6530    -4.0600                  /CO2 (g)

Calcite solubilty in fresh water, 25C with PCO2=1e-2.5 bar
Langumuir (1997), Calculated values in Table 6.3
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 4 3
ccsol.csv        140     150 3301400 3301401
0   0   0
    150  0.000E+00  -11.60 y                    /Ca+2
    140  0.000E+00   -7.00 y                    /CO3-2
    330  0.000E+00   -7.00 y                    /H+1

  3   2
5015001     8.4800     8.0000                  /calcite
3301403    20.6530    -4.0600                  /CO2 (g)

Calcite solubilty in fresh water, 25C with PCO2=1e-1.5 bar
Langumuir (1997), Calculated values in Table 6.3
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 4 3
ccsol.csv        140     150 3301400 3301401
```

```
0    0    0
     150   0.000E+00   -11.60 y                    /Ca+2
     140   0.000E+00    -7.00 y                    /CO3-2
     330   0.000E+00    -7.00 y                    /H+1

   3    2
5015001      8.4800      8.0000                   /calcite
3301403     19.6530     -4.0600                   /CO2 (g)
```

Note: The partial pressures in Langmuir (1997) are presented in terms of bars, while MINTEQA2 reads pressures in terms of atmospheres. For conversion, 1 bar = 0.98692 atm.

Validation Test Case 5—Surface Complexation (Double Diffuse-Layer Model). PHREEQC, Version 2.4.2 input files for Zn-sorption on ferrihydrite, using the parameters of Dzombak and Morel (1990). This input file is from Example 8 in the PHREEQC, Version 2.4.2 installation test problems (Parkhurst and Appelo, 1999).

```
TITLE Example 8.--Sorption of zinc on hydrous
                  iron oxides.
SURFACE_SPECIES
        Hfo_sOH  + H+ = Hfo_sOH2+
        log_k  7.18

        Hfo_sOH = Hfo_sO- + H+
        log_k  -8.82

        Hfo_sOH + Zn+2 = Hfo_sOZn+ + H+
        log_k  0.66

        Hfo_wOH  + H+ = Hfo_wOH2+
        log_k  7.18

        Hfo_wOH = Hfo_wO- + H+
        log_k  -8.82

        Hfo_wOH + Zn+2 = Hfo_wOZn+ + H+
        log_k  -2.32
SURFACE 1
        Hfo_sOH         5e-6    600.    0.09
        Hfo_wOH         2e-4
SOLUTION 1
        -units  mmol/kgw
        pH      8.0
        Zn      0.0001
        Na      100.    charge
        N(5)    100.
SOLUTION 2
        -units  mmol/kgw
        pH      8.0
        Zn      0.1
        Na      100.    charge
        N(5)    100.
USE solution none
#
# Model definitions
#
PHASES
        Fix_H+
        H+ = H+
        log_k  0.0
END
#
#   Zn = 1e-7
#
SELECTED_OUTPUT
        -file ex8.sel
        -molalities     Zn+2    Hfo_wOZn+       Hfo_sOZn+
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.0   NaOH    10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.25  NaOH    10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.5   NaOH    10.0
END
USE solution 1
```

```
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -5.75  NaOH     10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -6.0   NaOH     10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -6.25  NaOH     10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -6.5   NaOH     10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -6.75  NaOH     10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -7.0   NaOH     10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -7.25  NaOH     10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -7.5   NaOH     10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -7.75  NaOH     10.0
END
USE solution 1
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -8.0   NaOH     10.0
END
#
#    Zn = 1e-4
#
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -5.0   NaOH     10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -5.25  NaOH     10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -5.5   NaOH     10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -5.75  NaOH     10.0
END
USE solution 2
```

```
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -6.0    NaOH     10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -6.25   NaOH     10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -6.5    NaOH     10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -6.75   NaOH     10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -7.0    NaOH     10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -7.25   NaOH     10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -7.5    NaOH     10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -7.75   NaOH     10.0
END
USE solution 2
USE surface 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -8.0    NaOH     10.0
END
```

Validation Test Case 5—Surface Complexation (Double Diffuse-Layer Model). MINTEQA2, Version 4.02 input file for Zn-sorption on ferrihydrite, using the parameters of Dzombak and Morel (1990). This input file is constructed to match Example 8 in the PHREEQC, Version 2.4.2 installation test problems (Parkhurst and Appelo, 1999).

```
Zn-HFO sorption, Double Diffuse-Layer Model
Example 8; PHREEQC, Version 2.4.2 installation test files
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 1 3 3
13 H+1                    ACTIVITY   mol/L
1 330   1.000
  5.00   0.25
valid65.123       950 8119500 8129500
4   1   7
9.000E-02  600.00 0.000 0.000 81
    330  0.000E+00   -5.00 y                    /H+1
    500  1.000E-01   -1.00 y                    /Na+1
    492  1.000E-01   -1.00 y                    /NO3-1
    950  1.000E-07   -7.00 y                    /Zn+2
    813  1.000E-07   -7.00 y                    /ADS1PSIo
    811  5.000E-06   -5.30 y                    /ADS1TYP1
    812  2.000E-04   -3.70 y                    /ADS1TYP2

  2   4
9503300     -8.9600     55.8100                 /znoh+
```

```
9503301   -16.9000     0.0000                  /zn(oh)2 (aq)
9503302   -28.4000     0.0000                  /zn(oh)3-
9503303   -41.2000     0.0000                  /zn(oh)4-2
  3   1
    330     5.0000     0.0000                  /H+1
  6   3
    813     0.0000     0.0000                  /ADS1PSIo
9504921     0.4000    -4.6000                  /znno3+
9504922    -0.3000     0.0000                  /zn(no3)2 (aq)

  2   6
8113300 Hfo_sOH2+       0.0000    7.1800   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8113301 Hfo_sO-         0.0000   -8.8200   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8119500 Hf0_sOZn+       0.0000    0.6600   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 4   1.000 811   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8123300 Hfo_wOH2+       0.0000    7.1800   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 812   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8123301 Hf0_wO-         0.0000   -8.8200   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 812  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8129500 Hfo_wOZn+       0.0000   -2.3200   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 4   1.000 812   1.000 950  -1.000 330   1.000 813   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0

Zn-HFO sorption, Double Diffuse-Layer Model
Example 8; PHREEQC, Version 2.4.2 installation test files
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 1 3 3
13 H+1                    ACTIVITY   mol/L
1 330   1.000
  5.00   0.25
valid65.123       950 8119500 8129500
4   1   7
9.000E-02  600.00 0.000 0.000 81
    330  0.000E+00   -5.00 y                  /H+1
    500  1.000E-01   -1.00 y                  /Na+1
    492  1.000E-01   -1.00 y                  /NO3-1
    950  1.000E-04   -4.00 y                  /Zn+2
    813  1.000E-07   -7.00 y                  /ADS1PSIo
    811  5.000E-06   -5.30 y                  /ADS1TYP1
    812  2.000E-04   -3.70 y                  /ADS1TYP2

  2   4
9503300    -8.9600    55.8100                  /znoh+
9503301   -16.9000     0.0000                  /zn(oh)2 (aq)
9503302   -28.4000     0.0000                  /zn(oh)3-
9503303   -41.2000     0.0000                  /zn(oh)4-2
  3   1
    330     5.0000     0.0000                  /H+1
  6   3
    813     0.0000     0.0000                  /ADS1PSIo
9504921     0.4000    -4.6000                  /znno3+
9504922    -0.3000     0.0000                  /zn(no3)2 (aq)

  2   6
8113300 Hfo_sOH2+       0.0000    7.1800   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
  0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8113301 Hfo_sO-         0.0000   -8.8200   0.000   0.000 0.00 0.00 0.00   0.0000
 0.00 3   1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
```

```
  0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8119500 Hf0_sOZn+          0.0000    0.6600    0.000    0.000 0.00 0.00 0.00    0.0000
 0.00 4    1.000 811    1.000 950   -1.000 330    1.000 813    0.000    0    0.000    0
  0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8123300 Hfo_wOH2+          0.0000    7.1800    0.000    0.000 0.00 0.00 0.00    0.0000
 0.00 3    1.000 812    1.000 330    1.000 813    0.000    0    0.000    0    0.000    0
  0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8123301 Hf0_wO-            0.0000   -8.8200    0.000    0.000 0.00 0.00 0.00    0.0000
 0.00 3    1.000 812   -1.000 330   -1.000 813    0.000    0    0.000    0    0.000    0
  0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
8129500 Hfo_wOZn+          0.0000   -2.3200    0.000    0.000 0.00 0.00 0.00    0.0000
 0.00 4    1.000 812    1.000 950   -1.000 330    1.000 813    0.000    0    0.000    0
  0.000    0    0.000    0    0.000    0    0.000    0    0.000    0    0.000    0
0  0.000    0    0.000    0    0.000    0
```

Validation Test Case 6a—Redox Equilibria. MINTEQA2, Version 4.02 input file for redox Example 8.2 in Stumm and Morgan (1996). The simulation is intended to determine electron activity (pe).

```
Calculate electron activity (pe) for 10-5 M Fe(III) and 10-3 M Fe(
Example 8.2 from Stumm and Morgan (1996)
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    281  1.000E-05   -5.00 y                    /Fe+3
    280  1.000E-03   -3.00 y                    /Fe+2
      1  0.000E+00   -7.00                       /E-1

  3   1
2802810    13.0000   -42.7000                   /fe+2/fe+3
  6  10
      1     0.0000     0.0000                   /E-1
2813300    -2.1870    41.8100                   /feoh+2
2813301    -4.5940     0.0000                   /fe(oh)2+
2813302   -12.5600   103.8000                   /fe(oh)3 (aq)
2813303   -21.5880     0.0000                   /fe(oh)4-
2813304    -2.8540    57.6200                   /fe2(oh)2+4
2813305    -6.2880    65.2400                   /fe3(oh)4+5
2803300    -9.3970    55.8100                   /feoh+
2803301   -28.9910   126.4300                   /fe(oh)3-
2803302   -20.4940   119.6200                   /fe(oh)2 (aq)


Calculate electron activity (pe) for pH=7.5, pO2=0.22 atm
Example 8.2 from Stumm and Morgan (1996)
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.50 y                    /H+1
      1  0.000E+00   -7.00                      /E-1
    500  1.000E-03   -3.00                      /Na+1
    180  1.000E-03   -3.00                      /Cl-1

  3   2
3300021   -82.4222   571.6600                   /O2 (g)
    330     7.5000     0.0000                   /H+1
  6   1
      1     0.0000     0.0000                   /E-1


Calculate electron activity (pe) for 10-5 M Mn(II) and pyrolusite
Example 8.2 from Stumm and Morgan (1996)
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -8.00 y                    /H+1
      1  0.000E+00   -7.00                      /E-1
    470  1.000E-05   -5.00                      /Mn+2

  3   2
2047000   -40.8400   272.0000                   /pyrolusite
    330     8.0000     0.0000                   /H+1
  6   1
      1     0.0000     0.0000                   /E-1
```

Validation Test Case 6b—Redox Equilibria. MINTEQA2, Version 4.02 input file for redox Example 8.4 in Stumm and Morgan (1996). The simulation is intended to determine HS^-–SO_4^{2-} speciation as a function of electron activity (pe).

```
Redox equilbria test; 10-4 M SO4-2/HS- system
Based on Example 8.4 from Stumm and Morgan (1996)
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 1 2 2
48 E-1                    ACTIVITY   mol/L
1   1   1.000
 -9.00   0.10
valid66.123      730      732
0   0   0
    330  0.000E+00  -10.00 y                    /H+1
    730  1.000E-04   -4.00 y                    /HS-1
    732  0.000E+00  -16.00 y                    /SO4-2
      1  0.000E+00   -7.00 y                    /E-1

  3   3
7307320    34.0200   -60.1400                   /hs-/so4-2
    330    10.0000     0.0000                   /H+1
      1     7.0000     0.0000                   /E-1
  6   3
3307300     7.0200   -22.0000                   /h2s (aq)
3307320     1.9900    22.0000                   /hso4-
3307301   -17.3000    49.4000                   /s-2
```

Validation Test Case 7a—Temperature Effects. PHREEQC, Version 2.4.2 input file for temperature effects on saturation of gypsum and anhydrite. Pure water with 1.0 moles of anhydrite and 1.0 moles of gypsum. This input file is from Example 2 in the PHREEQC, Version 2.4.2 installation test problems (Parkhurst and Appelo, 1999).

```
TITLE Example 2.--Temperature dependence of solubility
                  of gypsum and anhydrite
SOLUTION 1 Pure water
        pH      7.0
        temp    25.0
EQUILIBRIUM_PHASES 1
        Gypsum          0.0     1.0
        Anhydrite       0.0     1.0
REACTION_TEMPERATURE 1
        25.0 75.0 in 51 steps
SELECTED_OUTPUT
        -file   ex2.sel
        -si     anhydrite  gypsum
END
```

Validation Test Case 7a—Temperature Effects. MINTEQA2, Version 4.02 input file for temperature effects on saturation of gypsum and anhydrite. Pure water with 1.0 moles of anhydrite and 1.0 moles of gypsum, based on Example 2 in the PHREEQC, Version 2.4.2 installation test problems (Parkhurst and Appelo, 1999). Thermodynamic data modified to match PHREEQC, Version 2.4.2.

```
Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  4   2
6015000     4.3600     7.1550   1.000E+00      /anhydrite
6015001     4.5800     0.4560   1.000E+00      /gypsum


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
30.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  4   2
6015000     4.3600     7.1550   1.000E+00      /anhydrite
6015001     4.5800     0.4560   1.000E+00      /gypsum


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
35.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  4   2
6015000     4.3600     7.1550   1.000E+00      /anhydrite
6015001     4.5800     0.4560   1.000E+00      /gypsum
```

```
Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
40.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  4   2
6015000     4.3600     7.1550   1.000E+00      /anhydrite
6015001     4.5800     0.4560   1.000E+00      /gypsum


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
45.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  4   2
6015000     4.3600     7.1550   1.000E+00      /anhydrite
6015001     4.5800     0.4560   1.000E+00      /gypsum


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
50.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  4   2
6015000     4.3600     7.1550   1.000E+00      /anhydrite
6015001     4.5800     0.4560   1.000E+00      /gypsum


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
55.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  4   2
6015000     4.3600     7.1550   1.000E+00      /anhydrite
6015001     4.5800     0.4560   1.000E+00      /gypsum


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
60.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  4   2
6015000     4.3600     7.1550   1.000E+00      /anhydrite
6015001     4.5800     0.4560   1.000E+00      /gypsum


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
65.00 MOLAL  0.000  0.00000E+00
```

```
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  4   2
6015000     4.3600     7.1550   1.000E+00      /anhydrite
6015001     4.5800     0.4560   1.000E+00      /gypsum


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
70.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  4   2
6015000     4.3600     7.1550   1.000E+00      /anhydrite
6015001     4.5800     0.4560   1.000E+00      /gypsum


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
75.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  4   2
6015000     4.3600     7.1550   1.000E+00      /anhydrite
6015001     4.5800     0.4560   1.000E+00      /gypsum
```

Validation Test Case 7b—Temperature Effects. MINTEQA2, Version 4.02 input file for temperature effects on saturation of gypsum and anhydrite. Pure water assuming infinite gypsum (25° to 55 °C) and infinite anhydrite (60° to 75 °C). Thermodynamic data modified to match PHREEQC, Version 2.4.2.

```
Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  3   1
6015001     4.5800     0.4560                   /gypsum


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
30.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  3   1
6015001     4.5800     0.4560                   /gypsum


Anhydrite/Gypsum solubility as function of temperature
```

```
Test Example 2 for PHREEQC, Version 2.4.2
35.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  3   1
6015001     4.5800     0.4560                   /gypsum


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
40.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  3   1
6015001     4.5800     0.4560                   /gypsum


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
45.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  3   1
6015001     4.5800     0.4560                   /gypsum


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
50.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  3   1
6015001     4.5800     0.4560                   /gypsum


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
55.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2

  3   1
6015001     4.5800     0.4560                   /gypsum


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
60.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                    /H+1
    150  0.000E+00   -7.00 y                    /Ca+2
    732  0.000E+00   -7.00 y                    /SO4-2
```

```
  3   1
6015000     4.3600     7.1550                    /anhydrite


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
65.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                   /H+1
    150  0.000E+00   -7.00 y                   /Ca+2
    732  0.000E+00   -7.00 y                   /SO4-2

  3   1
6015000     4.3600     7.1550                    /anhydrite


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
70.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                   /H+1
    150  0.000E+00   -7.00 y                   /Ca+2
    732  0.000E+00   -7.00 y                   /SO4-2

  3   1
6015000     4.3600     7.1550                    /anhydrite


Anhydrite/Gypsum solubility as function of temperature
Test Example 2 for PHREEQC, Version 2.4.2
75.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 0 0 0
0   0   0
    330  0.000E+00   -7.00 y                   /H+1
    150  0.000E+00   -7.00 y                   /Ca+2
    732  0.000E+00   -7.00 y                   /SO4-2

  3   1
6015000     4.3600     7.1550                    /anhydrite
```

Validation Test Case 8a—Np and U speciation. PHREEQC, Version 2.4.2 input files for neptunium and uranium speciation as a function of pH. T = 25 °C, $P_{CO2} = 10^{-3.5}$ atm, $P_{O2} = 10^{-0.66}$ atm, (a) Neptunium speciation with $Np_{total} = 10^{-7}$ m. Neptunium oxidation states change with pH and both Np(V)-species and Np(VI)-species are written to the output file np_phrq2.123; (b) Uranium speciation with $U_{total} = 10^{-7}$ m. Uranium speciation is dominated by U(VI) over entire pH range, an only U(VI) species are written to u_phrq2.123.

```
TITLE Test Example: Speciation of Np(V), 1.0e-7 molal NpO2+, \
PCO2=1e-3.5; Speciation over pH range

SOLUTION 1
        -units   mol/kgw
        pH       7.00
        redox    O(0)/O(-2)
        temp     25.0
        Na                0.100      charge
        N(+5)             0.100      as NO3-
        Np(+5)            0.0000001  as NpO2+
        O(0)              1.0        O2(g) -0.66

PHASES 1
     Fix_H+
     H+ = H+
     log_k = 0.0
END

SELECTED_OUTPUT
-file np_phrq2.123
-molalities  NpO2+ NpO2OH NpO2(OH)2- NpO2CO3- NpO2(CO3)2-3 NpO2(CO3)3-5 \
NpO2(CO3)2(OH)-4 NpO2(CO3)2-2 NpO2(CO3)3-4

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -4.00  NaOH  10.0
        CO2(g)   -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -4.25  NaOH  10.0
        CO2(g)   -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -4.50  NaOH  10.0
        CO2(g)   -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -4.75  NaOH  10.0
        CO2(g)   -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.00  NaOH  10.0
        CO2(g)   -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.25  NaOH  10.0
        CO2(g)   -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -5.50  NaOH  10.0
```

```
        CO2(g)    -3.5    1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -5.75   NaOH   10.0
        CO2(g)    -3.5    1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -6.00   NaOH   10.0
        CO2(g)    -3.5    1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -6.25   NaOH   10.0
        CO2(g)    -3.5    1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -6.50   NaOH   10.0
        CO2(g)    -3.5    1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -6.75   NaOH   10.0
        CO2(g)    -3.5    1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -7.00   NaOH   10.0
        CO2(g)    -3.5    1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -7.25   NaOH   10.0
        CO2(g)    -3.5    1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -7.50   NaOH   10.0
        CO2(g)    -3.5    1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -7.75   NaOH   10.0
        CO2(g)    -3.5    1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -8.00   NaOH   10.0
        CO2(g)    -3.5    1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -8.25   NaOH   10.0
        CO2(g)    -3.5    1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -8.50   NaOH   10.0
        CO2(g)    -3.5    1.0
```

```
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -8.75  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -9.00  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -9.25  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -9.50  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -9.75  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -10.00  NaOH  10.0
        CO2(g)    -3.5   1.0
END


TITLE Test Example: Speciation of U(VI), 1.0e-7 molal UO2+2, \
PCO2=1e-3.5; Speciation over pH range

SOLUTION 1
        -units    mol/kgw
        pH        7.00
        redox     O(0)/O(-2)
        temp      25.0
        Na                0.100       charge
        N(+5)             0.100       as NO3
        U(+6)             0.0000001   as UO2
        O(0)              1.0        O2(g) -0.66

SOLUTION_SPECIES
UO2+2 + 2H2O = UO2(OH)2 + 2H+
        log_k     -11.7000
        delta_h    18.095    kcal
        -gamma      3.0      0
PHASES 1
     Fix_H+
     H+ = H+
     log_k = 0.0
END
SELECTED_OUTPUT
-file u_phrq2.123
-molalities  UO2+2 UO2NO3+ UO2CO3 UO2(CO3)2-2 UO2(CO3)3-4 \
(UO2)2CO3(OH)3- UO2OH+ UO2(OH)2 UO2(OH)3- UO2(OH)4-2 \
(UO2)2(OH)2+2  (UO2)3(OH)5+

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -4.00  NaOH  10.0
        CO2(g)    -3.5   1.0
END
```

```
Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -4.25  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -4.50  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -4.75  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -5.00  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -5.25  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -5.50  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -5.75  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -6.00  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -6.25  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -6.50  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -6.75  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -7.00  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
```

```
EQUILIBRIUM_PHASES 1
        Fix_H+    -7.25  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -7.50  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -7.75  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -8.00  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -8.25  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -8.50  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -8.75  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -9.00  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -9.25  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -9.50  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+    -9.75  NaOH  10.0
        CO2(g)    -3.5   1.0
END

Use Solution 1
EQUILIBRIUM_PHASES 1
        Fix_H+   -10.00  NaOH  10.0
        CO2(g)    -3.5   1.0
END
```

Validation Test Case 8b—Np and U speciation. MINTEQA2, Version 4.02 input files for neptunium and uranium speciation as a function of pH. T = 25 °C, $P_{CO2} = 10^{-3.5}$ atm, $P_{O2} = 10^{-0.66}$ atm, (a) Neptunium speciation with $Np_{total} = 10^{-7}$ m. Neptunium oxidation states change with pH and both Np(V)-species and Np(VI)-species are written to the output file np_mint2.123; (b) Uranium speciation with $U_{total} = 10^{-7}$ m. Uranium speciation is dominated by U(VI) over entire pH range, an only U(VI) species are written to u_mint2.123.

```
Np(V) speciation, Np = 1e-7 M, PCO2=1e-3.5 atm
Variable pH, T = 25C,  PO2=0.22 atm

25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 1 6 3
25 H+1                    ACTIVITY   mol/L
1 330   1.000
  4.00   0.25
np_mint2.123     552 5523300 5523301 5521400 5521401 5521402
0   0   0
    330  0.000E+00   -4.00 y                    /H+1
    552  1.000E-07   -7.00 y                    /NpO2+
    500  1.000E-01   -1.00 y                    /Na+1
    492  1.000E-01   -1.00 y                    /NO3-1
    140  0.000E+00   -7.00 y                    /CO3-2
      1  0.000E+00   -7.00                       /E-1
    551  0.000E+00   -7.00 y                    /Np+4
    553  0.000E+00   -7.00 y                    /NpO2+2

  3   5
3301403    21.6470    -4.0600                  /CO2 (g)
5525510   -10.2100   149.5000                  /npo2+1/np+4
5535510   -29.8000   266.9500                  /npo2+2/np+4
3300021   -82.4318   571.6600                  /O2 (g)
    330     4.0000     0.0000                  /H+1
  6   1
      1     0.0000     0.0000                  /E-1


Np(V) speciation, Np = 1e-7 M, PCO2=1e-3.5 atm
Variable pH, T = 25C,  PO2=0.22 atm

25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 1 3 3
25 H+1                    ACTIVITY   mol/L
1 330   1.000
  4.00   0.25
np_mint2.123 5521403 5531401 5531402
0   0   0
    330  0.000E+00   -4.00 y                    /H+1
    552  1.000E-07   -7.00 y                    /NpO2+
    500  1.000E-01   -1.00 y                    /Na+1
    492  1.000E-01   -1.00 y                    /NO3-1
    140  0.000E+00   -7.00 y                    /CO3-2
      1  0.000E+00   -7.00                       /E-1
    551  0.000E+00   -7.00 y                    /Np+4
    553  0.000E+00   -7.00 y                    /NpO2+2

  3   5
3301403    21.6470    -4.0600                  /CO2 (g)
5525510   -10.2100   149.5000                  /npo2+1/np+4
5535510   -29.8000   266.9500                  /npo2+2/np+4
3300021   -82.4318   571.6600                  /O2 (g)
    330     4.0000     0.0000                  /H+1
  6   1
      1     0.0000     0.0000                  /E-1


U(VI) speciation, U = 1e-7 M, PCO2=1e-3.5 atm
Variable pH, T = 25C, PO2=0.22 atm
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 1 6 3
25 H+1                    ACTIVITY   mol/L
```

```
1 330   1.000
  4.00   0.25
u_mint2.123      893 8934920 8931400 8931401 8931402 8931405
0   0   0
    330  0.000E+00   -4.00 y                    /H+1
    893  1.000E-07   -7.00 y                    /UO2+2
    500  1.000E-01   -1.00 y                    /Na+1
    492  1.000E-01   -1.00 y                    /NO3-1
    140  0.000E+00   -7.00 y                    /CO3-2
      1  0.000E+00   -7.00                      /E-1
    891  0.000E+00   -7.00 y                    /U+4
    892  0.000E+00   -7.00 y                    /UO2+1

  2   1
8933301   -11.7000    75.7100                  /uo2(oh)2(aq)
  3   5
3301403    21.6470    -4.0600                  /CO2 (g)
3300021   -82.4318   571.6600                  /O2 (g)
8918930     9.0400  -143.8600                  /u+4/uo2+2
8928930     1.4800    -6.1300                  /uo2+/uo2+2
    330     4.0000     0.0000                  /H+1
  6   1
      1     0.0000     0.0000                  /E-1


U(VI) speciation, U = 1e-7 M, PCO2=1e-3.5 atm
Variable pH, T = 25C,  PO2=0.22 atm
25.00 MOLAL  0.000  0.00000E+00
0 0 1 0 1 0 0 0 1 1 1 6 3
25 H+1                    ACTIVITY   mol/L
1 330   1.000
  4.00   0.25
u_mint2.123  8933300 8933301 8933302 8933303 8933305 8933307
0   0   0
    330  0.000E+00   -4.00 y                    /H+1
    893  1.000E-07   -7.00 y                    /UO2+2
    500  1.000E-01   -1.00 y                    /Na+1
    492  1.000E-01   -1.00 y                    /NO3-1
    140  0.000E+00   -7.00 y                    /CO3-2
      1  0.000E+00   -7.00                      /E-1
    891  0.000E+00   -7.00 y                    /U+4
    892  0.000E+00   -7.00 y                    /UO2+1

  2   1
8933301   -11.7000    75.7100                  /uo2(oh)2(aq)
  3   5
3301403    21.6470    -4.0600                  /CO2 (g)
3300021   -82.4318   571.6600                  /O2 (g)
8918930     9.0400  -143.8600                  /u+4/uo2+2
8928930     1.4800    -6.1300                  /uo2+/uo2+2
    330     4.0000     0.0000                  /H+1
  6   1
      1     0.0000     0.0000                  /E-1
```