

1/27

SOFTWARE RELEASE NOTICE

1. SRN Number: <b>GHGC-SRN-189</b>		
2. Project Title: <b>RT</b>		Project No. <b>20-1402-871</b>
3. SRN Title: <b>PHREEQC, Version 1.6</b>		
4. Originator/Requestor: <b>David Turner</b>		Date: <b>4/15/99</b>
5. Summary of Actions		
<input checked="" type="checkbox"/> Release of new software <input type="checkbox"/> Release of modified software: <input type="checkbox"/> Enhancements made <input type="checkbox"/> Corrections made <input type="checkbox"/> Change of access software <input checked="" type="checkbox"/> Software Retirement <i>ECP 1/24/2003</i>		
6. Persons Authorized Access		
Name	Read Only/Read-Write	Addition/Change/Delete
<b>D.R. Turner</b>	<b>RO</b>	<b>A</b>
<b>J.W. Bradbury</b>	<b>RO</b>	<b>A</b>
<b>Others as Needed</b>	<b>RO</b>	<b>A</b>
7. Element Manager Approval: <b>English Pearcy</b> <i>ECP</i>		Date: <i>4/16/99</i>
8. Remarks: <b>Acquired software: Not to be modified.</b>		

2/27

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: <input type="checkbox"/> Automated Data System <input checked="" type="checkbox"/> Computer Program <input type="checkbox"/> Subroutine/Module		09. Processing Mode: <input type="checkbox"/> Interactive <input type="checkbox"/> Batch <input checked="" type="checkbox"/> Combination		10. Application Area a. General: <input checked="" type="checkbox"/> Scientific/Engineering <input type="checkbox"/> Auxiliary Analyses <input type="checkbox"/> Total System PA <input type="checkbox"/> Subsystem PA <input type="checkbox"/> 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: <input checked="" type="checkbox"/> Available <input type="checkbox"/> Limited <input type="checkbox"/> In-House ONLY			24. Documentation Availability: <input checked="" type="checkbox"/> Available <input type="checkbox"/> Preliminary <input type="checkbox"/> In-House ONLY		
25. Software Contact: United States Geological Survey David L. Parkhurst					Date: 1/16/98

*Bill M... 4/16/99 QA*

3/27

TO: Bruce Mabrito  
FROM: David Turner *DR*  
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

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.

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

SOLUTION\_MASTER\_SPECIES  
SOLUTION\_SPECIES  
PHASES  
EXCHANGE\_MASTER\_SPECIES  
EXCHANGE\_SPECIES  
SURFACE\_MASTER\_SPECIES  
SURFACE\_SPECIES  
END

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

-----  
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

6/27

PHASES

Uraninite  
UO2 + 4 H+ = U+4 + 2 H2O  
log\_k -3.490  
delta\_h -18.630 kcal

END

-----  
TITLE  
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Example 1.--Add uranium and speciate seawater.

-----  
Beginning of initial solution calculations.  
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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
S(6)	2.926e-02	2.926e-02
Si	7.382e-05	7.382e-05
U	1.437e-08	1.437e-08

Equilibrium with O2(g)

-----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-----

Species	Molality	Activity	Log Molality	Log Activity	Log 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

Na	Mn(NO3)2	1.375e-20	1.606e-20	-19.862	-19.794	0.067
	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



```

-----
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
    
```

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

```

-----
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-----
Species Molality Activity Log Molality Log Activity Log 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
    
```

LEP 6



Example 11

Selected Output  
CNWRA-Generated

4/15/99

-----  
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	Na0.62Ca0.37Al1.38Si2.625O8

Redox mole transfers:

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

Model contains minimum number of phases.

=====

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 c11: 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:
  Solution 1 1.000e+00 1.000e+00
  Solution 2 1.000e+00 1.000e+00

Phase mole transfers:
  Minimum Maximum
  Halite 1.600e-05 1.490e-05 NaCl
  Gypsum 1.500e-05 1.413e-05 CaSO4:2H2O
  Kaolinite -3.316e-05 -5.518e-05 Al2Si2O5(OH)4
  Ca-Montmorillon -8.156e-05 -1.107e-04
  Ca0.165Al2.33Si3.67O10(OH)2
  CO2(g) 2.909e-04 2.346e-04 CO2
  Calcite 1.258e-04 1.028e-04 CaCO3
  Biotite 1.370e-05 1.317e-05 KMg3AlSi3O10(OH)2
  Plagioclase 1.758e-04 1.582e-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.
-----
```

```
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:
  Solution 1 1.000e+00 1.000e+00
  Solution 2 1.000e+00 1.000e+00

Phase mole transfers:
  Minimum Maximum
  Halite 1.600e-05 1.490e-05 NaCl
  Gypsum 1.500e-05 1.413e-05 CaSO4:2H2O
  Kaolinite -1.282e-04 -1.403e-04 Al2Si2O5(OH)4
  CO2(g) 3.044e-04 2.474e-04 CO2
  Calcite 1.124e-04 8.874e-05 CaCO3
  Chalcedony -1.093e-04 -1.483e-04 SiO2
  Biotite 1.370e-05 1.317e-05 KMg3AlSi3O10(OH)2
  Plagioclase 1.758e-04 1.582e-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 c11: 62
-----
End of simulation.
-----
Reading input data for simulation 2.
-----
End of run.
-----
```

13/27

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.