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SOFTWARE RELEASE NOTICE

1. SRN Number: **GHGC-SRN-189**

2. Project Title: **RT** | Project No.**20-1402-871**

3. SRN Title: **PHREEQC, Version 1.6**

4. Originator/Requestor: **David Turner** | Date: **4/15/99**

5. Summary of Actions

- ■ Release of new software
- □ Release of modified software:
  - □ Enhancements made
  - □ Corrections made
- □ Change of access software
- ☒ Software Retirement 1/24/2003

6. Persons Authorized Access

Name	Read Only/Read-Write	Addition/Change/Delete
D.R. Turner	**RO**	**A**
J.W. Bradbury	**RO**	**A**
Others as Needed	**RO**	**A**

7. Element Manager Approval: **English Pearcy** Date: 4/16/99

8. Remarks: **Acquired software: Not to be modified.**

CNWRA Form TOP-6 (05/98)

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SOFTWARE SUMMARY FORM

01. Summary Date: **4//15/99**	02. Summary prepared by (Name and phone) **David R. Turner (210) 522-2139**	03. Summary Action: **NEW**
04. Software Date: **1/16/98**	05. Short Title: **PHREEQC -Geochemical speciation code**	
06. Software Title: **PHREEQC Version 1.6**		07. Internal Software ID: **NONE**

08. Software Type: ☐ Automated Data System ■ Computer Program ☐ Subroutine/Module	09. Processing Mode: ☐ Interactive ☐ Batch ■ Combination	10. Application Area a. General: ■ Scientific/Engineering ☐ Auxiliary Analyses ☐ Total System PA ☐ Subsystem PA ☐ Other b. Specific:
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:
PHREEQC is a computer program written in the C programming language that is designed to form a wide variety of aqueous geochemical calculations.

14. Computer Platform **PC**	15. Computer Operating System: **DOS/Windows**	16. Programming Language(s): **C**	17. Number of Source Program Statements: **N/A**
18. Computer Memory Requirements: **64 Kb**	19. Tape Drives: **N/A**	20. Disk Units: **N/A**	21. Graphics: **N/A**

22. Other Operational Requirements: **N/A**

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

25. Software Contact: **United States Geological Survey**
David L. Parkhurst Date: **1/16/98**

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

4/16/99 QA

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TO: Bruce Mabrito
FROM: David Turner
SUBJECT: Installation and Testing of PHREEQC, Version 1.6 Acquired Software
DATE: April 15, 1999

The geochemical code PHREEQC, Version 1.6 was obtained as a compressed file (**phrqc1-6.exe**) from the U.S. Geological Survey anonymous FTP site. The FTP address is:

brrcrftp.cr.usgs.gov

On this site, the DOS/PC version of PHREEQC is located in the **geochem/pc/phreeqc** subdirectory. The compressed file **phrqc1-6.exe** contains the executable file, the source code (in C programming language), test problem input, and an electronic copy of the user's manual. This file is attached (3.5" floppy disk). The code can also be ordered from:

U.S. Geological Survey
NWIS Program Office
437 National Center
Reston, VA 22092

The compressed file was expanded and PHREEQC, Version 1.6 was installed and has been tested in the DOS shell for Windows NT 4.0. No problems were encountered during installation.

The test problems provided with the PHREEQC, Version 1.6 distribution file were run to test proper installation. Hardcopies and electronic files of the following are attached:

Input Files (from USGS)
Output Files (CNWRA-generated)

The input files received from the USGS are also included as electronic files on the attached disk (**phrqc1-6.exe**).

The abstract from the PHREEQC User's Manual (Parkhurst, 1995) is included here as background:

Abstract

PHREEQC is a computer program written in the C programming language that is designed to perform a wide variety of aqueous geochemical calculations. PHREEQC is based on an ion-association aqueous model and has capabilities for (1) speciation and saturation-index calculations, (2) reaction-path and advective-transport calculations involving specified irreversible reactions, mixing of solutions, mineral and gas equilibria, surface-complexation reactions, and ion-exchange reactions, and (3) inverse modeling, which finds sets of mineral and gas mole transfers that account for composition differences between waters, within specified compositional uncertainties. PHREEQC is derived from the Fortran program PHREEQE, but it has been completely rewritten in C with the addition many new capabilities. New features include the capabilities to use redox couples to distribute redox elements among their valence states in speciation calculations; to model ion-exchange and surface-complexation reactions; to model reactions with a fixed-pressure, multicomponent gas phase (that is, a gas bubble); to calculate the mass of water in the aqueous phase during reaction and transport calculations; to keep track of the moles of minerals present in the solid phases and determine automatically the thermodynamically stable phase

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assemblage; to simulate advective transport in combination with PHREEQC's reaction-modeling capability; and to make inverse modeling calculations that allow for uncertainties in the analytical data. The user interface is improved through the use of a simplified approach to redox reactions, which includes explicit mole-balance equations for hydrogen and oxygen; the use of a revised input that is modular and completely free format; and the use of mineral names and standard chemical symbolism rather than index numbers. The use of C eliminates nearly all limitations on array sizes, including numbers of elements, aqueous species, solutions, phases, and lengths of character strings. A new equation solver that optimizes a set of equalities subject to both equality and inequality constraints is used to determine the thermodynamically stable set of phases in equilibrium with a solution. A more complete Newton-Raphson formulation, master-species switching, and scaling of the algebraic equations reduce the number of failures of the numerical method in PHREEQC relative to PHREEQE. This report presents the equations that are the basis for chemical equilibrium and inverse-modeling calculations in PHREEQC, describes the input for the program, and presents twelve examples that demonstrate most of the program's capabilities.

Reference:

Parkhurst, D.L. 1995. *User's Guide to PHREEQC - A Computer Program for Speciation, Reaction-Path, Advective-Transport, and Inverse Geochemical Calculations*. Water Resources Investigations Report 95-4227. Lakewood, CO: United States Geological Survey.

PHREEQC, Version 1.6
Example 1, Input/Output
CNWRA-generated
4/15/99

```
------------------
Reading data base.
------------------

       SOLUTION_MASTER_SPECIES
       SOLUTION_SPECIES
       PHASES
       EXCHANGE_MASTER_SPECIES
       EXCHANGE_SPECIES
       SURFACE_MASTER_SPECIES
       SURFACE_SPECIES
       END
------------------------------------
Reading input data for simulation 1.
------------------------------------

       TITLE Example 1.--Add uranium and speciate seawater.
       SOLUTION 1  SEAWATER FROM NORDSTROM ET AL. (1979)
              units   ppm
              pH      8.22
              pe      8.451
              density 1.023
              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  pe
              Si              4.28
              Cl              19353.0
              Alkalinity      141.682 as HCO3
              S(6)            2712.0
              N(5)            0.29    as NO3
              N(-3)           0.03    as NH4
              U               3.3     ppb     N(5)/N(-3)
              O(0)            1.0     O2(g)   -0.7
       SOLUTION_MASTER_SPECIES
              U       U+4     0.0     238.0290     238.0290
              U(4)    U+4     0.0     238.0290
              U(5)    UO2+    0.0     238.0290
              U(6)    UO2+2   0.0     238.0290
       SOLUTION_SPECIES
              U+4 = U+4
                      log_k           0.0
              U+4 + 4 H2O = U(OH)4 + 4 H+
                      log_k           -8.538
                      delta_h         24.760 kcal
              U+4 + 5 H2O = U(OH)5- + 5 H+
                      log_k           -13.147
                      delta_h         27.580 kcal
              U+4 + 2 H2O = UO2+ + 4 H+ + e-
                      log_k           -6.432
                      delta_h         31.130 kcal
              U+4 + 2 H2O = UO2+2 + 4 H+ + 2 e-
                      log_k           -9.217
                      delta_h         34.430 kcal
              UO2+2 + H2O = UO2OH+ + H+
                      log_k           -5.782
                      delta_h         11.015 kcal
              2UO2+2 + 2H2O = (UO2)2(OH)2+2 + 2H+
                      log_k           -5.626
                      delta_h         -36.04 kcal
              3UO2+2 + 5H2O = (UO2)3(OH)5+ + 5H+
                      log_k           -15.641
                      delta_h         -44.27 kcal
              UO2+2 + CO3-2 = UO2CO3
                      log_k           10.064
                      delta_h         0.84 kcal
              UO2+2 + 2CO3-2 = UO2(CO3)2-2
                      log_k           16.977
                      delta_h         3.48 kcal
              UO2+2 + 3CO3-2 = UO2(CO3)3-4
                      log_k           21.397
                      delta_h         -8.78 kcal
```

```
       PHASES
              Uraninite
              UO2 + 4 H+ = U+4 + 2 H2O
              log_k           -3.490
              delta_h         -18.630 kcal
       END
-----
TITLE
-----

 Example 1.--Add uranium and speciate seawater.

-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1. SEAWATER FROM NORDSTROM ET AL. (1979)

-----------------------------Solution composition------------------------------

       Elements            Molality        Moles

       Alkalinity        2.406e-03   2.406e-03
       Ca                1.066e-02   1.066e-02
       Cl                5.657e-01   5.657e-01
       Fe                3.711e-08   3.711e-08
       K                 1.058e-02   1.058e-02
       Mg                5.507e-02   5.507e-02
       Mn                3.773e-09   3.773e-09
       N(-3)             1.724e-06   1.724e-06
       N(5)              4.847e-06   4.847e-06
       Na                4.854e-01   4.854e-01
       O(0)              3.746e-04   3.746e-04  Equilibrium with O2(g)
       S(6)              2.926e-02   2.926e-02
       Si                7.382e-05   7.382e-05
       U                 1.437e-08   1.437e-08

----------------------------Description of solution----------------------------

                                pH  =   8.220
                                pe  =   8.451
                  Activity of water  =   0.981
                     Ionic strength  =   6.748e-01
                  Mass of water (kg)  =   1.000e+00
             Total carbon (mol/kg)  =   2.180e-03
                Total CO2 (mol/kg)  =   2.180e-03
                  Temperature (deg C)  =  25.000
           Electrical balance (eq)  =   7.936e-04
                        Iterations  =   7
                           Total H  = 1.110147e+02
                           Total O  = 5.563047e+01

----------------------------------Redox couples---------------------------------

       Redox couple                pe  Eh (volts)

       N(-3)/N(5)             4.6750       0.2766
       O(-2)/O(0)            12.3893       0.7329

---------------------------Distribution of species----------------------------

                                                    Log         Log         Log
       Species            Molality    Activity  Molality  Activity     Gamma

       OH-               2.674e-06   1.629e-06    -5.573    -5.788    -0.215
       H+                7.981e-09   6.026e-09    -8.098    -8.220    -0.122
       H2O               5.551e+01   9.806e-01    -0.009    -0.009     0.000
C(4)            2.180e-03
       HCO3-             1.514e-03   1.023e-03    -2.820    -2.990    -0.170
       MgHCO3+           2.195e-04   1.640e-04    -3.658    -3.785    -0.127
       NaHCO3            1.667e-04   1.948e-04    -3.778    -3.710     0.067
       MgCO3             8.913e-05   1.041e-04    -4.050    -3.982     0.067
       NaCO3-            6.718e-05   5.020e-05    -4.173    -4.299    -0.127
       CaHCO3+           4.597e-05   3.106e-05    -4.337    -4.508    -0.170
       CO3-2             3.821e-05   7.959e-06    -4.418    -5.099    -0.681
       CaCO3             2.725e-05   3.183e-05    -4.565    -4.497     0.067
```

	CO2	1.210e-05	1.413e-05	-4.917	-4.850	0.067
	UO2(CO3)3-4	1.255e-08	1.184e-10	-7.901	-9.927	-2.025
	UO2(CO3)2-2	1.814e-09	5.653e-10	-8.741	-9.248	-0.506
	MnCO3	2.696e-10	3.150e-10	-9.569	-9.502	0.067
	MnHCO3+	6.077e-11	4.541e-11	-10.216	-10.343	-0.127
	UO2CO3	7.429e-12	8.678e-12	-11.129	-11.062	0.067
	FeCO3	1.952e-20	2.281e-20	-19.709	-19.642	0.067
	FeHCO3+	1.635e-20	1.222e-20	-19.786	-19.913	-0.127
Ca		1.066e-02				
	Ca+2	9.504e-03	2.380e-03	-2.022	-2.623	-0.601
	CaSO4	1.083e-03	1.266e-03	-2.965	-2.898	0.067
	CaHCO3+	4.597e-05	3.106e-05	-4.337	-4.508	-0.170
	CaCO3	2.725e-05	3.183e-05	-4.565	-4.497	0.067
	CaOH+	8.604e-08	6.429e-08	-7.065	-7.192	-0.127
	CaHSO4+	5.979e-11	4.467e-11	-10.223	-10.350	-0.127
Cl		5.657e-01				
	Cl-	5.657e-01	3.528e-01	-0.247	-0.452	-0.205
	MnCl+	9.582e-10	7.160e-10	-9.019	-9.145	-0.127
	MnCl2	9.439e-11	1.103e-10	-10.025	-9.958	0.067
	MnCl3-	1.434e-11	1.071e-11	-10.844	-10.970	-0.127
	FeCl+2	9.557e-19	2.978e-19	-18.020	-18.526	-0.506
	FeCl2+	6.281e-19	4.693e-19	-18.202	-18.329	-0.127
	FeCl+	7.786e-20	5.817e-20	-19.109	-19.235	-0.127
	FeCl3	1.417e-20	1.656e-20	-19.849	-19.781	0.067
Fe(2)		6.909e-19				
	Fe+2	5.205e-19	1.195e-19	-18.284	-18.923	-0.639
	FeCl+	7.786e-20	5.817e-20	-19.109	-19.235	-0.127
	FeSO4	4.845e-20	5.660e-20	-19.315	-19.247	0.067
	FeCO3	1.952e-20	2.281e-20	-19.709	-19.642	0.067
	FeHCO3+	1.635e-20	1.222e-20	-19.786	-19.913	-0.127
	FeOH+	8.227e-21	6.147e-21	-20.085	-20.211	-0.127
	FeHSO4+	3.000e-27	2.242e-27	-26.523	-26.649	-0.127
Fe(3)		3.711e-08				
	Fe(OH)3	2.841e-08	3.318e-08	-7.547	-7.479	0.067
	Fe(OH)4-	6.591e-09	4.924e-09	-8.181	-8.308	-0.127
	Fe(OH)2+	2.118e-09	1.583e-09	-8.674	-8.801	-0.127
	FeOH+2	9.425e-14	2.937e-14	-13.026	-13.532	-0.506
	FeSO4+	1.093e-18	8.167e-19	-17.961	-18.088	-0.127
	FeCl+2	9.557e-19	2.978e-19	-18.020	-18.526	-0.506
	FeCl2+	6.281e-19	4.693e-19	-18.202	-18.329	-0.127
	Fe+3	3.509e-19	2.796e-20	-18.455	-19.554	-1.099
	Fe(SO4)2-	6.372e-20	4.761e-20	-19.196	-19.322	-0.127
	FeCl3	1.417e-20	1.656e-20	-19.849	-19.781	0.067
	Fe2(OH)2+4	2.462e-24	2.322e-26	-23.609	-25.634	-2.025
	FeHSO4+2	4.228e-26	1.318e-26	-25.374	-25.880	-0.506
	Fe3(OH)4+5	1.122e-29	7.679e-33	-28.950	-32.115	-3.165
H(0)		0.000e+00				
	H2	0.000e+00	0.000e+00	-44.436	-44.369	0.067
K		1.058e-02				
	K+	1.042e-02	6.495e-03	-1.982	-2.187	-0.205
	KSO4-	1.627e-04	1.216e-04	-3.789	-3.915	-0.127
	KOH	3.137e-09	3.665e-09	-8.503	-8.436	0.067
Mg		5.507e-02				
	Mg+2	4.742e-02	1.371e-02	-1.324	-1.863	-0.539
	MgSO4	7.330e-03	8.562e-03	-2.135	-2.067	0.067
	MgHCO3+	2.195e-04	1.640e-04	-3.658	-3.785	-0.127
	MgCO3	8.913e-05	1.041e-04	-4.050	-3.982	0.067
	MgOH+	1.084e-05	8.100e-06	-4.965	-5.092	-0.127
Mn(2)		3.773e-09				
	Mn+2	2.171e-09	4.982e-10	-8.663	-9.303	-0.639
	MnCl+	9.582e-10	7.160e-10	-9.019	-9.145	-0.127
	MnCO3	2.696e-10	3.150e-10	-9.569	-9.502	0.067
	MnSO4	2.021e-10	2.360e-10	-9.695	-9.627	0.067
	MnCl2	9.439e-11	1.103e-10	-10.025	-9.958	0.067
	MnHCO3+	6.077e-11	4.541e-11	-10.216	-10.343	-0.127
	MnCl3-	1.434e-11	1.071e-11	-10.844	-10.970	-0.127
	MnOH+	2.789e-12	2.084e-12	-11.555	-11.681	-0.127
	Mn(NO3)2	1.375e-20	1.606e-20	-19.862	-19.794	0.067
Mn(3)		5.993e-26				
	Mn+3	5.993e-26	4.349e-27	-25.222	-26.362	-1.139
N(-3)		1.724e-06				
	NH4+	1.609e-06	9.049e-07	-5.794	-6.043	-0.250
	NH3	7.326e-08	8.558e-08	-7.135	-7.068	0.067
	NH4SO4-	4.157e-08	3.106e-08	-7.381	-7.508	-0.127
N(5)		4.847e-06				
	NO3-	4.847e-06	2.846e-06	-5.315	-5.546	-0.231

	Mn(NO3)2	1.375e-20	1.606e-20	-19.862	-19.794	0.067
Na		4.854e-01				
	Na+	4.791e-01	3.387e-01	-0.320	-0.470	-0.151
	NaSO4-	6.053e-03	4.523e-03	-2.218	-2.345	-0.127
	NaHCO3	1.667e-04	1.948e-04	-3.778	-3.710	0.067
	NaCO3-	6.718e-05	5.020e-05	-4.173	-4.299	-0.127
	NaOH	3.117e-07	3.641e-07	-6.506	-6.439	0.067
O(0)		3.746e-04				
	O2	1.873e-04	2.188e-04	-3.727	-3.660	0.067
S(6)		2.926e-02				
	SO4-2	1.463e-02	2.664e-03	-1.835	-2.574	-0.740
	MgSO4	7.330e-03	8.562e-03	-2.135	-2.067	0.067
	NaSO4-	6.053e-03	4.523e-03	-2.218	-2.345	-0.127
	CaSO4	1.083e-03	1.266e-03	-2.965	-2.898	0.067
	KSO4-	1.627e-04	1.216e-04	-3.789	-3.915	-0.127
	NH4SO4-	4.157e-08	3.106e-08	-7.381	-7.508	-0.127
	HSO4-	2.089e-09	1.561e-09	-8.680	-8.807	-0.127
	MnSO4	2.021e-10	2.360e-10	-9.695	-9.627	0.067
	CaHSO4+	5.979e-11	4.467e-11	-10.223	-10.350	-0.127
	FeSO4+	1.093e-18	8.167e-19	-17.961	-18.088	-0.127
	Fe(SO4)2-	6.372e-20	4.761e-20	-19.196	-19.322	-0.127
	FeSO4	4.845e-20	5.660e-20	-19.315	-19.247	0.067
	FeHSO4+2	4.228e-26	1.318e-26	-25.374	-25.880	-0.506
	FeHSO4+	3.000e-27	2.242e-27	-26.523	-26.649	-0.127
Si		7.382e-05				
	H4SiO4	7.110e-05	8.306e-05	-4.148	-4.081	0.067
	H3SiO4-	2.720e-06	2.032e-06	-5.565	-5.692	-0.127
	H2SiO4-2	7.362e-11	2.294e-11	-10.133	-10.639	-0.506
U(4)		1.034e-21				
	U(OH)5-	1.034e-21	7.726e-22	-20.985	-21.112	-0.127
	U(OH)4	1.652e-25	1.930e-25	-24.782	-24.715	0.067
	U+4	0.000e+00	0.000e+00	-46.997	-49.022	-2.025
U(5)		1.622e-18				
	UO2+	1.622e-18	1.212e-18	-17.790	-17.916	-0.127
U(6)		1.437e-08				
	UO2(CO3)3-4	1.255e-08	1.184e-10	-7.901	-9.927	-2.025
	UO2(CO3)2-2	1.814e-09	5.653e-10	-8.741	-9.248	-0.506
	UO2CO3	7.429e-12	8.678e-12	-11.129	-11.062	0.067
	UO2OH+	3.385e-14	2.530e-14	-13.470	-13.597	-0.127
	UO2+2	3.019e-16	9.409e-17	-15.520	-16.026	-0.506
	(UO2)2(OH)2+2	1.780e-21	5.547e-22	-20.750	-21.256	-0.506
	(UO2)3(OH)5+	2.908e-23	2.173e-23	-22.536	-22.663	-0.127

----------Saturation indices----------

Phase	SI	log IAP	log KT	
Anhydrite	-0.84	-5.20	-4.36	CaSO4
Aragonite	0.61	-7.72	-8.34	CaCO3
Calcite	0.76	-7.72	-8.48	CaCO3
Chalcedony	-0.51	-4.06	-3.55	SiO2
Chrysotile	3.36	35.56	32.20	Mg3Si2O5(OH)4
CO2(g)	-3.38	-21.53	-18.15	CO2
Dolomite	2.41	-14.68	-17.09	CaMg(CO3)2
Fe(OH)3(a)	0.19	-3.42	-3.61	Fe(OH)3
Goethite	6.09	-3.41	-9.50	FeOOH
Gypsum	-0.63	-5.21	-4.58	CaSO4:2H2O
H2(g)	-41.22	1.82	43.04	H2
Hausmannite	1.57	19.56	17.99	Mn3O4
Hematite	14.20	-6.81	-21.01	Fe2O3
Jarosite-K	-7.52	-42.23	-34.71	KFe3(SO4)2(OH)6
Manganite	2.39	6.21	3.82	MnOOH
Melanterite	-19.35	-21.56	-2.21	FeSO4:7H2O
NH3(g)	-8.84	2.18	11.01	NH3
O2(g)	-0.70	-3.66	-2.96	O2
Pyrochroite	-8.08	7.12	15.20	Mn(OH)2
Pyrolusite	6.96	5.30	-1.66	MnO2
Quartz	-0.08	-4.06	-3.98	SiO2
Rhodochrosite	-3.27	-14.40	-11.13	MnCO3
Sepiolite	1.16	16.92	15.76	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-1.74	16.92	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-13.13	-24.02	-10.89	FeCO3
SiO2(a)	-1.35	-4.06	-2.71	SiO2
Talc	6.04	27.44	21.40	Mg3Si4O10(OH)2
Uraninite	-12.67	4.39	17.06	UO2

PHREEQC, Version 1.6
Example 1, Output
From User's Manual (Parkhurst, 1995)

Table 4. Output for example 1

```
------------------
Reading data base.
------------------
        SOLUTION_SPECIES
        SOLUTION_MASTER_SPECIES
        PHASES
        EXCHANGE_MASTER_SPECIES
        EXCHANGE_SPECIES
        SURFACE_MASTER_SPECIES
        SURFACE_SPECIES
        END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------
        TITLE Example 1.--Add uranium and speciate seawater.
        SOLUTION 1  SEAWATER FROM NORDSTROM ET AL. (1979)
                units   ppm
                pH      8.22
                pe      8.451
                density 1.023
                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  pe
                Si              4.28
                Cl              19353.0
                Alkalinity      141.682 as HCO3
                S(6)            2712.0
                N(5)            0.29    as NO3
                N(-3)           0.03    as NH4
                U               3.3     ppb     N(5)/N(-3)
                O(0)            1.0     O2(g)   -0.7
        SOLUTION_MASTER_SPECIES
                U       U+4     0.0     238.0290        238.0290
                U(4)    U+4     0.0     238.0290
                U(5)    UO2+    0.0     238.0290
                U(6)    UO2+2   0.0     238.0290
        SOLUTION_SPECIES
                U+4 = U+4
                        log_k           0.0
                U+4 + 4 H2O = U(OH)4 + 4 H+
                        log_k           -8.538
                        delta_h         24.760 kcal
                U+4 + 5 H2O = U(OH)5- + 5 H+
                        log_k           -13.147
                        delta_h         27.580 kcal
                U+4 + 2 H2O = UO2+ + 4 H+ + e-
                        log_k           -6.432
                        delta_h         31.130 kcal
                U+4 + 2 H2O = UO2+2 + 4 H+ + 2 e-
                        log_k           -9.217
                        delta_h         34.430 kcal
                UO2+2 + H2O = UO2OH+ + H+
                        log_k           -5.782
                        delta_h         11.015 kcal
                2UO2+2 + 2H2O = (UO2)2(OH)2+2 + 2H+
                        log_k           -5.626
                        delta_h         -36.04 kcal
                3UO2+2 + 5H2O = (UO2)3(OH)5+ + 5H+
                        log_k           -15.641
                        delta_h         -44.27 kcal
                UO2+2 + CO3-2 = UO2CO3
                        log_k           10.064
                        delta_h         0.84 kcal
                UO2+2 + 2CO3-2 = UO2(CO3)2-2
                        log_k           16.977
                        delta_h         3.48 kcal
                UO2+2 + 3CO3-2 = UO2(CO3)3-4
                        log_k           21.397
                        delta_h         -8.78 kcal
        PHASES
                Uraninite
                UO2 + 4 H+ = U+4 + 2 H2O
                log_k           -3.490
                delta_h         -18.630 kcal
        END
-----
TITLE
-----

 Example 1.--Add uranium and speciate seawater.

-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.     SEAWATER FROM NORDSTROM ET AL. (1979)

-----------------------------Solution composition------------------------------
        Elements            Molality        Moles

        Alkalinity        2.406e-03   2.406e-03
        Ca                1.066e-02   1.066e-02
        Cl                5.657e-01   5.657e-01
        Fe                3.711e-08   3.711e-08
        K                 1.058e-02   1.058e-02
        Mg                5.507e-02   5.507e-02
        Mn                3.773e-09   3.773e-09
        N(-3)             1.724e-06   1.724e-06
        N(5)              4.847e-06   4.847e-06
        Na                4.854e-01   4.854e-01
        O(0)              3.746e-04   3.746e-04  Equilibrium with O2(g)
        S(6)              2.926e-02   2.926e-02
        Si                7.382e-05   7.382e-05
        U                 1.437e-08   1.437e-08

----------------------------Description of solution----------------------------
                                pH  =   8.220
                                pe  =   8.451
                  Activity of water  =   0.981
                     Ionic strength  =   6.750e-01
                  Mass of water (kg)  =   1.000e+00
             Total carbon (mol/kg)    =   2.180e-03
                Total CO2 (mol/kg)    =   2.180e-03
                Temperature (deg C)   =  25.000
        Electrical balance (eq)       =   7.936e-04
                          Iterations  =   7
                             Total H  = 1.110147e+02
                             Total O  = 5.563047e+01

---------------------------------Redox couples---------------------------------
        Redox couple                pe  Eh (volts)

        N(-3)/N(5)             4.6750       0.2767
        O(-2)/O(0)            12.3893       0.7333

----------------------------Distribution of species----------------------------

                                                                  Log         Log         Log
        Species               Molality    Activity  Log Molality  Activity    Gamma
        OH-                 2.678e-06   1.629e-06    -5.572      -5.788      -0.216
        H+                  7.987e-09   6.026e-09    -8.098      -8.220      -0.122
        H2O                 5.551e+01   9.806e-01    -0.009      -0.009       0.000
C(4)            2.180e-03
        HCO3-               1.515e-03   1.023e-03    -2.820      -2.990      -0.171
        MgHCO3+             2.190e-04   1.635e-04    -3.659      -3.786      -0.127
        NaHCO3              1.665e-04   1.945e-04    -3.779      -3.711       0.068
        MgCO3               8.885e-05   1.038e-04    -4.051      -3.984       0.068
        NaCO3-              6.716e-05   5.013e-05    -4.173      -4.300      -0.127
        CaHCO3+             4.585e-05   3.095e-05    -4.339      -4.509      -0.171
        CO3-2               3.836e-05   7.959e-06    -4.416      -5.099      -0.683
```

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Table 4. Output for example 1--Continued

	CaCO3	2.715e-05	3.171e-05	-4.566	-4.499	0.068
	CO2	1.209e-05	1.413e-05	-4.917	-4.850	0.068
	UO2(CO3)3-4	1.256e-08	1.169e-10	-7.901	-9.932	-2.031
	UO2(CO3)2-2	1.798e-09	5.583e-10	-8.745	-9.253	-0.508
	MnCO3	2.691e-10	3.144e-10	-9.570	-9.503	0.068
	MnHCO3+	6.071e-11	4.532e-11	-10.217	-10.344	-0.127
	UO2CO3	7.337e-12	8.570e-12	-11.134	-11.067	0.068
	FeCO3	1.952e-20	2.280e-20	-19.710	-19.642	0.068
	FeHCO3+	1.636e-20	1.221e-20	-19.786	-19.913	-0.127
Ca	1.066e-02					
	Ca+2	9.510e-03	2.372e-03	-2.022	-2.625	-0.603
	CaSO4	1.078e-03	1.260e-03	-2.967	-2.900	0.068
	CaHCO3+	4.585e-05	3.095e-05	-4.339	-4.509	-0.171
	CaCO3	2.715e-05	3.171e-05	-4.566	-4.499	0.068
	CaOH+	8.582e-08	6.406e-08	-7.066	-7.193	-0.127
Cl	5.657e-01					
	Cl-	5.657e-01	3.523e-01	-0.247	-0.453	-0.206
	MnCl+	9.561e-10	7.137e-10	-9.020	-9.146	-0.127
	MnCl2	9.396e-11	1.098e-10	-10.027	-9.960	0.068
	MnCl3-	1.427e-11	1.065e-11	-10.846	-10.973	-0.127
	FeCl+2	9.576e-19	2.974e-19	-18.019	-18.527	-0.508
	FeCl2+	6.270e-19	4.680e-19	-18.203	-18.330	-0.127
	FeCl+	7.781e-20	5.809e-20	-19.109	-19.236	-0.127
	FeCl3	1.412e-20	1.649e-20	-19.850	-19.783	0.068
Fe(2)	6.926e-19					
	Fe+2	5.223e-19	1.194e-19	-18.282	-18.923	-0.641
	FeCl+	7.781e-20	5.809e-20	-19.109	-19.236	-0.127
	FeSO4	4.839e-20	5.652e-20	-19.315	-19.248	0.068
	FeCO3	1.952e-20	2.280e-20	-19.710	-19.642	0.068
	FeHCO3+	1.636e-20	1.221e-20	-19.786	-19.913	-0.127
	FeOH+	8.233e-21	6.146e-21	-20.084	-20.211	-0.127
	FeHSO4+	2.999e-27	2.239e-27	-26.523	-26.650	-0.127
Fe(3)	3.711e-08					
	Fe(OH)3	2.840e-08	3.317e-08	-7.547	-7.479	0.068
	Fe(OH)4-	6.595e-09	4.924e-09	-8.181	-8.308	-0.127
	Fe(OH)2+	2.120e-09	1.582e-09	-8.674	-8.801	-0.127
	FeOH+2	9.456e-14	2.937e-14	-13.024	-13.532	-0.508
	FeSO4+	1.093e-18	8.156e-19	-17.962	-18.089	-0.127
	FeCl+2	9.576e-19	2.974e-19	-18.019	-18.527	-0.508
	FeCl2+	6.270e-19	4.680e-19	-18.203	-18.330	-0.127
	Fe+3	3.529e-19	2.795e-20	-18.452	-19.554	-1.101
	Fe(SO4)2-	6.362e-20	4.749e-20	-19.196	-19.323	-0.127
	FeCl3	1.412e-20	1.649e-20	-19.850	-19.783	0.068
	Fe2(OH)2+4	2.495e-24	2.321e-26	-23.603	-25.634	-2.031
	FeHSO4+2	4.238e-26	1.316e-26	-25.373	-25.881	-0.508
	Fe3(OH)4+5	1.146e-29	7.675e-33	-28.941	-32.115	-3.174
H(0)	0.000e+00					
	H2	0.000e+00	0.000e+00	-44.436	-44.369	0.068
K	1.058e-02					
	K+	1.041e-02	6.486e-03	-1.982	-2.188	-0.206
	KSO4-	1.637e-04	1.222e-04	-3.786	-3.913	-0.127
	KOH	3.133e-09	3.660e-09	-8.504	-8.437	0.068
Mg	5.507e-02					
	Mg+2	4.745e-02	1.367e-02	-1.324	-1.864	-0.541
	MgSO4	7.299e-03	8.526e-03	-2.137	-2.069	0.068
	MgHCO3+	2.190e-04	1.635e-04	-3.659	-3.786	-0.127
	MgCO3	8.885e-05	1.038e-04	-4.051	-3.984	0.068
	MgOH+	1.082e-05	8.074e-06	-4.966	-5.093	-0.127
Mn(2)	3.773e-09					
	Mn+2	2.174e-09	4.973e-10	-8.663	-9.303	-0.641
	MnCl+	9.561e-10	7.137e-10	-9.020	-9.146	-0.127
	MnCO3	2.691e-10	3.144e-10	-9.570	-9.503	0.068
	MnSO4	2.015e-10	2.353e-10	-9.696	-9.628	0.068
	MnCl2	9.396e-11	1.098e-10	-10.027	-9.960	0.068
	MnHCO3+	6.071e-11	4.532e-11	-10.217	-10.344	-0.127
	MnCl3-	1.427e-11	1.065e-11	-10.846	-10.973	-0.127
	MnOH+	2.786e-12	2.080e-12	-11.555	-11.682	-0.127
	Mn(NO3)2	1.369e-20	1.599e-20	-19.864	-19.796	0.068
Mn(3)	6.029e-26					
	Mn+3	6.029e-26	4.341e-27	-25.220	-26.362	-1.143
N(-3)	1.724e-06					
	NH4+	1.610e-06	9.042e-07	-5.793	-6.044	-0.251
	NH3	7.191e-08	8.400e-08	-7.143	-7.076	0.068
	NH4SO4-	4.153e-08	3.100e-08	-7.382	-7.509	-0.127
N(5)	4.847e-06					
	NO3-	4.847e-06	2.842e-06	-5.315	-5.546	-0.232
	Mn(NO3)2	1.369e-20	1.599e-20	-19.864	-19.796	0.068
Na	4.854e-01					
	Na+	4.791e-01	3.383e-01	-0.320	-0.471	-0.151
	NaSO4-	6.045e-03	4.512e-03	-2.219	-2.346	-0.127
	NaHCO3	1.665e-04	1.945e-04	-3.779	-3.711	0.068
	NaCO3-	6.716e-05	5.013e-05	-4.173	-4.300	-0.127
	NaOH	3.114e-07	3.637e-07	-6.507	-6.439	0.068
O(0)	3.746e-04					
	O2	1.873e-04	2.188e-04	-3.728	-3.660	0.068
S(6)	2.926e-02					
	SO4-2	1.467e-02	2.661e-03	-1.834	-2.575	-0.741
	MgSO4	7.299e-03	8.526e-03	-2.137	-2.069	0.068
	NaSO4-	6.045e-03	4.512e-03	-2.219	-2.346	-0.127
	CaSO4	1.078e-03	1.260e-03	-2.967	-2.900	0.068
	KSO4-	1.637e-04	1.222e-04	-3.786	-3.913	-0.127
	NH4SO4-	4.153e-08	3.100e-08	-7.382	-7.509	-0.127
	HSO4-	2.089e-09	1.559e-09	-8.680	-8.807	-0.127
	MnSO4	2.015e-10	2.353e-10	-9.696	-9.628	0.068
	FeSO4+	1.093e-18	8.156e-19	-17.962	-18.089	-0.127
	Fe(SO4)2-	6.362e-20	4.749e-20	-19.196	-19.323	-0.127
	FeSO4	4.839e-20	5.652e-20	-19.315	-19.248	0.068
	FeHSO4+2	4.238e-26	1.316e-26	-25.373	-25.881	-0.508
	FeHSO4+	2.999e-27	2.239e-27	-26.523	-26.650	-0.127
Si	7.382e-05					
	H4SiO4	7.110e-05	8.306e-05	-4.148	-4.081	0.068
	H3SiO4-	2.723e-06	2.032e-06	-5.565	-5.692	-0.127
	H2SiO4-2	7.388e-11	2.294e-11	-10.131	-10.639	-0.508
U(4)	1.022e-21					
	U(OH)5-	1.022e-21	7.631e-22	-20.990	-21.117	-0.127
	U(OH)4	1.632e-25	1.906e-25	-24.787	-24.720	0.068
	U+4	0.000e+00	0.000e+00	-46.996	-49.028	-2.031
U(5)	1.604e-18					
	UO2+	1.604e-18	1.197e-18	-17.795	-17.922	-0.127
U(6)	1.437e-08					
	UO2(CO3)3-4	1.256e-08	1.169e-10	-7.901	-9.932	-2.031
	UO2(CO3)2-2	1.798e-09	5.583e-10	-8.745	-9.253	-0.508
	UO2CO3	7.337e-12	8.570e-12	-11.134	-11.067	0.068
	UO2OH+	3.347e-14	2.498e-14	-13.475	-13.602	-0.127
	UO2+2	2.992e-16	9.293e-17	-15.524	-16.032	-0.508
	(UO2)2(OH)2+2	1.742e-21	5.411e-22	-20.759	-21.267	-0.508
	(UO2)3(OH)5+	2.804e-23	2.093e-23	-22.552	-22.679	-0.127

Saturation indices

Phase	SI	log IAP	log KT	
Anhydrite	-0.84	-5.20	-4.36	CaSO4
Aragonite	0.61	-7.72	-8.34	CaCO3
Calcite	0.76	-7.72	-8.48	CaCO3
Chalcedony	-0.51	-4.06	-3.55	SiO2
Chrysotile	3.36	35.56	32.20	Mg3Si2O5(OH)4
CO2(g)	-3.38	-21.53	-18.15	CO2
Dolomite	2.40	-14.69	-17.09	CaMg(CO3)2
Fe(OH)3(a)	0.19	-3.42	-3.61	Fe(OH)3
Goethite	6.09	-3.41	-9.50	FeOOH
Gypsum	-0.64	-5.22	-4.58	CaSO4:2H2O
H2(g)	-41.22	1.82	43.04	H2
Hausmannite	1.56	19.55	17.99	Mn3O4
Hematite	14.20	-6.81	-21.01	Fe2O3
Jarosite-K	-7.52	-42.23	-34.71	KFe3(SO4)2(OH)6
Manganite	2.39	6.21	3.82	MnOOH
Melanterite	-19.35	-21.56	-2.21	FeSO4:7H2O
NH3(g)	-8.85	2.18	11.02	NH3
O2(g)	-0.70	-3.66	-2.96	O2
Pyrochroite	-8.08	7.12	15.20	Mn(OH)2
Pyrolusite	6.96	5.30	-1.66	MnO2
Quartz	-0.08	-4.06	-3.98	SiO2
Rhodochrosite	-3.27	-14.40	-11.13	MnCO3
Sepiolite	1.15	16.91	15.76	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-1.75	16.91	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-13.13	-24.02	-10.89	FeCO3
SiO2(a)	-1.35	-4.06	-2.71	SiO2
Talc	6.04	27.44	21.40	Mg3Si4O10(OH)2
Uraninite	-12.67	4.39	17.06	UO2

PHREEQ, Version 1.6
Example 11
Selected Output
CNWRA-Generated
4/15/99

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Beginning of inverse modeling calculations.

Solution 1:

pH	6.200e+00	+	1.242e-02	=	6.212e+00
Al	0.000e+00	+	0.000e+00	=	0.000e+00
Alkalinity	3.280e-04	+	5.500e-06	=	3.335e-04
C(-4)	0.000e+00	+	0.000e+00	=	0.000e+00
C(4)	7.825e-04	+	0.000e+00	=	7.825e-04
Ca	7.800e-05	+	-3.900e-06	=	7.410e-05
Cl	1.400e-05	+	0.000e+00	=	1.400e-05
H(0)	0.000e+00	+	0.000e+00	=	0.000e+00
K	2.800e-05	+	-7.000e-07	=	2.730e-05
Mg	2.900e-05	+	0.000e+00	=	2.900e-05
Na	1.340e-04	+	0.000e+00	=	1.340e-04
O(0)	0.000e+00	+	0.000e+00	=	0.000e+00
S(-2)	0.000e+00	+	0.000e+00	=	0.000e+00
S(6)	1.000e-05	+	0.000e+00	=	1.000e-05
Si	2.730e-04	+	0.000e+00	=	2.730e-04

Solution 2:

pH	6.800e+00	+	-3.398e-03	=	6.797e+00
Al	0.000e+00	+	0.000e+00	=	0.000e+00
Alkalinity	8.951e-04	+	-1.796e-06	=	8.933e-04
C(-4)	0.000e+00	+	0.000e+00	=	0.000e+00
C(4)	1.199e-03	+	0.000e+00	=	1.199e-03
Ca	2.600e-04	+	6.501e-06	=	2.665e-04
Cl	3.000e-05	+	0.000e+00	=	3.000e-05
H(0)	0.000e+00	+	0.000e+00	=	0.000e+00
K	4.000e-05	+	1.000e-06	=	4.100e-05
Mg	7.101e-05	+	-8.979e-07	=	7.011e-05
Na	2.590e-04	+	0.000e+00	=	2.590e-04
O(0)	0.000e+00	+	0.000e+00	=	0.000e+00
S(-2)	0.000e+00	+	0.000e+00	=	0.000e+00
S(6)	2.500e-05	+	0.000e+00	=	2.500e-05
Si	4.100e-04	+	0.000e+00	=	4.100e-04

Solution fractions:

		Minimum	Maximum
Solution 1	1.000e+00	1.000e+00	1.000e+00
Solution 2	1.000e+00	1.000e+00	1.000e+00

Phase mole transfers:

		Minimum	Maximum	
Halite	1.600e-05	1.490e-05	1.710e-05	NaCl
Gypsum	1.500e-05	1.413e-05	1.588e-05	CaSO4:2H2O
Kaolinite	-3.316e-05	-5.518e-05	-1.140e-05	Al2Si2O5(OH)4
Ca-Montmorillon	-8.156e-05	-1.107e-04	-5.213e-05	Ca0.165Al2.33Si3.67O10(OH)2
CO2(g)	2.909e-04	2.346e-04	3.543e-04	CO2
Calcite	1.258e-04	1.028e-04	1.326e-04	CaCO3
Biotite	1.370e-05	1.317e-05	1.370e-05	KMg3AlSi3O10(OH)2
Plagioclase	1.758e-04	1.582e-04	1.935e-04	Na0.62Ca0.37Al1.38Si2.62O8

Redox mole transfers:

Sum of residuals: 5.573e+00
Maximum fractional error in element concentration: 5.000e-02

Model contains minimum number of phases.
==========

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Solution 1:

pH	6.200e+00	+	1.242e-02	=	6.212e+00
Al	0.000e+00	+	0.000e+00	=	0.000e+00
Alkalinity	3.280e-04	+	5.500e-06	=	3.335e-04
C(-4)	0.000e+00	+	0.000e+00	=	0.000e+00
C(4)	7.825e-04	+	0.000e+00	=	7.825e-04
Ca	7.800e-05	+	-3.900e-06	=	7.410e-05
Cl	1.400e-05	+	0.000e+00	=	1.400e-05
H(0)	0.000e+00	+	0.000e+00	=	0.000e+00
K	2.800e-05	+	-7.000e-07	=	2.730e-05
Mg	2.900e-05	+	0.000e+00	=	2.900e-05
Na	1.340e-04	+	0.000e+00	=	1.340e-04
O(0)	0.000e+00	+	0.000e+00	=	0.000e+00
S(-2)	0.000e+00	+	0.000e+00	=	0.000e+00
S(6)	1.000e-05	+	0.000e+00	=	1.000e-05
Si	2.730e-04	+	0.000e+00	=	2.730e-04

Solution 2:

pH	6.800e+00	+	-3.399e-03	=	6.797e+00
Al	0.000e+00	+	0.000e+00	=	0.000e+00
Alkalinity	8.951e-04	+	-1.796e-06	=	8.933e-04
C(-4)	0.000e+00	+	0.000e+00	=	0.000e+00
C(4)	1.199e-03	+	0.000e+00	=	1.199e-03
Ca	2.600e-04	+	6.501e-06	=	2.665e-04
Cl	3.000e-05	+	0.000e+00	=	3.000e-05
H(0)	0.000e+00	+	0.000e+00	=	0.000e+00
K	4.000e-05	+	1.000e-06	=	4.100e-05
Mg	7.101e-05	+	-8.980e-07	=	7.011e-05
Na	2.590e-04	+	0.000e+00	=	2.590e-04
O(0)	0.000e+00	+	0.000e+00	=	0.000e+00
S(-2)	0.000e+00	+	0.000e+00	=	0.000e+00
S(6)	2.500e-05	+	0.000e+00	=	2.500e-05
Si	4.100e-04	+	0.000e+00	=	4.100e-04

Solution fractions:

		Minimum	Maximum
Solution 1	1.000e+00	1.000e+00	1.000e+00
Solution 2	1.000e+00	1.000e+00	1.000e+00

Phase mole transfers:

		Minimum	Maximum	
Halite	1.600e-05	1.490e-05	1.710e-05	NaCl
Gypsum	1.500e-05	1.413e-05	1.588e-05	CaSO4:2H2O
Kaolinite	-1.282e-04	-1.403e-04	-1.159e-04	Al2Si2O5(OH)4
CO2(g)	3.044e-04	2.474e-04	3.684e-04	CO2
Calcite	1.124e-04	8.874e-05	1.198e-04	CaCO3
Chalcedony	-1.093e-04	-1.483e-04	-6.986e-05	SiO2
Biotite	1.370e-05	1.317e-05	1.370e-05	KMg3AlSi3O10(OH)2
Plagioclase	1.758e-04	1.582e-04	1.935e-04	Na0.62Ca0.37Al1.38Si2.625O8

Redox mole transfers:

Sum of residuals: 5.573e+00
Maximum fractional error in element concentration: 5.000e-02

Model contains minimum number of phases.

==========

Summary of inverse modeling:

Number of models found: 2
Number of minimal models found: 2
Number of infeasible sets of phases saved: 20
Number of calls to cl1: 62

End of simulation.

Reading input data for simulation 2.

End of run.

Table 20. Selected output for example 11

PHREEQC, Version 1.6
Example 11, Selected Output
From User's Manual (Parkhurst, 1995)

```
-----------------------------------------
Beginning of inverse modeling calculations.
-----------------------------------------


Solution 1:
                pH      6.200e+00  +   1.242e-02  =   6.212e+00
                Al      0.000e+00  +   0.000e+00  =   0.000e+00
        Alkalinity      3.280e-04  +   5.500e-06  =   3.335e-04
             C(-4)      0.000e+00  +   0.000e+00  =   0.000e+00
              C(4)      7.825e-04  +   0.000e+00  =   7.825e-04
                Ca      7.800e-05  +  -3.900e-06  =   7.410e-05
                Cl      1.400e-05  +   0.000e+00  =   1.400e-05
              H(0)      0.000e+00  +   0.000e+00  =   0.000e+00
                 K      2.800e-05  +  -7.000e-07  =   2.730e-05
                Mg      2.900e-05  +   0.000e+00  =   2.900e-05
                Na      1.340e-04  +   0.000e+00  =   1.340e-04
              O(0)      0.000e+00  +   0.000e+00  =   0.000e+00
             S(-2)      0.000e+00  +   0.000e+00  =   0.000e+00
              S(6)      1.000e-05  +   0.000e+00  =   1.000e-05
                Si      2.730e-04  +   0.000e+00  =   2.730e-04

Solution 2:
                pH      6.800e+00  +  -3.399e-03  =   6.797e+00
                Al      0.000e+00  +   0.000e+00  =   0.000e+00
        Alkalinity      8.951e-04  +  -1.796e-06  =   8.933e-04
             C(-4)      0.000e+00  +   0.000e+00  =   0.000e+00
              C(4)      1.199e-03  +   0.000e+00  =   1.199e-03
                Ca      2.600e-04  +   6.501e-06  =   2.665e-04
                Cl      3.000e-05  +   0.000e+00  =   3.000e-05
              H(0)      0.000e+00  +   0.000e+00  =   0.000e+00
                 K      4.000e-05  +   1.000e-06  =   4.100e-05
                Mg      7.101e-05  +  -8.979e-07  =   7.011e-05
                Na      2.590e-04  +   0.000e+00  =   2.590e-04
              O(0)      0.000e+00  +   0.000e+00  =   0.000e+00
             S(-2)      0.000e+00  +   0.000e+00  =   0.000e+00
              S(6)      2.500e-05  +   0.000e+00  =   2.500e-05
                Si      4.100e-04  +   0.000e+00  =   4.100e-04

Solution fractions:                      Minimum         Maximum
   Solution    1      1.000e+00        1.000e+00       1.000e+00
   Solution    2      1.000e+00        1.000e+00       1.000e+00

Phase mole transfers:                    Minimum         Maximum
          Halite      1.600e-05        1.490e-05       1.710e-05   NaCl
          Gypsum      1.500e-05        1.413e-05       1.588e-05   CaSO4:2H2O
       Kaolinite     -3.316e-05       -5.518e-05      -1.140e-05   Al2Si2O5(OH)4
Ca-Montmorillon     -8.156e-05       -1.107e-04      -5.213e-05
Ca0.165Al2.33Si3.67O10(OH)2
         CO2(g)      2.909e-04        2.346e-04       3.543e-04   CO2
         Calcite      1.258e-04        1.028e-04       1.326e-04   CaCO3
         Biotite     1.370e-05        1.317e-05       1.370e-05   KMg3AlSi3O10(OH)2
    Plagioclase      1.758e-04        1.582e-04       1.935e-04
Na0.62Ca0.37Al1.38Si2.62SO8

Redox mole transfers:

Sum of residuals:                                        5.573e+00
Maximum fractional error in element concentration:       5.000e-02

Model contains minimum number of phases.
================================================================================
```

```
Solution 1:
                pH      6.200e+00  +   1.242e-02  =   6.212e+00
                Al      0.000e+00  +   0.000e+00  =   0.000e+00
        Alkalinity      3.280e-04  +   5.500e-06  =   3.335e-04
             C(-4)      0.000e+00  +   0.000e+00  =   0.000e+00
              C(4)      7.825e-04  +   0.000e+00  =   7.825e-04
                Ca      7.800e-05  +  -3.900e-06  =   7.410e-05
                Cl      1.400e-05  +   0.000e+00  =   1.400e-05
              H(0)      0.000e+00  +   0.000e+00  =   0.000e+00
                 K      2.800e-05  +  -7.000e-07  =   2.730e-05
                Mg      2.900e-05  +   0.000e+00  =   2.900e-05
                Na      1.340e-04  +   0.000e+00  =   1.340e-04
              O(0)      0.000e+00  +   0.000e+00  =   0.000e+00
             S(-2)      0.000e+00  +   0.000e+00  =   0.000e+00
              S(6)      1.000e-05  +   0.000e+00  =   1.000e-05
                Si      2.730e-04  +   0.000e+00  =   2.730e-04

Solution 2:
                pH      6.800e+00  +  -3.399e-03  =   6.797e+00
                Al      0.000e+00  +   0.000e+00  =   0.000e+00
        Alkalinity      8.951e-04  +  -1.796e-06  =   8.933e-04
             C(-4)      0.000e+00  +   0.000e+00  =   0.000e+00
              C(4)      1.199e-03  +   0.000e+00  =   1.199e-03
                Ca      2.600e-04  +   6.501e-06  =   2.665e-04
                Cl      3.000e-05  +   0.000e+00  =   3.000e-05
              H(0)      0.000e+00  +   0.000e+00  =   0.000e+00
                 K      4.000e-05  +   1.000e-06  =   4.100e-05
                Mg      7.101e-05  +  -8.980e-07  =   7.011e-05
                Na      2.590e-04  +   0.000e+00  =   2.590e-04
              O(0)      0.000e+00  +   0.000e+00  =   0.000e+00
             S(-2)      0.000e+00  +   0.000e+00  =   0.000e+00
              S(6)      2.500e-05  +   0.000e+00  =   2.500e-05
                Si      4.100e-04  +   0.000e+00  =   4.100e-04

Solution fractions:                      Minimum         Maximum
   Solution    1      1.000e+00        1.000e+00       1.000e+00
   Solution    2      1.000e+00        1.000e+00       1.000e+00

Phase mole transfers:                    Minimum         Maximum
          Halite      1.600e-05        1.490e-05       1.710e-05   NaCl
          Gypsum      1.500e-05        1.413e-05       1.588e-05   CaSO4:2H2O
       Kaolinite     -1.282e-04       -1.403e-04      -1.159e-04   Al2Si2O5(OH)4
         CO2(g)      3.044e-04        2.474e-04       3.684e-04   CO2
         Calcite      1.124e-04        8.874e-05       1.198e-04   CaCO3
       Chalcedony    -1.093e-04       -1.483e-04      -6.986e-05   SiO2
         Biotite     1.370e-05        1.317e-05       1.370e-05   KMg3AlSi3O10(OH)2
    Plagioclase      1.758e-04        1.582e-04       1.935e-04
Na0.62Ca0.37Al1.38Si2.62SO8

Redox mole transfers:

Sum of residuals:                                        5.573e+00
Maximum fractional error in element concentration:       5.000e-02

Model contains minimum number of phases.
================================================================================


Summary of inverse modeling:

                Number of models found: 2
                Number of minimal models found: 2
                Number of infeasible sets of phases saved: 20
                Number of calls to cl1: 62
------------------
End of simulation.
------------------
------------------------------------
Reading input data for simulation 2.
------------------------------------
-----------
End of run.
-----------
```

Information on Pages 14 through 27 contains User's Guide to PHREEQA-A Computer Program for Speciation, Reaction-Path, Advective-Transport, and Inverse Geochemical Calculations copyright information and is therefore not included in this file.