

Input file: C:\Users\weissd2k\OneDrive - Imperial College London\3 Teaching\Lectures
 \60055 Contaminant Transport\PHREEQC\examples\ex1 U Speciation Calculation.pqi
 Output file: C:\Users\weissd2k\OneDrive - Imperial College London\3 Teaching\Lectures
 \60055 Contaminant Transport\PHREEQC\examples\ex1 U Speciation Calculation.pqi
 Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.7.3-15968\database
 \phreeqc.dat

 Reading data base.

SOLUTION_MASTER_SPECIES
 SOLUTION_SPECIES
 PHASES
 EXCHANGE_MASTER_SPECIES
 EXCHANGE_SPECIES
 SURFACE_MASTER_SPECIES
 SURFACE_SPECIES
 RATES
 END

 Reading input data for simulation 1.

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.7.3-15968\database
 \phreeqc.dat

TITLE Example 1.--Add uranium and speciate seawater.
 SOLUTION 1 SEAWATER FROM NORDSTROM AND OTHERS (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 gfw 62.0
 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

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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

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PHASES

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Uraninite
UO2 + 4 H+ = U+4 + 2 H2O
      log_k      -3.490
      delta_h    -18.630 kcal

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END

TITLE

Example 1.--Add uranium and speciate seawater.

Beginning of initial solution calculations.

Initial solution 1. SEAWATER FROM NORDSTROM AND OTHERS (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)	4.376e-04	4.376e-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
Specific Conductance (µS/cm, 25°C) = 52630
Density (g/cm³) = 1.02323
Volume (L) = 1.01282
Activity of water = 0.981
Ionic strength (mol/kgw) = 6.747e-01
Mass of water (kg) = 1.000e+00
Total carbon (mol/kg) = 2.182e-03
Total CO2 (mol/kg) = 2.182e-03
Temperature (°C) = 25.00

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Electrical balance (eq) = 7.936e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.07
Iterations = 7
Total H = 1.110147e+02
Total O = 5.563054e+01

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

Redox couple	pe	Eh (volts)
N(-3)/N(5)	4.6750	0.2766
O(-2)/O(0)	12.4062	0.7339

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm ³ /mol
OH-	2.705e-06	1.647e-06	-5.568	-5.783	-0.215	-2.63
H+	7.984e-09	6.026e-09	-8.098	-8.220	-0.122	0.00
H2O	5.551e+01	9.806e-01	1.744	-0.009	0.000	18.07
C(4)	2.182e-03					
HCO3-	1.485e-03	1.003e-03	-2.828	-2.999	-0.171	26.98
MgHCO3+	2.560e-04	1.610e-04	-3.592	-3.793	-0.201	5.82
NaHCO3	1.658e-04	1.936e-04	-3.781	-3.713	0.067	1.80
MgCO3	8.747e-05	1.022e-04	-4.058	-3.991	0.067	-17.09
NaCO3-	6.682e-05	4.990e-05	-4.175	-4.302	-0.127	2.88
CaHCO3+	4.453e-05	3.081e-05	-4.351	-4.511	-0.160	9.96
CO3-2	3.752e-05	7.803e-06	-4.426	-5.108	-0.682	-1.97
CaCO3	2.703e-05	3.158e-05	-4.568	-4.501	0.067	-14.60
CO2	1.186e-05	1.385e-05	-4.926	-4.858	0.067	34.43
UO2 (CO3) 3-4	1.252e-08	1.173e-10	-7.902	-9.931	-2.028	(0)
UO2 (CO3) 2-2	1.837e-09	5.716e-10	-8.736	-9.243	-0.507	(0)
MnCO3	2.550e-10	2.979e-10	-9.593	-9.526	0.067	(0)
MnHCO3+	6.475e-11	4.294e-11	-10.189	-10.367	-0.178	(0)
UO2CO3	7.662e-12	8.950e-12	-11.116	-11.048	0.067	(0)
(CO2) 2	3.015e-12	3.522e-12	-11.521	-11.453	0.067	68.87
FeCO3	1.796e-20	2.098e-20	-19.746	-19.678	0.067	(0)
FeHCO3+	1.505e-20	1.124e-20	-19.823	-19.949	-0.127	(0)
Ca	1.066e-02					
Ca+2	9.634e-03	2.409e-03	-2.016	-2.618	-0.602	-16.69
CaSO4	9.548e-04	1.115e-03	-3.020	-2.953	0.067	7.50
CaHCO3+	4.453e-05	3.081e-05	-4.351	-4.511	-0.160	9.96
CaCO3	2.703e-05	3.158e-05	-4.568	-4.501	0.067	-14.60
CaOH+	8.711e-08	6.505e-08	-7.060	-7.187	-0.127	(0)
CaHSO4+	5.915e-11	4.418e-11	-10.228	-10.355	-0.127	(0)
Cl	5.657e-01					
Cl-	5.657e-01	3.568e-01	-0.247	-0.448	-0.200	18.79
MnCl+	1.053e-09	6.985e-10	-8.977	-9.156	-0.178	-2.79
MnCl2	9.314e-11	1.088e-10	-10.031	-9.963	0.067	85.89
MnCl3-	1.612e-11	1.069e-11	-10.793	-10.971	-0.178	45.79
FeCl+2	1.519e-18	2.939e-19	-17.818	-18.532	-0.713	(0)
FeCl2+	7.062e-19	4.684e-19	-18.151	-18.329	-0.178	(0)
FeCl+	7.392e-20	5.521e-20	-19.131	-19.258	-0.127	(0)
FeCl3	1.431e-20	1.671e-20	-19.844	-19.777	0.067	(0)
Fe(2)	6.492e-19					
Fe+2	4.892e-19	1.121e-19	-18.311	-18.950	-0.640	-20.71
FeCl+	7.392e-20	5.521e-20	-19.131	-19.258	-0.127	(0)
FeSO4	4.443e-20	5.190e-20	-19.352	-19.285	0.067	18.97
FeCO3	1.796e-20	2.098e-20	-19.746	-19.678	0.067	(0)
FeHCO3+	1.505e-20	1.124e-20	-19.823	-19.949	-0.127	(0)
FeOH+	8.698e-21	5.768e-21	-20.061	-20.239	-0.178	(0)
Fe (OH) 2	6.840e-24	7.990e-24	-23.165	-23.097	0.067	(0)
Fe (OH) 3-	7.284e-26	4.831e-26	-25.138	-25.316	-0.178	(0)
FeHSO4+	2.753e-27	2.056e-27	-26.560	-26.687	-0.127	(0)
Fe(3)	3.711e-08					
Fe (OH) 3	2.771e-08	3.237e-08	-7.557	-7.490	0.067	(0)
Fe (OH) 4-	7.114e-09	4.804e-09	-8.148	-8.318	-0.171	(0)

	Fe (OH) 2+	2.287e-09	1.544e-09	-8.641	-8.811	-0.171	(0)
	FeOH+2	1.481e-13	2.866e-14	-12.829	-13.543	-0.713	(0)
	FeCl+2	1.519e-18	2.939e-19	-17.818	-18.532	-0.713	(0)
	FeSO4+	1.174e-18	7.786e-19	-17.930	-18.109	-0.178	(0)
	FeCl2+	7.062e-19	4.684e-19	-18.151	-18.329	-0.178	(0)
	Fe+3	3.432e-19	2.727e-20	-18.464	-19.564	-1.100	(0)
	Fe (SO4) 2-	5.939e-20	4.436e-20	-19.226	-19.353	-0.127	(0)
	FeCl3	1.431e-20	1.671e-20	-19.844	-19.777	0.067	(0)
	Fe2 (OH) 2+4	2.359e-24	2.210e-26	-23.627	-25.656	-2.028	(0)
	FeHSO4+2	4.038e-26	1.256e-26	-25.394	-25.901	-0.507	(0)
	Fe3 (OH) 4+5	1.053e-29	7.130e-33	-28.978	-32.147	-3.169	(0)
H (0)	0.000e+00						
	H2	0.000e+00	0.000e+00	-44.470	-44.402	0.067	28.61
K	1.058e-02						
	K+	1.040e-02	6.483e-03	-1.983	-2.188	-0.205	9.66
	KSO4-	1.756e-04	1.186e-04	-3.755	-3.926	-0.171	34.85
Mg	5.507e-02						
	Mg+2	4.754e-02	1.372e-02	-1.323	-1.863	-0.540	-20.41
	MgSO4	7.170e-03	8.375e-03	-2.144	-2.077	0.067	5.84
	MgHCO3+	2.560e-04	1.610e-04	-3.592	-3.793	-0.201	5.82
	MgCO3	8.747e-05	1.022e-04	-4.058	-3.991	0.067	-17.09
	MgOH+	1.151e-05	8.107e-06	-4.939	-5.091	-0.152	(0)
Mn (2)	3.773e-09						
	Mn+2	2.097e-09	4.806e-10	-8.678	-9.318	-0.640	-16.36
	MnCl+	1.053e-09	6.985e-10	-8.977	-9.156	-0.178	-2.79
	MnCO3	2.550e-10	2.979e-10	-9.593	-9.526	0.067	(0)
	MnSO4	1.905e-10	2.225e-10	-9.720	-9.653	0.067	22.54
	MnCl2	9.314e-11	1.088e-10	-10.031	-9.963	0.067	85.89
	MnHCO3+	6.475e-11	4.294e-11	-10.189	-10.367	-0.178	(0)
	MnCl3-	1.612e-11	1.069e-11	-10.793	-10.971	-0.178	45.79
	MnOH+	3.031e-12	2.010e-12	-11.518	-11.697	-0.178	(0)
	Mn (OH) 3-	4.949e-20	3.282e-20	-19.305	-19.484	-0.178	(0)
	Mn (NO3) 2	1.325e-20	1.548e-20	-19.878	-19.810	0.067	41.04
Mn (3)	5.279e-26						
	Mn+3	5.279e-26	4.195e-27	-25.277	-26.377	-1.100	(0)
N (-3)	1.724e-06						
	NH4+	1.610e-06	9.048e-07	-5.793	-6.043	-0.250	18.44
	NH3	7.326e-08	8.557e-08	-7.135	-7.068	0.067	24.42
	NH4SO4-	4.064e-08	3.035e-08	-7.391	-7.518	-0.127	39.98
N (5)	4.847e-06						
	NO3-	4.847e-06	2.844e-06	-5.314	-5.546	-0.232	30.29
	Mn (NO3) 2	1.325e-20	1.548e-20	-19.878	-19.810	0.067	41.04
Na	4.854e-01						
	Na+	4.785e-01	3.434e-01	-0.320	-0.464	-0.144	-0.50
	NaSO4-	6.637e-03	4.482e-03	-2.178	-2.349	-0.171	21.21
	NaHCO3	1.658e-04	1.936e-04	-3.781	-3.713	0.067	1.80
	NaCO3-	6.682e-05	4.990e-05	-4.175	-4.302	-0.127	2.88
	NaOH	4.843e-17	5.657e-17	-16.315	-16.247	0.067	(0)
O (0)	4.376e-04						
	O2	2.188e-04	2.556e-04	-3.660	-3.592	0.067	30.40
S (6)	2.926e-02						
	SO4-2	1.432e-02	2.604e-03	-1.844	-2.584	-0.740	17.49
	MgSO4	7.170e-03	8.375e-03	-2.144	-2.077	0.067	5.84
	NaSO4-	6.637e-03	4.482e-03	-2.178	-2.349	-0.171	21.21
	CaSO4	9.548e-04	1.115e-03	-3.020	-2.953	0.067	7.50
	KSO4-	1.756e-04	1.186e-04	-3.755	-3.926	-0.171	34.85
	NH4SO4-	4.064e-08	3.035e-08	-7.391	-7.518	-0.127	39.98
	HSO4-	2.042e-09	1.525e-09	-8.690	-8.817	-0.127	40.96
	MnSO4	1.905e-10	2.225e-10	-9.720	-9.653	0.067	22.54
	CaHSO4+	5.915e-11	4.418e-11	-10.228	-10.355	-0.127	(0)
	FeSO4+	1.174e-18	7.786e-19	-17.930	-18.109	-0.178	(0)
	Fe (SO4) 2-	5.939e-20	4.436e-20	-19.226	-19.353	-0.127	(0)
	FeSO4	4.443e-20	5.190e-20	-19.352	-19.285	0.067	18.97
	FeHSO4+2	4.038e-26	1.256e-26	-25.394	-25.901	-0.507	(0)
	FeHSO4+	2.753e-27	2.056e-27	-26.560	-26.687	-0.127	(0)
Si	7.382e-05						
	H4SiO4	7.061e-05	8.248e-05	-4.151	-4.084	0.067	52.08
	H3SiO4-	3.210e-06	2.018e-06	-5.494	-5.695	-0.201	28.72

H2SiO4-2	1.096e-10	2.279e-11	-9.960	-10.642	-0.682	(0)
U(4)	1.088e-21					
U(OH) 5-	1.088e-21	8.128e-22	-20.963	-21.090	-0.127	(0)
U(OH) 4	1.738e-25	2.030e-25	-24.760	-24.692	0.067	(0)
U+4	0.000e+00	0.000e+00	-46.972	-49.000	-2.028	(0)
U(5)	1.707e-18					
UO2+	1.707e-18	1.275e-18	-17.768	-17.894	-0.127	(0)
U(6)	1.437e-08					
UO2 (CO3) 3-4	1.252e-08	1.173e-10	-7.902	-9.931	-2.028	(0)
UO2 (CO3) 2-2	1.837e-09	5.716e-10	-8.736	-9.243	-0.507	(0)
UO2CO3	7.662e-12	8.950e-12	-11.116	-11.048	0.067	(0)
UO2OH+	3.563e-14	2.661e-14	-13.448	-13.575	-0.127	(0)
UO2+2	3.182e-16	9.898e-17	-15.497	-16.004	-0.507	(0)
(UO2) 2 (OH) 2+2	1.973e-21	6.139e-22	-20.705	-21.212	-0.507	(0)
(UO2) 3 (OH) 5+	3.387e-23	2.530e-23	-22.470	-22.597	-0.127	(0)

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

Phase	SI**	log IAP	log K(298 K,	1 atm)	
Anhydrite	-0.93	-5.20	-4.28	CaSO4	
Aragonite	0.61	-7.73	-8.34	CaCO3	
Calcite	0.75	-7.73	-8.48	CaCO3	
Chalcedony	-0.52	-4.07	-3.55	SiO2	
Chrysotile	3.36	35.56	32.20	Mg3Si2O5 (OH) 4	
CO2 (g)	-3.39	-4.86	-1.47	CO2	
Dolomite	2.39	-14.70	-17.08	CaMg (CO3) 2	
Fe (OH) 3 (a)	0.18	5.07	4.89	Fe (OH) 3	
Goethite	6.08	5.08	-1.00	FeOOH	
Gypsum	-0.64	-5.22	-4.58	CaSO4:2H2O	
H2 (g)	-41.30	-44.40	-3.10	H2	
H2O (g)	-1.51	-0.01	1.50	H2O	
Halite	-2.48	-0.91	1.57	NaCl	
Hausmannite	1.55	62.58	61.03	Mn3O4	
Hematite	14.17	10.17	-4.01	Fe2O3	
Jarosite-K	-7.57	-16.78	-9.21	KFe3 (SO4) 2 (OH) 6	
Manganite	2.39	27.73	25.34	MnOOH	
Melanterite	-19.39	-21.59	-2.21	FeSO4:7H2O	
NH3 (g)	-8.86	-7.07	1.80	NH3	
O2 (g)	-0.70	-3.59	-2.89	O2	Pressure 0.2 atm, phi 1.000
Pyrochroite	-8.10	7.10	15.20	Mn (OH) 2	
Pyrolusite	6.97	48.35	41.38	MnO2:H2O	
Quartz	-0.09	-4.07	-3.98	SiO2	
Rhodochrosite	-3.30	-14.43	-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	-13.17	-24.06	-10.89	FeCO3	
SiO2 (a)	-1.35	-4.07	-2.71	SiO2	
Sylvite	-3.54	-2.64	0.90	KCl	
Talc	6.03	27.43	21.40	Mg3Si4O10 (OH) 2	
Uraninite	-12.65	-16.14	-3.49	UO2	

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.066 Seconds.
