Supplementary information - Appendix 1

Biogeochemistry of U, Ni, and As in two meromictic pit lakes at the Cluff Lake uranium mine, northern Saskatchewan

von Gunten Konstantin¹, Tyler Warchola¹, Mark Donner², Manuel Cossio¹, Weiduo Hao¹, Christopher Boothman³, Jonathan Lloyd³, Tariq Siddique², Camille A. Partin⁴, Shannon Flynn¹, Arden Rosaasen⁵, Kurt Konhauser¹, Daniel S. Alessi¹

¹Department of Earth and Atmospheric Sciences, University of Alberta, 1-26 Earth Sciences Building, Edmonton, T6G 2R3, Canada

²Department of Renewable Resources, University of Alberta, 751 General Services Building, Edmonton, Alberta, T6G 2H1, Canada

³School of Earth and Environmental Sciences, University of Manchester, Oxford Road, Manchester, M13 9PL, United Kingdom

⁴Department of Geological Sciences, University of Saskatchewan, 114 Science Place, Saskatoon, Saskatchewan, S7N 5E2, Canada

⁵AREVA Resources Canada, 817 45 St W, Saskatoon, Saskatchewan, S7K 3X5, Canada

Appendix 1: PHREEQC output for D-pit and DJX-pit thermodynamic calculations

1.1 D-pit, 0.5 m

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
Al	2.224e-06	2.224e+00
As	1.335e-08	1.335e-02
B	4.347e-06	4.347e+00
Ba	2.913e-08	2.913e-02
Br	2.503e-07	2.503e-01
C	1.133e-03	1.133e+03
Ca	2.731e-04	2.731e+02
Cl	5.465e-05	5.465e+01
Fe	1.422e-05	1.422e+01
K	4.563e-05	4.563e+01
Li	7.204e-07	7.204e-01
Mg	2.997e-04	2.996e+02
Mn	2.914e-06	2.914e+00
Na	9.817e-05	9.817e+01
Ni	5.112e-08	5.112e-02
S	6.563e-05	6.562e+01
Si	1.099e-04	1.099e+02
Sr	7.306e-07	7.306e-01
U	5.041e-07	5.041e-01

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

pH	=	7.220	Charge balance
pe	=	2.850	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength (mol/kgw)	=	1.889e-03	
Mass of water (kg)	=	1.000e+06	
Total alkalinity (eq/kg)	=	1.018e-03	
Total CO2 (mol/kg)	=	1.133e-03	
Temperature (°C)	=	20.80	
Pressure (atm)	=	1.04	
Electrical balance (eq)	=	1.290e+02	
Percent error, 100*(Cat-[An])/(Cat+[An])	=	5.18	
Iterations	=	3	
Total H	=	1.110141e+08	
Total O	=	5.551034e+07	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm ³ /mol
OH-	1.268e-07	1.208e-07	-6.897	-6.918	-0.021	(0)
H+	6.302e-08	6.026e-08	-7.200	-7.220	-0.020	0.00
H2O	5.551e+01	1.000e+00	1.744	-0.000	0.000	18.05
Al	2.224e-06					
Al (OH) 3	1.346e-06	1.346e-06	-5.871	-5.871	0.000	(0)
Al (OH) 4-	8.099e-07	7.722e-07	-6.092	-6.112	-0.021	(0)
Al (OH) 2+	6.755e-08	6.444e-08	-7.170	-7.191	-0.020	(0)
AlOH+2	4.532e-10	3.755e-10	-9.344	-9.425	-0.082	(0)
Al+3	4.414e-12	2.946e-12	-11.355	-11.531	-0.176	(0)
AlSO4+	1.550e-13	1.478e-13	-12.810	-12.830	-0.021	(0)
Al (SO4) 2-	6.109e-16	5.825e-16	-15.214	-15.235	-0.021	(0)
As (3)	1.259e-14					
H3AsO3	1.248e-14	1.249e-14	-13.904	-13.904	0.000	(0)
H2AsO3-	1.098e-16	1.047e-16	-15.959	-15.980	-0.021	(0)
HAsO3-2	1.384e-21	1.142e-21	-20.859	-20.942	-0.083	(0)
H4AsO3+	3.911e-22	3.728e-22	-21.408	-21.429	-0.021	(0)
AsO3-3	9.720e-28	6.315e-28	-27.012	-27.200	-0.187	(0)
As (5)	1.335e-08					
HAsO4-2	1.023e-08	8.447e-09	-7.990	-8.073	-0.083	(0)
H2AsO4-	3.116e-09	2.970e-09	-8.506	-8.527	-0.021	(0)
AsO4-3	4.925e-13	3.200e-13	-12.308	-12.495	-0.187	(0)
H3AsO4	3.005e-14	3.007e-14	-13.522	-13.522	0.000	(0)
B	4.347e-06					
H3BO3	4.308e-06	4.309e-06	-5.366	-5.366	0.000	(0)
H2BO3-	3.992e-08	3.801e-08	-7.399	-7.420	-0.021	(0)
Ba	2.913e-08					
Ba+2	2.913e-08	2.411e-08	-7.536	-7.618	-0.082	(0)
BaOH+	1.278e-14	1.219e-14	-13.893	-13.914	-0.021	(0)
Br	2.503e-07					
Br-	2.503e-07	2.386e-07	-6.602	-6.622	-0.021	(0)
NiBr+	6.343e-15	6.046e-15	-14.198	-14.219	-0.021	(0)
C (4)	1.133e-03					
HCO3-	1.001e-03	9.548e-04	-3.000	-3.020	-0.020	(0)
H2CO3	1.246e-04	1.246e-04	-3.905	-3.904	0.000	(0)
MgHCO3+	2.795e-06	2.664e-06	-5.554	-5.574	-0.021	(0)
CaHCO3+	2.033e-06	1.940e-06	-5.692	-5.712	-0.020	(0)
CO3-2	8.182e-07	6.778e-07	-6.087	-6.169	-0.082	(0)
UO2 (CO3) 2-2	4.183e-07	3.453e-07	-6.379	-6.462	-0.083	(0)
CaCO3	1.964e-07	1.964e-07	-6.707	-6.707	0.000	(0)
MgCO3	1.484e-07	1.485e-07	-6.828	-6.828	0.000	(0)
UO2CO3	6.844e-08	6.847e-08	-7.165	-7.165	0.000	(0)
NaHCO3	4.591e-08	4.593e-08	-7.338	-7.338	0.000	(0)
MnHCO3+	4.034e-08	3.847e-08	-7.394	-7.415	-0.021	(0)
NiCO3	4.025e-08	4.026e-08	-7.395	-7.395	0.000	(0)
UO2 (CO3) 3-4	1.645e-08	7.644e-09	-7.784	-8.117	-0.333	(0)
NiHCO3+	1.013e-09	9.659e-10	-8.994	-9.015	-0.021	(0)
NaCO3-	9.936e-10	9.479e-10	-9.003	-9.023	-0.020	(0)
Ni (CO3) 2-2	5.745e-11	4.743e-11	-10.241	-10.324	-0.083	(0)
Ca	2.731e-04					
Ca+2	2.687e-04	2.230e-04	-3.571	-3.652	-0.081	(0)
CaSO4	2.212e-06	2.213e-06	-5.655	-5.655	0.000	(0)
CaHCO3+	2.033e-06	1.940e-06	-5.692	-5.712	-0.020	(0)
CaCO3	1.964e-07	1.964e-07	-6.707	-6.707	0.000	(0)
CaOH+	6.893e-10	6.579e-10	-9.162	-9.182	-0.020	(0)
Cl	5.465e-05					
Cl-	5.465e-05	5.206e-05	-4.262	-4.284	-0.021	(0)
MnCl+	5.225e-10	4.984e-10	-9.282	-9.302	-0.021	(0)
NiCl+	1.097e-12	1.045e-12	-11.960	-11.981	-0.021	(0)
MnCl2	7.044e-15	7.048e-15	-14.152	-14.152	0.000	(0)
UO2Cl+	7.219e-16	6.881e-16	-15.142	-15.162	-0.021	(0)
NiCl2	1.980e-16	1.981e-16	-15.703	-15.703	0.000	(0)
FeCl+2	9.703e-19	8.030e-19	-18.013	-18.095	-0.082	(0)
MnCl3-	1.734e-19	1.654e-19	-18.761	-18.781	-0.021	(0)
FeCl2+	2.241e-22	2.137e-22	-21.650	-21.670	-0.021	(0)
FeCl3	1.112e-27	1.113e-27	-26.954	-26.954	0.000	(0)
UCl+3	1.118e-39	7.264e-40	-38.952	-39.139	-0.187	(0)
Fe (2)	1.378e-05					
Fe+2	1.364e-05	1.131e-05	-4.865	-4.946	-0.081	(0)
FeSO4	9.387e-08	9.391e-08	-7.027	-7.027	0.000	(0)
FeOH+	4.528e-08	4.319e-08	-7.344	-7.365	-0.021	(0)
Fe (OH) 2	4.210e-12	4.212e-12	-11.376	-11.376	0.000	(0)
Fe (OH) 3-	2.611e-15	2.491e-15	-14.583	-14.604	-0.021	(0)
Fe (HS) 2	0.000e+00	0.000e+00	-111.571	-111.570	0.000	(0)
Fe (HS) 3-	0.000e+00	0.000e+00	-167.300	-167.320	-0.021	(0)
Fe (3)	4.397e-07					
Fe (OH) 2+	3.608e-07	3.442e-07	-6.443	-6.463	-0.020	(0)
Fe (OH) 3	6.709e-08	6.712e-08	-7.173	-7.173	0.000	(0)
Fe (OH) 4-	1.168e-08	1.114e-08	-7.933	-7.953	-0.020	(0)
FeOH+2	5.891e-11	4.875e-11	-10.230	-10.312	-0.082	(0)
Fe+3	8.759e-16	5.846e-16	-15.058	-15.233	-0.176	(0)
FeSO4+	2.341e-16	2.233e-16	-15.631	-15.651	-0.021	(0)
FeCl+2	9.703e-19	8.030e-19	-18.013	-18.095	-0.082	(0)
Fe (SO4) 2-	3.676e-19	3.504e-19	-18.435	-18.455	-0.021	(0)
Fe2 (OH) 2+4	1.642e-19	7.627e-20	-18.785	-19.118	-0.333	(0)
FeCl2+	2.241e-22	2.137e-22	-21.650	-21.670	-0.021	(0)
Fe3 (OH) 4+5	1.783e-23	5.381e-24	-22.749	-23.269	-0.520	(0)
FeCl3	1.112e-27	1.113e-27	-26.954	-26.954	0.000	(0)
H (0)	1.070e-23					
H2	5.349e-24	5.352e-24	-23.272	-23.272	0.000	(0)
K	4.563e-05					
K+	4.561e-05	4.345e-05	-4.341	-4.362	-0.021	(0)
KSO4-	1.499e-08	1.430e-08	-7.824	-7.845	-0.020	(0)
Li	7.204e-07					
Li+	7.202e-07	6.873e-07	-6.143	-6.163	-0.020	(0)
LiSO4-	1.587e-10	1.514e-10	-9.799	-9.820	-0.021	(0)
Mg	2.997e-04					
Mg+2	2.946e-04	2.449e-04	-3.531	-3.611	-0.080	(0)
MgHCO3+	2.795e-06	2.664e-06	-5.554	-5.574	-0.021	(0)
MgSO4	2.124e-06	2.125e-06	-5.673	-5.673	0.000	(0)
MgCO3	1.484e-07	1.485e-07	-6.828	-6.828	0.000	(0)

MgOH+	4.823e-09	4.604e-09	-8.317	-8.337	-0.020	(0)
Mn (2)	2.914e-06					
Mn+2	2.852e-06	2.366e-06	-5.545	-5.626	-0.081	(0)
MnHCO3+	4.034e-08	3.847e-08	-7.394	-7.415	-0.021	(0)
MnSO4	2.061e-08	2.062e-08	-7.686	-7.686	0.000	(0)
MnOH+	7.478e-10	7.133e-10	-9.126	-9.147	-0.021	(0)
MnCl+	5.225e-10	4.984e-10	-9.282	-9.302	-0.021	(0)
MnCl2	7.044e-15	7.048e-15	-14.152	-14.152	0.000	(0)
Mn (OH) 3-	1.797e-19	1.714e-19	-18.745	-18.766	-0.021	(0)
MnCl3-	1.734e-19	1.654e-19	-18.761	-18.781	-0.021	(0)
Mn (3)	1.453e-28					
Mn+3	1.453e-28	9.701e-29	-27.838	-28.013	-0.176	(0)
Mn (6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-56.395	-56.477	-0.082	(0)
Mn (7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-63.269	-63.290	-0.021	(0)
Na	9.817e-05					
Na+	9.810e-05	9.354e-05	-4.008	-4.029	-0.021	(0)
NaHCO3	4.591e-08	4.593e-08	-7.338	-7.338	0.000	(0)
NaSO4-	2.413e-08	2.302e-08	-7.617	-7.638	-0.020	(0)
NaCO3-	9.936e-10	9.479e-10	-9.003	-9.023	-0.020	(0)
Ni	5.112e-08					
NiCO3	4.025e-08	4.026e-08	-7.395	-7.395	0.000	(0)
Ni+2	9.706e-09	8.014e-09	-8.013	-8.096	-0.083	(0)
NiHCO3+	1.013e-09	9.659e-10	-8.994	-9.015	-0.021	(0)
NiSO4	7.597e-11	7.600e-11	-10.119	-10.119	0.000	(0)
Ni (CO3) 2-2	5.745e-11	4.743e-11	-10.241	-10.324	-0.083	(0)
NiOH+	1.427e-11	1.361e-11	-10.845	-10.866	-0.021	(0)
NiCl+	1.097e-12	1.045e-12	-11.960	-11.981	-0.021	(0)
Ni (OH) 2	2.206e-13	2.207e-13	-12.656	-12.656	0.000	(0)
NiBr+	6.343e-15	6.046e-15	-14.198	-14.219	-0.021	(0)
Ni (SO4) 2-2	2.588e-16	2.136e-16	-15.587	-15.670	-0.083	(0)
NiCl2	1.980e-16	1.981e-16	-15.703	-15.703	0.000	(0)
Ni (OH) 3-	3.843e-17	3.663e-17	-16.415	-16.436	-0.021	(0)
O (0)	0.000e+00					
O2	0.000e+00	0.000e+00	-47.212	-47.212	0.000	(0)
S (-2)	0.000e+00					
HS-	0.000e+00	0.000e+00	-57.766	-57.787	-0.021	(0)
H2S	0.000e+00	0.000e+00	-58.009	-58.008	0.000	(0)
S5-2	0.000e+00	0.000e+00	-60.176	-60.259	-0.083	(0)
S6-2	0.000e+00	0.000e+00	-60.365	-60.448	-0.083	(0)
S4-2	0.000e+00	0.000e+00	-60.414	-60.498	-0.083	(0)
S-2	0.000e+00	0.000e+00	-63.530	-63.612	-0.082	(0)
S3-2	0.000e+00	0.000e+00	-63.875	-63.958	-0.083	(0)
S2-2	0.000e+00	0.000e+00	-65.131	-65.214	-0.083	(0)
Fe (HS) 2	0.000e+00	0.000e+00	-111.571	-111.570	0.000	(0)
Fe (HS) 3-	0.000e+00	0.000e+00	-167.300	-167.320	-0.021	(0)
S (6)	6.563e-05					
SO4-2	6.114e-05	5.046e-05	-4.214	-4.297	-0.083	(0)
CaSO4	2.212e-06	2.213e-06	-5.655	-5.655	0.000	(0)
MgSO4	2.124e-06	2.125e-06	-5.673	-5.673	0.000	(0)
FeSO4	9.387e-08	9.391e-08	-7.027	-7.027	0.000	(0)
NaSO4-	2.413e-08	2.302e-08	-7.617	-7.638	-0.020	(0)
MnSO4	2.061e-08	2.062e-08	-7.686	-7.686	0.000	(0)
KSO4-	1.499e-08	1.430e-08	-7.824	-7.845	-0.020	(0)
HSO4-	2.756e-10	2.627e-10	-9.560	-9.580	-0.021	(0)
LiSO4-	1.587e-10	1.514e-10	-9.799	-9.820	-0.021	(0)
NiSO4	7.597e-11	7.600e-11	-10.119	-10.119	0.000	(0)
UO2SO4	1.872e-13	1.873e-13	-12.728	-12.727	0.000	(0)
AlSO4+	1.550e-13	1.478e-13	-12.810	-12.830	-0.021	(0)
Al (SO4) 2-	6.109e-16	5.825e-16	-15.214	-15.235	-0.021	(0)
UO2 (SO4) 2-2	3.329e-16	2.748e-16	-15.478	-15.561	-0.083	(0)
Ni (SO4) 2-2	2.588e-16	2.136e-16	-15.587	-15.670	-0.083	(0)
FeSO4+	2.341e-16	2.233e-16	-15.631	-15.651	-0.021	(0)
Fe (SO4) 2-	3.676e-19	3.504e-19	-18.435	-18.455	-0.021	(0)
USO4+2	1.316e-35	1.086e-35	-34.881	-34.964	-0.083	(0)
U (SO4) 2	9.678e-36	9.682e-36	-35.014	-35.014	0.000	(0)
Si	1.099e-04					
H4SiO4	1.097e-04	1.097e-04	-3.960	-3.960	0.000	(0)
H3SiO4-	1.809e-07	1.725e-07	-6.742	-6.763	-0.021	(0)
UO2H3SiO4+	6.240e-11	5.948e-11	-10.205	-10.226	-0.021	(0)
H2SiO4-2	4.261e-12	3.530e-12	-11.370	-11.452	-0.082	(0)
Sr	7.306e-07					
Sr+2	7.306e-07	6.046e-07	-6.136	-6.219	-0.082	(0)
SrOH+	4.923e-13	4.695e-13	-12.308	-12.328	-0.021	(0)
U (3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-47.804	-47.991	-0.187	(0)
U (4)	4.206e-14					
U (OH) 5-	4.195e-14	3.999e-14	-13.377	-13.398	-0.021	(0)
U (OH) 4	1.079e-16	1.080e-16	-15.967	-15.967	0.000	(0)
U (OH) 3+	2.626e-20	2.504e-20	-19.581	-19.601	-0.021	(0)
U (OH) 2+2	9.512e-25	7.853e-25	-24.022	-24.105	-0.083	(0)
UOH+3	3.432e-30	2.230e-30	-29.464	-29.652	-0.187	(0)
USO4+2	1.316e-35	1.086e-35	-34.881	-34.964	-0.083	(0)
U (SO4) 2	9.678e-36	9.682e-36	-35.014	-35.014	0.000	(0)
U+4	1.753e-36	8.142e-37	-35.756	-36.089	-0.333	(0)
UCl+3	1.118e-39	7.264e-40	-38.952	-39.139	-0.187	(0)
U6 (OH) 15+9	0.000e+00	0.000e+00	-123.779	-125.465	-1.685	(0)
U (5)	8.026e-12					
UO2+	8.026e-12	7.650e-12	-11.096	-11.116	-0.021	(0)
U (6)	5.041e-07					
UO2 (CO3) 2-2	4.183e-07	3.453e-07	-6.379	-6.462	-0.083	(0)
UO2CO3	6.844e-08	6.847e-08	-7.165	-7.165	0.000	(0)
UO2 (CO3) 3-4	1.645e-08	7.644e-09	-7.784	-8.117	-0.333	(0)
UO2OH+	9.076e-10	8.651e-10	-9.042	-9.063	-0.021	(0)
UO2H3SiO4+	6.240e-11	5.948e-11	-10.205	-10.226	-0.021	(0)
UO2+2	9.938e-12	8.205e-12	-11.003	-11.086	-0.083	(0)
UO2SO4	1.872e-13	1.873e-13	-12.728	-12.727	0.000	(0)
(UO2) 3 (OH) 5+	1.017e-13	9.697e-14	-12.993	-13.013	-0.021	(0)
(UO2) 2 (OH) 2+2	3.974e-14	3.281e-14	-13.401	-13.484	-0.083	(0)
UO2Cl+	7.219e-16	6.881e-16	-15.142	-15.162	-0.021	(0)
UO2 (SO4) 2-2	3.329e-16	2.748e-16	-15.478	-15.561	-0.083	(0)

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

Phase	SI**	log IAP	log K(293 K, 1 atm)
Akermanite	-23.79	24.49	48.27 Ca2MgSi2O7
Al (OH) 3 (a)	-0.53	10.13	10.66 Al (OH) 3
Al2O3	-2.72	20.26	22.98 Al2O3
Al4 (OH) 10SO4	-0.92	21.78	22.70 Al4 (OH) 10SO4
AlAsO4:2H2O	-8.19	-3.39	4.80 AlAsO4:2H2O
Albite	-2.27	1.44	3.72 NaAlSi3O8
Albite (low)	-1.33	1.44	2.77 NaAlSi3O8
AlOHSO4	-5.38	-8.61	-3.23 AlOHSO4
AlumK	-19.24	-24.49	-5.25 KAl (SO4) 2:12H2O
Alunite	-2.84	-4.23	-1.39 KAl3 (SO4) 2 (OH) 6
Analcime	-1.56	5.40	6.96 NaAlSi2O6:H2O
Anhydrite	-3.35	-7.95	-4.60 CaSO4
Annite	5.61	29.59	23.98 KFe3AlSi3O10 (OH) 2
Anorthite	-3.04	23.13	26.17 CaAl2Si2O8
Aragonite	-1.51	-9.82	-8.31 CaCO3
Arsenolite	-52.66	-55.61	-2.95 As4O6
Artinite	-8.85	1.05	9.90 MgCO3:Mg (OH) 2:3H2O
As2O5	-33.80	-27.04	6.76 As2O5
B UO2 (OH) 2	-2.33	3.35	5.69 UO2 (OH) 2
Ba3 (AsO4) 2	2.36	-6.58	-8.94 Ba3 (AsO4) 2
Barite	-1.87	-11.91	-10.04 BaSO4
Birnessite	-14.37	3.72	18.09 MnO2
Bixbyite	-12.26	-12.71	-0.45 Mn2O3
Boehmite	1.26	10.13	8.87 AlOOH
Brucite	-6.23	10.83	17.06 Mg (OH) 2
Bunsenite	-6.36	6.34	12.70 NiO
Ca-Nontronite	24.33	3.44	-20.89 Fe2Al.33Si3.67O10 (OH) 2Ca0.165
Ca-Olivine	-20.60	17.62	38.22 Ca2SiO4
Ca3 (AsO4) 2:6H2O	-16.98	5.32	22.30 Ca3 (AsO4) 2:6H2O
Ca3SiO5	-46.58	28.41	74.98 Ca3SiO5
Calcite	-1.37	-9.82	-8.45 CaCO3
Celestine	-4.06	-10.52	-6.46 SrSO4
CH4 (g)	-60.43	-101.17	-40.74 CH4
Chalcedony	-0.39	-3.96	-3.57 SiO2
Chrysotile	-8.17	24.57	32.74 Mg3Si2O5 (OH) 4
Claudetite	-52.41	-55.61	-3.20 As4O6
Clinoenstatite	-4.68	6.87	11.55 MgSiO3
CO2 (g)	-2.44	-20.61	-18.17 CO2
Cristobalite	-0.32	-3.96	-3.64 SiO2
Diaspore	3.00	10.13	7.13 AlOOH
Diopside	-6.53	13.70	20.22 CaMgSi2O6
Dolomite	-2.69	-19.60	-16.91 CaMg (CO3) 2
Epsomite	-5.74	-7.91	-2.17 MgSO4:7H2O
Fe (OH) 2.7ClO.3	6.02	2.98	-3.04 Fe (OH) 2.7ClO.3
Fe2 (SO4) 3	-47.56	-43.36	4.20 Fe2 (SO4) 3
Fe3 (OH) 8	2.13	22.35	20.22 Fe3 (OH) 8
FeAsO4:2H2O	-7.50	-7.10	0.40 FeAsO4:2H2O
Ferrihydrite	1.54	6.43	4.89 Fe (OH) 3
FeS (ppt)	-51.60	-55.51	-3.92 FeS
Forsterite	-11.11	17.70	28.81 Mg2SiO4
Gehlenite	-20.16	37.88	58.04 Ca2Al2SiO7
Gibbsite (C)	1.12	10.13	9.01 Al (OH) 3
Goethite	5.78	6.43	0.65 FeOOH
Greenalite	-0.25	20.56	20.81 Fe3Si2O5 (OH) 4
Greigite	-192.65	-237.68	-45.03 Fe3S4
Gummite	-7.29	3.35	10.64 UO3
Gypsum	-3.34	-7.95	-4.61 CaSO4:2H2O
Halite	-9.88	-8.31	1.57 NaCl
Halloysite	2.93	12.34	9.41 Al2Si2O5 (OH) 4
Hausmannite	-15.80	46.58	62.38 Mn3O4
Hematite	16.54	12.85	-3.68 Fe2O3
Hercynite	1.77	29.75	27.98 FeAl2O4
Huntite	-9.46	-39.16	-29.70 CaMg3 (CO3) 4
Hydromagnesite	-20.07	-28.29	-8.22 Mg5 (CO3) 4 (OH) 2:4H2O
Jarosite-H	-6.67	-18.19	-11.52 (H3O) Fe3 (SO4) 2 (OH) 6
Jarosite-K	-0.86	-15.34	-14.47 KFe3 (SO4) 2 (OH) 6
Jarosite-Na	-4.18	-15.00	-10.82 NaFe3 (SO4) 2 (OH) 6
K-Nontronite	18.16	2.61	-15.55 Fe2Al.33Si3.67O10 (OH) 2K0.33
Kalsilite	-4.11	9.03	13.14 KAlSiO4
Kaolinite	6.24	12.34	6.10 Al2Si2O5 (OH) 4
Larnite	-22.12	17.62	39.74 Ca2SiO4
Laumontite	0.22	15.21	14.99 CaAl2Si4O12:4H2O
Leonhardtite	13.03	30.42	17.38 Ca2Al4Si8O24:7H2O
Lepidocrocite	5.06	6.43	1.37 FeOOH
Leucite	-1.59	5.07	6.65 KAlSi2O6
Lime	-22.49	10.79	33.28 CaO
Mackinawite	-50.87	-55.51	-4.65 FeS
Magadiite	-10.23	-24.53	-14.30 NaSi7O13 (OH) 3:3H2O
Maghemite	6.47	12.85	6.39 Fe2O3
Magnesite	-1.82	-9.78	-7.96 MgCO3
Magnetite	18.08	22.35	4.27 Fe3O4
Manganite	-6.12	-6.35	-0.24 MnOOH
Melanterite	-6.74	-9.24	-2.50 FeSO4:7H2O
Merwinite	-34.39	35.27	69.66 Ca3MgSi2O8
Mg-Ferrite	6.22	23.68	17.46 MgFe2O4
Mg-Nontronite	24.04	3.45	-20.59 Fe2Al.33Si3.67O10 (OH) 2Mg0.165
Microcline	0.36	1.11	0.74 KAlSi3O8
Millerite	-50.59	-58.66	-8.07 NiS
Mirabilite	-11.04	-12.36	-1.31 Na2SO4:10H2O
Mn2 (SO4) 3	-63.62	-68.92	-5.30 Mn2 (SO4) 3
Mn3 (AsO4) 2:8H2O	-13.10	-0.60	12.50 Mn3 (AsO4) 2:8H2O
MnCl2:4H2O	-16.72	-14.19	2.53 MnCl2:4H2O
MnS (Green)	-60.05	-56.19	3.86 MnS
MnSO4	-12.75	-9.92	2.83 MnSO4
Monticellite	-13.13	17.66	30.79 CaMgSiO4
Montmorillonite	6.23	8.90	2.67 Mg0.485Fe.22Al1.71Si3.81O10 (OH) 2
Morenosite	-10.00	-12.39	-2.39 NiSO4:7H2O
Muscovite	7.76	21.37	13.61 KAl3Si3O10 (OH) 2
Na-Nontronite	17.22	2.72	-14.50 Fe2Al.33Si3.67O10 (OH) 2Na0.33

Natron	-12.75	-14.23	-1.48	Na2CO3:10H2O
Nepheline	-5.21	9.36	14.57	NaAlSiO4
Nesquehonite	-4.22	-9.78	-5.56	MgCO3:3H2O
Ni(OH)2	-4.14	6.34	10.48	Ni(OH)2
Ni2SiO4	-6.16	8.73	14.89	Ni2SiO4
Ni3(AsO4)2:8H2O	-23.71	-8.01	15.70	Ni3(AsO4)2:8H2O
Ni4(OH)6SO4	-25.36	6.64	32.00	Ni4(OH)6SO4
NiCO3	-7.53	-14.27	-6.74	NiCO3
Nsutite	-13.79	3.72	17.50	MnO2
O2(g)	-44.24	40.28	84.52	O2
Oripment	-160.99	-222.83	-61.84	As2S3
P-Wollstanite	-7.24	6.83	14.07	CaSiO3
Periclase	-11.06	10.83	21.89	MgO
Phlogopite	-33.61	33.60	67.20	KMg3AlSi3O10(OH)2
Portlandite	-12.21	10.79	23.00	Ca(OH)2
Pyrite	-81.78	-100.38	-18.60	FeS2
Pyrocroite	-6.51	8.81	15.32	Mn(OH)2
Pyrolusite	-12.45	3.72	16.17	MnO2
Pyrophyllite	6.02	4.42	-1.60	Al2Si4O10(OH)2
Quartz	0.11	-3.96	-4.07	SiO2
Realgar	-68.91	-88.98	-20.07	AsS
Retgersite	-10.34	-12.39	-2.05	NiSO4:6H2O
Rhodochrosite	-1.41	-11.79	-10.39	MnCO3
Rutherfordine	-2.80	-17.25	-14.45	UO2CO3
Sanidine(H)	-0.10	1.11	1.21	KAlSi3O8
Schoepite	-2.18	3.35	5.53	UO2(OH)2:H2O
Sepiolite(a)	-9.00	9.78	18.78	Mg2Si3O7.5OH:3H2O
Sepiolite(c)	-6.42	9.78	16.20	Mg2Si3O7.5OH:3H2O
Siderite	-0.62	-11.12	-10.49	FeCO3
SiO2(a)	-0.90	-3.96	-3.06	SiO2
SiO2(am)	-1.21	-3.96	-2.75	SiO2
Spinel	-6.18	31.09	37.27	MgAl2O4
Strontianite	-3.14	-12.39	-9.24	SrCO3
Sulfur	-42.80	-44.87	-2.07	S
Talc	-6.77	16.65	23.42	Mg3Si4O10(OH)2
Thenardite	-12.18	-12.36	-0.17	Na2SO4
Thermonatrite	-14.38	-14.23	0.15	Na2CO3:H2O
Tremolite	-13.51	44.04	57.56	Ca2Mg5Si8O22(OH)2
U3O8(C)	-3.67	18.65	22.32	U3O8
U4O9(C)	-6.37	-8.70	-2.32	U4O9
UO2(am)	-8.42	-7.21	1.21	UO2
UO3(C)	-4.57	3.35	7.92	UO3
Uraninite	-2.70	-7.21	-4.50	UO2
Uranophane	-7.91	9.58	17.49	Ca(UO2)2(SiO3OH)2
USiO4(C)	-3.70	-11.17	-7.47	USiO4
Wairakite	-4.32	15.21	19.53	CaAl2Si4O12:2H2O
Witherite	-5.20	-13.79	-8.59	BaCO3
Wollastonite	-6.37	6.83	13.20	CaSiO3

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

End of simulation.

1.2 D-pit, 5 m

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
Al	2.409e-06	2.409e+00
As	4.004e-08	4.004e-02
B	4.902e-06	4.902e+00
Ba	4.369e-08	4.369e-02
Br	2.628e-07	2.628e-01
C	2.128e-03	2.128e+03
Ca	3.171e-04	3.171e+02
Cl	6.451e-05	6.451e+01
Fe	3.801e-05	3.801e+01
K	4.877e-05	4.877e+01
Li	7.204e-07	7.204e-01
Mg	3.656e-04	3.656e+02
Mn	1.173e-05	1.173e+01
N	8.571e-06	8.571e+00
Na	1.179e-04	1.179e+02
Ni	6.815e-08	6.815e-02
S	6.875e-05	6.875e+01
Si	1.474e-04	1.474e+02
Sr	8.676e-07	8.676e-01
U	2.815e-07	2.815e-01

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

pH	=	6.400	Charge balance
pe	=	3.370	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength (mol/kgw)	=	2.340e-03	
Mass of water (kg)	=	1.000e+06	
Total alkalinity (eq/kg)	=	1.296e-03	
Total CO2 (mol/kg)	=	2.128e-03	
Temperature (°C)	=	3.90	

Pressure (atm) = 1.40
 Electrical balance (eq) = 1.523e+02
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 4.90
 Iterations = 3
 Total H = 1.110160e+08
 Total O = 5.551349e+07

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm ³ /mol
H+	4.177e-07	3.981e-07	-6.379	-6.400	-0.021	0.00
OH-	4.784e-09	4.541e-09	-8.320	-8.343	-0.023	(0)
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.02
Al	2.409e-06					
Al(OH)3	1.799e-06	1.800e-06	-5.745	-5.745	0.000	(0)
Al(OH)2+	5.987e-07	5.691e-07	-6.223	-6.245	-0.022	(0)
AlOH+2	7.742e-09	6.322e-09	-8.111	-8.199	-0.088	(0)
Al+3	1.750e-09	1.135e-09	-8.757	-8.945	-0.188	(0)
Al(OH)4-	1.652e-09	1.570e-09	-8.782	-8.804	-0.022	(0)
AlSO4+	4.932e-11	4.685e-11	-10.307	-10.329	-0.022	(0)
Al(SO4)2-	1.863e-13	1.770e-13	-12.730	-12.752	-0.022	(0)
As(3)	5.530e-11					
H3AsO3	5.526e-11	5.529e-11	-10.258	-10.257	0.000	(0)
H2AsO3-	3.723e-14	3.536e-14	-13.429	-13.452	-0.022	(0)
H4AsO3+	1.148e-17	1.091e-17	-16.940	-16.962	-0.022	(0)
HAsO3-2	3.234e-20	2.630e-20	-19.490	-19.580	-0.090	(0)
AsO3-3	1.862e-27	1.170e-27	-26.730	-26.932	-0.202	(0)
As(5)	3.999e-08					
H2AsO4-	2.732e-08	2.594e-08	-7.564	-7.586	-0.022	(0)
HAsO4-2	1.267e-08	1.030e-08	-7.897	-7.987	-0.090	(0)
H3AsO4	1.454e-12	1.454e-12	-11.838	-11.837	0.000	(0)
AsO4-3	5.970e-14	3.751e-14	-13.224	-13.426	-0.202	(0)
B	4.902e-06					
H3BO3	4.897e-06	4.900e-06	-5.310	-5.310	0.000	(0)
H2BO3-	4.963e-09	4.707e-09	-8.304	-8.327	-0.023	(0)
Ba	4.369e-08					
Ba+2	4.369e-08	3.564e-08	-7.360	-7.448	-0.089	(0)
BaOH+	5.936e-16	5.641e-16	-15.227	-15.249	-0.022	(0)
Br	2.628e-07					
Br-	2.628e-07	2.496e-07	-6.580	-6.603	-0.022	(0)
NiBr+	2.901e-14	2.755e-14	-13.537	-13.560	-0.022	(0)
C(4)	2.128e-03					
HCO3-	1.283e-03	1.220e-03	-2.892	-2.914	-0.022	(0)
H2CO3	8.383e-04	8.388e-04	-3.077	-3.076	0.000	(0)
MgHCO3+	3.509e-06	3.333e-06	-5.455	-5.477	-0.022	(0)
CaHCO3+	1.785e-06	1.697e-06	-5.748	-5.770	-0.022	(0)
UO2CO3	1.833e-07	1.834e-07	-6.737	-6.737	0.000	(0)
MnHCO3+	1.300e-07	1.235e-07	-6.886	-6.908	-0.022	(0)
CO3-2	1.012e-07	8.264e-08	-6.995	-7.083	-0.088	(0)
UO2(CO3)2-2	9.486e-08	7.716e-08	-7.023	-7.113	-0.090	(0)
NaHCO3	4.425e-08	4.427e-08	-7.354	-7.354	0.000	(0)
CaCO3	2.208e-08	2.209e-08	-7.656	-7.656	0.000	(0)
NiCO3	2.137e-08	2.138e-08	-7.670	-7.670	0.000	(0)
MgCO3	1.682e-08	1.683e-08	-7.774	-7.774	0.000	(0)
NiHCO3+	3.569e-09	3.389e-09	-8.447	-8.470	-0.022	(0)
UO2(CO3)3-4	1.729e-09	7.569e-10	-8.762	-9.121	-0.359	(0)
NaCO3-	5.737e-11	5.453e-11	-10.241	-10.263	-0.022	(0)
Ni(CO3)2-2	3.776e-12	3.071e-12	-11.423	-11.513	-0.090	(0)
Ca	3.171e-04					
Ca+2	3.130e-04	2.563e-04	-3.504	-3.591	-0.087	(0)
CaSO4	2.245e-06	2.246e-06	-5.649	-5.649	0.000	(0)
CaHCO3+	1.785e-06	1.697e-06	-5.748	-5.770	-0.022	(0)
CaCO3	2.208e-08	2.209e-08	-7.656	-7.656	0.000	(0)
CaOH+	2.638e-11	2.509e-11	-10.579	-10.601	-0.022	(0)
Cl	6.451e-05					
Cl-	6.450e-05	6.121e-05	-4.190	-4.213	-0.023	(0)
MnCl+	2.458e-09	2.336e-09	-8.609	-8.632	-0.022	(0)
NiCl+	5.638e-12	5.354e-12	-11.249	-11.271	-0.022	(0)
MnCl2	3.882e-14	3.884e-14	-13.411	-13.411	0.000	(0)
UO2Cl+	1.636e-14	1.553e-14	-13.786	-13.809	-0.022	(0)
NiCl2	1.192e-15	1.193e-15	-14.924	-14.923	0.000	(0)
FeCl+2	2.053e-18	1.674e-18	-17.688	-17.776	-0.089	(0)
MnCl3-	1.128e-18	1.072e-18	-17.948	-17.970	-0.022	(0)
FeCl2+	9.895e-22	9.404e-22	-21.005	-21.027	-0.022	(0)
FeCl3	5.753e-27	5.756e-27	-26.240	-26.240	0.000	(0)
UCl+3	6.664e-35	4.187e-35	-34.176	-34.378	-0.202	(0)
Fe(2)	3.799e-05					
Fe+2	3.779e-05	3.091e-05	-4.423	-4.510	-0.087	(0)
FeSO4	1.885e-07	1.886e-07	-6.725	-6.724	0.000	(0)
FeOH+	4.738e-09	4.503e-09	-8.324	-8.347	-0.022	(0)
Fe(OH)2	1.335e-14	1.336e-14	-13.874	-13.874	0.000	(0)
Fe(OH)3-	1.050e-18	9.978e-19	-17.979	-18.001	-0.022	(0)
Fe(HS)2	0.000e+00	0.000e+00	-99.211	-99.210	0.000	(0)
Fe(HS)3-	0.000e+00	0.000e+00	-148.976	-148.999	-0.022	(0)
Fe(3)	2.719e-08					
Fe(OH)2+	2.642e-08	2.511e-08	-7.578	-7.600	-0.022	(0)
Fe(OH)3	7.409e-10	7.413e-10	-9.130	-9.130	0.000	(0)
Fe(OH)4-	1.959e-11	1.863e-11	-10.708	-10.730	-0.022	(0)
FeOH+2	9.722e-12	7.929e-12	-11.012	-11.101	-0.089	(0)
Fe+3	2.870e-15	1.861e-15	-14.542	-14.730	-0.188	(0)
FeSO4+	5.120e-16	4.866e-16	-15.291	-15.313	-0.022	(0)
FeCl+2	2.053e-18	1.674e-18	-17.688	-17.776	-0.089	(0)
Fe(SO4)2-	7.705e-19	7.318e-19	-18.113	-18.136	-0.022	(0)
Fe2(OH)2+4	9.877e-21	4.324e-21	-20.005	-20.364	-0.359	(0)
FeCl2+	9.895e-22	9.404e-22	-21.005	-21.027	-0.022	(0)
Fe3(OH)4+5	7.441e-26	2.047e-26	-25.128	-25.689	-0.561	(0)
FeCl3	5.753e-27	5.756e-27	-26.240	-26.240	0.000	(0)
H(0)	5.123e-23					
H2	2.562e-23	2.563e-23	-22.591	-22.591	0.000	(0)
K	4.877e-05					
K+	4.876e-05	4.627e-05	-4.312	-4.335	-0.023	(0)

KSO4-	1.196e-08	1.137e-08	-7.922	-7.944	-0.022	(0)
Li	7.204e-07					
Li+	7.202e-07	6.849e-07	-6.143	-6.164	-0.022	(0)
LiSO4-	1.635e-10	1.554e-10	-9.786	-9.809	-0.022	(0)
Mg	3.656e-04					
Mg+2	3.598e-04	2.951e-04	-3.444	-3.530	-0.086	(0)
MgHCO3+	3.509e-06	3.333e-06	-5.455	-5.477	-0.022	(0)
MgSO4	2.277e-06	2.278e-06	-5.643	-5.642	0.000	(0)
MgCO3	1.682e-08	1.683e-08	-7.774	-7.774	0.000	(0)
MgOH+	1.794e-10	1.707e-10	-9.746	-9.768	-0.022	(0)
Mn (2)	1.173e-05					
Mn+2	1.153e-05	9.432e-06	-4.938	-5.025	-0.087	(0)
MnHCO3+	1.300e-07	1.235e-07	-6.886	-6.908	-0.022	(0)
MnSO4	6.745e-08	6.749e-08	-7.171	-7.171	0.000	(0)
MnCl+	2.458e-09	2.336e-09	-8.609	-8.632	-0.022	(0)
MnOH+	1.007e-10	9.570e-11	-9.997	-10.019	-0.022	(0)
MnCl2	3.882e-14	3.884e-14	-13.411	-13.411	0.000	(0)
MnCl3-	1.128e-18	1.072e-18	-17.948	-17.970	-0.022	(0)
Mn (OH) 3-	2.495e-21	2.371e-21	-20.603	-20.625	-0.022	(0)
Mn (NO3) 2	0.000e+00	0.000e+00	-91.706	-91.706	0.000	(0)
Mn (3)	2.908e-26					
Mn+3	2.908e-26	1.885e-26	-25.536	-25.725	-0.188	(0)
Mn (6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-67.072	-67.161	-0.089	(0)
Mn (7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-74.637	-74.660	-0.023	(0)
N (-3)	8.571e-06					
NH4+	8.563e-06	8.122e-06	-5.067	-5.090	-0.023	(0)
NH4SO4-	5.722e-09	5.438e-09	-8.242	-8.265	-0.022	(0)
NH3	2.327e-09	2.328e-09	-8.633	-8.633	0.000	(0)
N (3)	6.989e-33					
NO2-	6.989e-33	6.637e-33	-32.156	-32.178	-0.022	(0)
N (5)	0.000e+00					
NO3-	0.000e+00	0.000e+00	-43.629	-43.651	-0.023	(0)
Mn (NO3) 2	0.000e+00	0.000e+00	-91.706	-91.706	0.000	(0)
Na	1.179e-04					
Na+	1.178e-04	1.119e-04	-3.929	-3.951	-0.022	(0)
NaHCO3	4.425e-08	4.427e-08	-7.354	-7.354	0.000	(0)
NaSO4-	2.655e-08	2.524e-08	-7.576	-7.598	-0.022	(0)
NaCO3-	5.737e-11	5.453e-11	-10.241	-10.263	-0.022	(0)
Ni	6.815e-08					
Ni+2	4.291e-08	3.490e-08	-7.367	-7.457	-0.090	(0)
NiCO3	2.137e-08	2.138e-08	-7.670	-7.670	0.000	(0)
NiHCO3+	3.569e-09	3.389e-09	-8.447	-8.470	-0.022	(0)
NiSO4	2.908e-10	2.909e-10	-9.536	-9.536	0.000	(0)
NiCl+	5.638e-12	5.354e-12	-11.249	-11.271	-0.022	(0)
Ni (CO3) 2-2	3.776e-12	3.071e-12	-11.423	-11.513	-0.090	(0)
NiOH+	2.583e-12	2.453e-12	-11.588	-11.610	-0.022	(0)
NiBr+	2.901e-14	2.755e-14	-13.537	-13.560	-0.022	(0)
Ni (OH) 2	2.202e-14	2.203e-14	-13.657	-13.657	0.000	(0)
Ni (SO4) 2-2	1.214e-15	9.872e-16	-14.916	-15.006	-0.090	(0)
NiCl2	1.192e-15	1.193e-15	-14.924	-14.923	0.000	(0)
Ni (OH) 3-	5.830e-19	5.536e-19	-18.234	-18.257	-0.022	(0)
O (0)	0.000e+00					
O2	0.000e+00	0.000e+00	-54.526	-54.525	0.000	(0)
S (-2)	0.000e+00					
H2S	0.000e+00	0.000e+00	-50.950	-50.949	0.000	(0)
HS-	0.000e+00	0.000e+00	-51.803	-51.825	-0.023	(0)
S6-2	0.000e+00	0.000e+00	-55.217	-55.306	-0.090	(0)
S5-2	0.000e+00	0.000e+00	-55.450	-55.539	-0.090	(0)
S4-2	0.000e+00	0.000e+00	-55.706	-55.796	-0.090	(0)
S-2	0.000e+00	0.000e+00	-58.930	-59.019	-0.089	(0)
S3-2	0.000e+00	0.000e+00	-59.198	-59.288	-0.090	(0)
S2-2	0.000e+00	0.000e+00	-60.500	-60.590	-0.090	(0)
Fe (HS) 2	0.000e+00	0.000e+00	-99.211	-99.210	0.000	(0)
Fe (HS) 3-	0.000e+00	0.000e+00	-148.976	-148.999	-0.022	(0)
S (6)	6.875e-05					
SO4-2	6.393e-05	5.197e-05	-4.194	-4.284	-0.090	(0)
MgSO4	2.277e-06	2.278e-06	-5.643	-5.642	0.000	(0)
CaSO4	2.245e-06	2.246e-06	-5.649	-5.649	0.000	(0)
FeSO4	1.885e-07	1.886e-07	-6.725	-6.724	0.000	(0)
MnSO4	6.745e-08	6.749e-08	-7.171	-7.171	0.000	(0)
NaSO4-	2.655e-08	2.524e-08	-7.576	-7.598	-0.022	(0)
KSO4-	1.196e-08	1.137e-08	-7.922	-7.944	-0.022	(0)
NH4SO4-	5.722e-09	5.438e-09	-8.242	-8.265	-0.022	(0)
HSO4-	1.203e-09	1.143e-09	-8.920	-8.942	-0.022	(0)
NiSO4	2.908e-10	2.909e-10	-9.536	-9.536	0.000	(0)
LiSO4-	1.635e-10	1.554e-10	-9.786	-9.809	-0.022	(0)
AlSO4+	4.932e-11	4.685e-11	-10.307	-10.329	-0.022	(0)
UO2SO4	2.472e-12	2.474e-12	-11.607	-11.607	0.000	(0)
Al (SO4) 2-	1.863e-13	1.770e-13	-12.730	-12.752	-0.022	(0)
UO2 (SO4) 2-2	4.140e-15	3.367e-15	-14.383	-14.473	-0.090	(0)
Ni (SO4) 2-2	1.214e-15	9.872e-16	-14.916	-15.006	-0.090	(0)
FeSO4+	5.120e-16	4.866e-16	-15.291	-15.313	-0.022	(0)
Fe (SO4) 2-	7.705e-19	7.318e-19	-18.113	-18.136	-0.022	(0)
USO4+2	1.293e-30	1.052e-30	-29.888	-29.978	-0.090	(0)
U (SO4) 2	6.422e-31	6.425e-31	-30.192	-30.192	0.000	(0)
Si	1.474e-04					
H4SiO4	1.474e-04	1.475e-04	-3.831	-3.831	0.000	(0)
H3SiO4-	1.371e-08	1.302e-08	-7.863	-7.885	-0.022	(0)
UO2H3SiO4+	2.783e-10	2.643e-10	-9.556	-9.578	-0.022	(0)
H2SiO4-2	4.726e-15	3.859e-15	-14.325	-14.413	-0.088	(0)
Sr	8.676e-07					
Sr+2	8.676e-07	7.076e-07	-6.062	-6.150	-0.089	(0)
SrOH+	1.927e-14	1.831e-14	-13.715	-13.737	-0.022	(0)
U (3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-44.274	-44.476	-0.202	(0)
U (4)	2.661e-14					
U (OH) 5-	2.602e-14	2.471e-14	-13.585	-13.607	-0.022	(0)
U (OH) 4	5.911e-16	5.914e-16	-15.228	-15.228	0.000	(0)
U (OH) 3+	1.189e-18	1.129e-18	-17.925	-17.947	-0.022	(0)
U (OH) 2+2	4.806e-22	3.909e-22	-21.318	-21.408	-0.090	(0)
UOH+3	2.452e-26	1.540e-26	-25.611	-25.812	-0.202	(0)

USO4+2	1.293e-30	1.052e-30	-29.888	-29.978	-0.090	(0)
U(SO4)2	6.422e-31	6.425e-31	-30.192	-30.192	0.000	(0)
U+4	2.573e-31	1.126e-31	-30.590	-30.948	-0.359	(0)
UCl+3	6.664e-35	4.187e-35	-34.176	-34.378	-0.202	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-105.101	-106.918	-1.816	(0)
U(5)	7.502e-11					
UO2+	7.502e-11	7.125e-11	-10.125	-10.147	-0.022	(0)
U(6)	2.814e-07					
UO2CO3	1.833e-07	1.834e-07	-6.737	-6.737	0.000	(0)
UO2(CO3)2-2	9.486e-08	7.716e-08	-7.023	-7.113	-0.090	(0)
UO2(CO3)3-4	1.729e-09	7.569e-10	-8.762	-9.121	-0.359	(0)
UO2OH+	1.036e-09	9.842e-10	-8.984	-9.007	-0.022	(0)
UO2H3SiO4+	2.783e-10	2.643e-10	-9.556	-9.578	-0.022	(0)
UO2+2	2.203e-10	1.792e-10	-9.657	-9.747	-0.090	(0)
UO2SO4	2.472e-12	2.474e-12	-11.607	-11.607	0.000	(0)
(UO2)2(OH)2+2	1.515e-13	1.232e-13	-12.820	-12.909	-0.090	(0)
UO2Cl+	1.636e-14	1.553e-14	-13.786	-13.809	-0.022	(0)
(UO2)3(OH)5+	6.166e-15	5.856e-15	-14.210	-14.232	-0.022	(0)
UO2(SO4)2-2	4.140e-15	3.367e-15	-14.383	-14.473	-0.090	(0)

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

Phase	SI**	log IAP	log K(277 K, 1 atm)
Akermanite	-31.71	20.03	51.74 Ca2MgSi2O7
Al(OH)3(a)	-1.63	10.25	11.89 Al(OH)3
Al2O3	-2.47	20.51	22.98 Al2O3
Al4(OH)10SO4	1.24	23.94	22.70 Al4(OH)10SO4
AlAsO4·2H2O	-6.38	-1.58	4.80 AlAsO4·2H2O
Albite	-3.41	1.21	4.62 NaAlSi3O8
Albite(low)	-2.35	1.21	3.56 NaAlSi3O8
AlOHSO4	-3.60	-6.83	-3.23 AlOHSO4
AlumK	-16.27	-21.85	-5.57 KAl(SO4)2·12H2O
Alunite	0.23	-1.34	-1.57 KAl3(SO4)2(OH)6
Analcime	-2.95	5.04	7.99 NaAlSi2O6·H2O
Anhydrite	-3.45	-7.88	-4.43 CaSO4
Annite	-1.26	25.70	26.96 KFe3AlSi3O10(OH)2
Anorthite	-7.32	22.06	29.37 CaAl2Si2O8
Aragonite	-2.44	-10.67	-8.23 CaCO3
Arsenolite	-37.43	-41.03	-3.60 As4O6
Artinite	-12.55	-1.34	11.20 MgCO3·Mg(OH)2·3H2O
As2O5	-30.68	-23.67	7.00 As2O5
B_UO2(OH)2	-3.26	3.05	6.31 UO2(OH)2
Ba3(AsO4)2	1.44	-7.62	-9.06 Ba3(AsO4)2
Barite	-1.41	-11.73	-10.33 BaSO4
Birnessite	-14.85	3.25	18.09 MnO2
Bixbyite	-13.29	-13.05	0.24 Mn2O3
Boehmite	0.11	10.25	10.15 AlOOH
Brucite	-8.96	9.27	18.23 Mg(OH)2
Bunsenite	-8.44	5.34	13.79 NiO
Ca-Nontronite	20.67	-0.22	-20.89 Fe2Al.33Si3.67O10(OH)2Ca0.165
Ca-Olivine	-26.12	14.59	40.70 Ca2SiO4
Ca3(AsO4)2·6H2O	-18.35	3.95	22.30 Ca3(AsO4)2·6H2O
Ca3SiO5	-56.01	23.79	79.80 Ca3SiO5
Calcite	-2.28	-10.67	-8.40 CaCO3
Celestite	-4.00	-10.43	-6.44 SrSO4
CH4(g)	-54.54	-98.04	-43.50 CH4
Chalcedony	-0.05	-3.83	-3.78 SiO2
Chrysotile	-14.97	20.15	35.12 Mg3Si2O5(OH)4
Claudetite	-37.22	-41.03	-3.81 As4O6
Clinoenstatite	-7.02	5.44	12.46 MgSiO3
CO2(g)	-1.69	-19.88	-18.19 CO2
Cristobalite	0.06	-3.83	-3.89 SiO2
Diaspore	2.01	10.25	8.25 AlOOH
Diopside	-10.87	10.82	21.69 CaMgSi2O6
Dolomite	-4.75	-21.29	-16.54 CaMg(CO3)2
Epsomite	-5.52	-7.81	-2.30 MgSO4·7H2O
Fe(OH)2·7ClO.3	4.33	1.29	-3.04 Fe(OH)2·7ClO.3
Fe2(SO4)3	-49.19	-42.31	6.88 Fe2(SO4)3
Fe3(OH)8	-2.99	17.23	20.22 Fe3(OH)8
FeAsO4·2H2O	-7.77	-7.37	0.40 FeAsO4·2H2O
Ferrihydrite	-0.42	4.47	4.89 Fe(OH)3
FeS(ppt)	-46.02	-49.94	-3.92 FeS
Forsterite	-16.30	14.71	31.01 Mg2SiO4
Gehlenite	-28.21	35.10	63.30 Ca2Al2SiO7
Gibbsite(C)	0.21	10.25	10.04 Al(OH)3
Goethite	3.16	4.47	1.31 FeOOH
Greenalite	-3.60	17.21	20.81 Fe3Si2O5(OH)4
Greigite	-170.64	-215.67	-45.03 Fe3S4
Gummite	-8.63	3.05	11.69 UO3
Gypsum	-3.25	-7.88	-4.62 CaSO4·2H2O
Halite	-9.70	-8.16	1.53 NaCl
Halloysite	1.64	12.85	11.21 Al2Si2O5(OH)4
Hausmannite	-23.15	42.86	66.01 Mn3O4
Hematite	11.23	8.94	-2.29 Fe2O3
Hercynite	-2.74	28.80	31.54 FeAl2O4
Huntite	-13.98	-42.51	-28.53 CaMg3(CO3)4
Hydromagnesite	-27.33	-33.18	-5.85 Mg5(CO3)4(OH)2·4H2O
Jarosite-H	-11.74	-20.76	-9.02 (H3O)Fe3(SO4)2(OH)6
Jarosite-K	-5.64	-18.69	-13.05 KFe3(SO4)2(OH)6
Jarosite-Na	-9.13	-18.31	-9.18 NaFe3(SO4)2(OH)6
K-Nontronite	14.49	-1.06	-15.55 Fe2Al.33Si3.67O10(OH)2K0.33
Kalsilite	-5.96	8.49	14.45 KAlSiO4
Kaolinite	5.15	12.85	7.70 Al2Si2O5(OH)4
Larnite	-27.75	14.59	42.34 Ca2SiO4
Laumontite	-2.88	14.39	17.28 CaAl2Si4O12·4H2O
Leonhardite	7.53	28.79	21.26 Ca2Al4Si8O24·7H2O
Lepidocrocite	3.10	4.47	1.37 FeOOH
Leucite	-3.00	4.66	7.66 KAlSi2O6
Lime	-26.17	9.21	35.38 CaO
Mackinawite	-45.29	-49.94	-4.65 FeS
Magadiite	-10.07	-24.37	-14.30 NaSi7O13(OH)3·3H2O
Maghemite	2.55	8.94	6.39 Fe2O3

Magnesite	-2.93	-10.61	-7.68	MgCO3
Magnetite	10.68	17.23	6.55	Fe3O4
Manganite	-6.29	-6.52	-0.24	MnOOH
Melanterite	-6.16	-8.79	-2.63	FeSO4:7H2O
Merwinite	-45.29	29.23	74.52	Ca3MgSi2O8
Mg-Ferrite	-2.28	18.21	20.48	MgFe2O4
Mg-Nontronite	20.38	-0.21	-20.59	Fe2Al.33Si3.67O10 (OH) 2Mg0.165
Microcline	-0.48	0.83	1.30	KAlSi3O8
Millerite	-44.70	-52.88	-8.18	NiS
Mirabilite	-10.01	-12.19	-2.18	Na2SO4:10H2O
Mn2(SO4)3	-60.77	-64.30	-3.53	Mn2(SO4)3
Mn3(AsO4)2:8H2O	-12.85	-0.35	12.50	Mn3(AsO4)2:8H2O
MnCl2:4H2O	-15.19	-13.45	1.74	MnCl2:4H2O
MnS(Green)	-54.57	-50.45	4.12	MnS
MnSO4	-12.84	-9.31	3.53	MnSO4
Monticellite	-18.38	14.65	33.03	CaMgSiO4
Montmorillonite	5.75	8.42	2.67	Mg0.485Fe.22Al1.71Si3.81O10 (OH) 2
Morenosite	-9.22	-11.74	-2.53	NiSO4:7H2O
Muscovite	5.03	21.34	16.30	KAl3Si3O10 (OH) 2
Na-Nontronite	13.57	-0.93	-14.50	Fe2Al.33Si3.67O10 (OH) 2Na0.33
Natron	-12.79	-14.99	-2.19	Na2CO3:10H2O
Nepheline	-7.20	8.87	16.07	NaAlSiO4
Nesquehonite	-5.31	-10.61	-5.30	MgCO3:3H2O
Ni(OH)2	-3.76	5.34	9.10	Ni(OH)2
Ni2SiO4	-9.55	6.85	16.40	Ni2SiO4
Ni3(AsO4)2:8H2O	-23.35	-7.65	15.70	Ni3(AsO4)2:8H2O
Ni4(OH)6SO4	-27.71	4.29	32.00	Ni4(OH)6SO4
NiCO3	-8.25	-14.54	-6.29	NiCO3
Nsutite	-14.26	3.25	17.50	MnO2
O2(g)	-51.51	39.08	90.59	O2
Oripment	-129.59	-195.19	-65.60	As2S3
P-Wollstanite	-9.64	5.38	15.02	CaSiO3
Periclase	-14.26	9.27	23.53	MgO
Phlogopite	-42.48	28.64	71.12	KMg3AlSi3O10 (OH) 2
Portlandite	-15.18	9.21	24.39	Ca(OH)2
Pyrite	-69.51	-88.62	-19.11	FeS2
Pyrocroite	-8.57	7.77	16.35	Mn(OH)2
Pyrolusite	-14.24	3.25	17.49	MnO2
Pyrophyllite	6.78	5.19	-1.60	Al2Si4O10 (OH) 2
Quartz	0.52	-3.83	-4.35	SiO2
Realgar	-56.80	-78.25	-21.45	AsS
Retgersite	-9.64	-11.74	-2.10	NiSO4:6H2O
Rhodochrosite	-1.81	-12.11	-10.29	MnCO3
Rutherfordine	-2.37	-16.83	-14.46	UO2CO3
Sanidine(H)	-1.03	0.83	1.86	KAlSi3O8
Schoepite	-3.02	3.05	6.08	UO2(OH)2:H2O
Sepiolite(a)	-11.73	7.05	18.78	Mg2Si3O7.5OH:3H2O
Sepiolite(c)	-10.39	7.05	17.44	Mg2Si3O7.5OH:3H2O
Siderite	-1.34	-11.59	-10.25	FeCO3
SiO2(a)	-0.57	-3.83	-3.27	SiO2
SiO2(am)	-0.90	-3.83	-2.93	SiO2
Spinel	-11.53	29.78	41.31	MgAl2O4
Strontianite	-4.02	-13.23	-9.21	SrCO3
Sulfur	-36.81	-38.69	-1.88	S
Talc	-12.52	12.49	25.01	Mg3Si4O10 (OH) 2
Thenardite	-12.04	-12.19	-0.15	Na2SO4
Thermonatrite	-15.27	-14.99	0.28	Na2CO3:H2O
Tremolite	-27.82	34.12	61.94	Ca2Mg5Si8O22 (OH) 2
U3O8(C)	-4.55	23.03	27.58	U3O8
U4O9(C)	-4.12	-1.85	2.27	U4O9
UO2(am)	-7.75	-5.35	2.40	UO2
UO2(NO3)2	-110.54	-97.05	13.49	UO2(NO3)2
UO2(NO3)2:2H2O	-102.24	-97.05	5.19	UO2(NO3)2:2H2O
UO2(NO3)2:3H2O	-100.83	-97.05	3.78	UO2(NO3)2:3H2O
UO2(NO3)2:6H2O	-99.08	-97.05	2.03	UO2(NO3)2:6H2O
UO3(C)	-5.74	3.05	8.80	UO3
Uraninite	-1.69	-5.35	-3.66	UO2
Uranophane	-9.84	7.65	17.49	Ca(UO2)2(SiO3OH)2
USiO4(C)	-2.37	-9.18	-6.81	USiO4
Wairakite	-8.00	14.39	22.40	CaAl2Si4O12:2H2O
Witherite	-5.93	-14.53	-8.61	BaCO3
Wollastonite	-8.71	5.38	14.08	CaSiO3

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

 End of simulation.

1.3 *D-pit, 10 m*

 Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
 Using pressure 1.

-----Solution composition-----			
Elements	Molality	Moles	
Al	2.706e-06	2.706e+00	
As	5.339e-08	5.339e-02	
B	5.180e-06	5.180e+00	
Ba	7.282e-08	7.282e-02	
Br	2.253e-07	2.253e-01	
C	2.148e-03	2.148e+03	
Ca	3.289e-04	3.289e+02	

Cl	6.338e-05	6.338e+01
Fe	5.928e-05	5.928e+01
K	5.033e-05	5.033e+01
Li	5.763e-07	5.763e-01
Mg	3.713e-04	3.713e+02
Mn	2.424e-05	2.424e+01
N	1.150e-05	1.150e+01
Na	1.251e-04	1.251e+02
Ni	1.022e-07	1.022e-01
S	7.188e-05	7.188e+01
Si	1.523e-04	1.523e+02
Sr	8.904e-07	8.904e-01
U	2.689e-07	2.689e-01

```

-----Description of solution-----
                                pH = 6.250      Charge balance
                                pe = 3.329      Adjusted to redox equilibrium
                                Activity of water = 1.000
                                Ionic strength (mol/kgw) = 2.370e-03
                                Mass of water (kg) = 1.000e+06
                                Total alkalinity (eq/kg) = 1.130e-03
                                Total CO2 (mol/kg) = 2.148e-03
                                Temperature (°C) = 3.60
                                Pressure (atm) = 1.87
                                Electrical balance (eq) = 4.287e+02
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 14.02
                                Iterations = 3
                                Total H = 1.110163e+08
                                Total O = 5.551358e+07

```

```

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

```

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	5.902e-07	5.623e-07	-6.229	-6.250	-0.021	0.00
OH-	3.301e-09	3.133e-09	-8.481	-8.504	-0.023	(0)
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.02
Al	2.706e-06					
Al(OH)3	1.826e-06	1.827e-06	-5.739	-5.738	0.000	(0)
Al(OH)2+	8.581e-07	8.155e-07	-6.066	-6.089	-0.022	(0)
AlOH+2	1.532e-08	1.249e-08	-7.815	-7.903	-0.088	(0)
Al+3	5.012e-09	3.243e-09	-8.300	-8.489	-0.189	(0)
Al(OH)4-	1.089e-09	1.034e-09	-8.963	-8.985	-0.022	(0)
AlSO4+	1.460e-10	1.386e-10	-9.836	-9.858	-0.022	(0)
Al(SO4)2-	5.727e-13	5.439e-13	-12.242	-12.264	-0.022	(0)
As(3)	2.901e-10					
H3AsO3	2.900e-10	2.901e-10	-9.538	-9.537	0.000	(0)
H2AsO3-	1.366e-13	1.297e-13	-12.865	-12.887	-0.023	(0)
H4AsO3+	8.514e-17	8.084e-17	-16.070	-16.092	-0.023	(0)
HAsO3-2	8.280e-20	6.727e-20	-19.082	-19.172	-0.090	(0)
AsO3-3	3.340e-27	2.093e-27	-26.476	-26.679	-0.203	(0)
As(5)	5.310e-08					
H2AsO4-	3.998e-08	3.796e-08	-7.398	-7.421	-0.023	(0)
HAsO4-2	1.312e-08	1.066e-08	-7.882	-7.972	-0.090	(0)
H3AsO4	2.994e-12	2.996e-12	-11.524	-11.523	0.000	(0)
AsO4-3	4.345e-14	2.723e-14	-13.362	-13.565	-0.203	(0)
B	5.180e-06					
H3BO3	5.176e-06	5.179e-06	-5.286	-5.286	0.000	(0)
H2BO3-	3.692e-09	3.501e-09	-8.433	-8.456	-0.023	(0)
Ba	7.282e-08					
Ba+2	7.282e-08	5.933e-08	-7.138	-7.227	-0.089	(0)
BaOH+	6.795e-16	6.456e-16	-15.168	-15.190	-0.022	(0)
Br	2.253e-07					
Br-	2.253e-07	2.139e-07	-6.647	-6.670	-0.023	(0)
NiBr+	4.280e-14	4.064e-14	-13.369	-13.391	-0.023	(0)
C(4)	2.148e-03					
HCO3-	1.117e-03	1.062e-03	-2.952	-2.974	-0.022	(0)
H2CO3	1.025e-03	1.026e-03	-2.989	-2.989	0.000	(0)
MgHCO3+	3.087e-06	2.931e-06	-5.510	-5.533	-0.023	(0)
CaHCO3+	1.596e-06	1.517e-06	-5.797	-5.819	-0.022	(0)
MnHCO3+	2.317e-07	2.201e-07	-6.635	-6.657	-0.022	(0)
UO2CO3	2.024e-07	2.026e-07	-6.694	-6.693	0.000	(0)
UO2(CO3)2-2	6.348e-08	5.158e-08	-7.197	-7.288	-0.090	(0)
CO3-2	6.182e-08	5.042e-08	-7.209	-7.297	-0.088	(0)
NaHCO3	4.047e-08	4.050e-08	-7.393	-7.393	0.000	(0)
NiCO3	2.245e-08	2.246e-08	-7.649	-7.649	0.000	(0)
CaCO3	1.394e-08	1.395e-08	-7.856	-7.856	0.000	(0)
MgCO3	1.037e-08	1.038e-08	-7.984	-7.984	0.000	(0)
NiHCO3+	5.296e-09	5.028e-09	-8.276	-8.299	-0.023	(0)
UO2(CO3)3-4	7.255e-10	3.162e-10	-9.139	-9.500	-0.361	(0)
NaCO3-	3.651e-11	3.470e-11	-10.438	-10.460	-0.022	(0)
Ni(CO3)2-2	2.422e-12	1.968e-12	-11.616	-11.706	-0.090	(0)
Ca	3.289e-04					
Ca+2	3.248e-04	2.657e-04	-3.488	-3.576	-0.087	(0)
CaSO4	2.413e-06	2.415e-06	-5.617	-5.617	0.000	(0)
CaHCO3+	1.596e-06	1.517e-06	-5.797	-5.819	-0.022	(0)
CaCO3	1.394e-08	1.395e-08	-7.856	-7.856	0.000	(0)
CaOH+	1.882e-11	1.790e-11	-10.725	-10.747	-0.022	(0)
Cl	6.338e-05					
Cl-	6.338e-05	6.012e-05	-4.198	-4.221	-0.023	(0)
MnCl+	4.992e-09	4.743e-09	-8.302	-8.324	-0.022	(0)
NiCl+	9.536e-12	9.053e-12	-11.021	-11.043	-0.023	(0)
MnCl2	7.742e-14	7.746e-14	-13.111	-13.111	0.000	(0)
UO2Cl+	2.898e-14	2.751e-14	-13.538	-13.560	-0.023	(0)
NiCl2	1.980e-15	1.981e-15	-14.703	-14.703	0.000	(0)
FeCl+2	2.780e-18	2.265e-18	-17.556	-17.645	-0.089	(0)
MnCl3-	2.210e-18	2.099e-18	-17.656	-17.678	-0.022	(0)
FeCl2+	1.330e-21	1.263e-21	-20.876	-20.898	-0.022	(0)
FeCl3	7.591e-27	7.595e-27	-26.120	-26.119	0.000	(0)
UCl+3	5.962e-34	3.736e-34	-33.225	-33.428	-0.203	(0)
Fe(2)	5.926e-05					

Fe+2	5.896e-05	4.817e-05	-4.229	-4.317	-0.088	(0)
FeSO4	3.036e-07	3.038e-07	-6.518	-6.517	0.000	(0)
FeOH+	5.096e-09	4.842e-09	-8.293	-8.315	-0.022	(0)
Fe(OH)2	9.865e-15	9.870e-15	-14.006	-14.006	0.000	(0)
Fe(OH)3-	5.477e-19	5.203e-19	-18.261	-18.284	-0.022	(0)
Fe(HS)2	0.000e+00	0.000e+00	-95.537	-95.537	0.000	(0)
Fe(HS)3-	0.000e+00	0.000e+00	-143.563	-143.585	-0.023	(0)
Fe(3)	1.884e-08					
Fe(OH)2+	1.846e-08	1.754e-08	-7.734	-7.756	-0.022	(0)
Fe(OH)3	3.665e-10	3.667e-10	-9.436	-9.436	0.000	(0)
FeOH+2	9.404e-12	7.662e-12	-11.027	-11.116	-0.089	(0)
Fe(OH)4-	6.865e-12	6.525e-12	-11.163	-11.185	-0.022	(0)
Fe+3	4.005e-15	2.591e-15	-14.397	-14.587	-0.189	(0)
FeSO4+	7.360e-16	6.993e-16	-15.133	-15.155	-0.022	(0)
FeCl+2	2.780e-18	2.265e-18	-17.556	-17.645	-0.089	(0)
Fe(SO4)2-	1.151e-18	1.092e-18	-17.939	-17.962	-0.023	(0)
Fe2(OH)2+4	9.398e-21	4.095e-21	-20.027	-20.388	-0.361	(0)
FeCl2+	1.330e-21	1.263e-21	-20.876	-20.898	-0.022	(0)
Fe3(OH)4+5	4.950e-26	1.352e-26	-25.305	-25.869	-0.564	(0)
FeCl3	7.591e-27	7.595e-27	-26.120	-26.119	0.000	(0)
H(0)	1.235e-22					
H2	6.175e-23	6.178e-23	-22.209	-22.209	0.000	(0)
K	5.033e-05					
K+	5.032e-05	4.774e-05	-4.298	-4.321	-0.023	(0)
KSO4-	1.276e-08	1.213e-08	-7.894	-7.916	-0.022	(0)
Li	5.763e-07					
Li+	5.761e-07	5.478e-07	-6.239	-6.261	-0.022	(0)
LiSO4-	1.360e-10	1.292e-10	-9.866	-9.889	-0.022	(0)
Mg	3.713e-04					
Mg+2	3.658e-04	2.997e-04	-3.437	-3.523	-0.087	(0)
MgHCO3+	3.087e-06	2.931e-06	-5.510	-5.533	-0.023	(0)
MgSO4	2.398e-06	2.400e-06	-5.620	-5.620	0.000	(0)
MgCO3	1.037e-08	1.038e-08	-7.984	-7.984	0.000	(0)
MgOH+	1.253e-10	1.191e-10	-9.902	-9.924	-0.022	(0)
Mn(2)	2.424e-05					
Mn+2	2.386e-05	1.950e-05	-4.622	-4.710	-0.088	(0)
MnHCO3+	2.317e-07	2.201e-07	-6.635	-6.657	-0.022	(0)
MnSO4	1.444e-07	1.445e-07	-6.840	-6.840	0.000	(0)
MnCl+	4.992e-09	4.743e-09	-8.302	-8.324	-0.022	(0)
MnOH+	1.434e-10	1.362e-10	-9.844	-9.866	-0.022	(0)
MnCl2	7.742e-14	7.746e-14	-13.111	-13.111	0.000	(0)
MnCl3-	2.210e-18	2.099e-18	-17.656	-17.678	-0.022	(0)
Mn(OH)3-	1.833e-21	1.741e-21	-20.737	-20.759	-0.022	(0)
Mn(NO3)2	0.000e+00	0.000e+00	-95.099	-95.099	0.000	(0)
Mn(3)	5.776e-26					
Mn+3	5.776e-26	3.737e-26	-25.238	-25.428	-0.189	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-68.245	-68.334	-0.089	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-75.873	-75.896	-0.023	(0)
N(-3)	1.150e-05					
NH4+	1.149e-05	1.089e-05	-4.940	-4.963	-0.023	(0)
NH4SO4-	7.985e-09	7.586e-09	-8.098	-8.120	-0.022	(0)
NH3	2.155e-09	2.157e-09	-8.666	-8.666	0.000	(0)
N(3)	2.559e-34					
NO2-	2.559e-34	2.429e-34	-33.592	-33.614	-0.023	(0)
N(5)	0.000e+00					
NO3-	0.000e+00	0.000e+00	-45.483	-45.506	-0.023	(0)
Mn(NO3)2	0.000e+00	0.000e+00	-95.099	-95.099	0.000	(0)
Na	1.251e-04					
Na+	1.251e-04	1.188e-04	-3.903	-3.925	-0.022	(0)
NaHCO3	4.047e-08	4.050e-08	-7.393	-7.393	0.000	(0)
NaSO4-	2.926e-08	2.780e-08	-7.534	-7.556	-0.022	(0)
NaCO3-	3.651e-11	3.470e-11	-10.438	-10.460	-0.022	(0)
Ni	1.022e-07					
Ni+2	7.395e-08	6.009e-08	-7.131	-7.221	-0.090	(0)
NiCO3	2.245e-08	2.246e-08	-7.649	-7.649	0.000	(0)
NiHCO3+	5.296e-09	5.028e-09	-8.276	-8.299	-0.023	(0)
NiSO4	5.190e-10	5.193e-10	-9.285	-9.285	0.000	(0)
NiCl+	9.536e-12	9.053e-12	-11.021	-11.043	-0.023	(0)
NiOH+	3.074e-12	2.918e-12	-11.512	-11.535	-0.023	(0)
Ni(CO3)2-2	2.422e-12	1.968e-12	-11.616	-11.706	-0.090	(0)
NiBr+	4.280e-14	4.064e-14	-13.369	-13.391	-0.023	(0)
Ni(OH)2	1.901e-14	1.903e-14	-13.721	-13.721	0.000	(0)
Ni(SO4)2-2	2.262e-15	1.838e-15	-14.645	-14.736	-0.090	(0)
NiCl2	1.980e-15	1.981e-15	-14.703	-14.703	0.000	(0)
Ni(OH)3-	3.566e-19	3.385e-19	-18.448	-18.470	-0.023	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-55.402	-55.401	0.000	(0)
S(-2)	0.000e+00					
H2S	0.000e+00	0.000e+00	-49.054	-49.054	0.000	(0)
HS-	0.000e+00	0.000e+00	-50.062	-50.085	-0.023	(0)
S6-2	0.000e+00	0.000e+00	-53.626	-53.716	-0.090	(0)
S5-2	0.000e+00	0.000e+00	-53.867	-53.957	-0.090	(0)
S4-2	0.000e+00	0.000e+00	-54.124	-54.214	-0.090	(0)
S-2	0.000e+00	0.000e+00	-57.350	-57.439	-0.089	(0)
S3-2	0.000e+00	0.000e+00	-57.616	-57.706	-0.090	(0)
S2-2	0.000e+00	0.000e+00	-58.919	-59.009	-0.090	(0)
Fe(HS)2	0.000e+00	0.000e+00	-95.537	-95.537	0.000	(0)
Fe(HS)3-	0.000e+00	0.000e+00	-143.563	-143.585	-0.023	(0)
S(6)	7.188e-05					
SO4-2	6.656e-05	5.405e-05	-4.177	-4.267	-0.090	(0)
CaSO4	2.413e-06	2.415e-06	-5.617	-5.617	0.000	(0)
MgSO4	2.398e-06	2.400e-06	-5.620	-5.620	0.000	(0)
FeSO4	3.036e-07	3.038e-07	-6.518	-6.517	0.000	(0)
MnSO4	1.444e-07	1.445e-07	-6.840	-6.840	0.000	(0)
NaSO4-	2.926e-08	2.780e-08	-7.534	-7.556	-0.022	(0)
KSO4-	1.276e-08	1.213e-08	-7.894	-7.916	-0.022	(0)
NH4SO4-	7.985e-09	7.586e-09	-8.098	-8.120	-0.022	(0)
HSO4-	1.755e-09	1.666e-09	-8.756	-8.778	-0.022	(0)
NiSO4	5.190e-10	5.193e-10	-9.285	-9.285	0.000	(0)
AlSO4+	1.460e-10	1.386e-10	-9.836	-9.858	-0.022	(0)
LiSO4-	1.360e-10	1.292e-10	-9.866	-9.889	-0.022	(0)

UO2SO4	4.601e-12	4.604e-12	-11.337	-11.337	0.000	(0)
Al (SO4) 2-	5.727e-13	5.439e-13	-12.242	-12.264	-0.022	(0)
UO2 (SO4) 2-2	8.006e-15	6.505e-15	-14.097	-14.187	-0.090	(0)
Ni (SO4) 2-2	2.262e-15	1.838e-15	-14.645	-14.736	-0.090	(0)
FeSO4+	7.360e-16	6.993e-16	-15.133	-15.155	-0.022	(0)
Fe (SO4) 2-	1.151e-18	1.092e-18	-17.939	-17.962	-0.023	(0)
USO4+2	1.238e-29	1.006e-29	-28.907	-28.997	-0.090	(0)
U (SO4) 2	6.339e-30	6.343e-30	-29.198	-29.198	0.000	(0)
Si	1.523e-04					
H4SiO4	1.523e-04	1.524e-04	-3.817	-3.817	0.000	(0)
H3SiO4-	9.842e-09	9.344e-09	-8.007	-8.029	-0.023	(0)
UO2H3SiO4+	3.681e-10	3.495e-10	-9.434	-9.457	-0.023	(0)
H2SiO4-2	2.295e-15	1.872e-15	-14.639	-14.728	-0.088	(0)
Sr	8.904e-07					
Sr+2	8.904e-07	7.254e-07	-6.050	-6.139	-0.089	(0)
SrOH+	1.360e-14	1.292e-14	-13.866	-13.889	-0.022	(0)
U (3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-43.287	-43.490	-0.203	(0)
U (4)	4.200e-14					
U (OH) 5-	4.068e-14	3.863e-14	-13.391	-13.413	-0.023	(0)
U (OH) 4	1.312e-15	1.313e-15	-14.882	-14.882	0.000	(0)
U (OH) 3+	3.744e-18	3.554e-18	-17.427	-17.449	-0.023	(0)
U (OH) 2+2	2.159e-21	1.754e-21	-20.666	-20.756	-0.090	(0)
UOH+3	1.581e-25	9.910e-26	-24.801	-25.004	-0.203	(0)
USO4+2	1.238e-29	1.006e-29	-28.907	-28.997	-0.090	(0)
U (SO4) 2	6.339e-30	6.343e-30	-29.198	-29.198	0.000	(0)
U+4	2.394e-30	1.043e-30	-29.621	-29.982	-0.361	(0)
UCl+3	5.962e-34	3.736e-34	-33.225	-33.428	-0.203	(0)
U6 (OH) 15+9	0.000e+00	0.000e+00	-101.538	-103.364	-1.826	(0)
U (5)	1.498e-10					
UO2+	1.498e-10	1.422e-10	-9.824	-9.847	-0.023	(0)
U (6)	2.687e-07					
UO2CO3	2.024e-07	2.026e-07	-6.694	-6.693	0.000	(0)
UO2 (CO3) 2-2	6.348e-08	5.158e-08	-7.197	-7.288	-0.090	(0)
UO2OH+	1.301e-09	1.235e-09	-8.886	-8.908	-0.023	(0)
UO2 (CO3) 3-4	7.255e-10	3.162e-10	-9.139	-9.500	-0.361	(0)
UO2+2	3.986e-10	3.239e-10	-9.399	-9.490	-0.090	(0)
UO2H3SiO4+	3.681e-10	3.495e-10	-9.434	-9.457	-0.023	(0)
UO2SO4	4.601e-12	4.604e-12	-11.337	-11.337	0.000	(0)
(UO2) 2 (OH) 2+2	2.436e-13	1.979e-13	-12.613	-12.704	-0.090	(0)
UO2Cl+	2.898e-14	2.751e-14	-13.538	-13.560	-0.023	(0)
UO2 (SO4) 2-2	8.006e-15	6.505e-15	-14.097	-14.187	-0.090	(0)
(UO2) 3 (OH) 5+	6.177e-15	5.864e-15	-14.209	-14.232	-0.023	(0)

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

Phase	SI**	log IAP	log K (276 K, 2 atm)	
Akermanite	-32.61	19.19	51.81	Ca2MgSi2O7
Al (OH) 3 (a)	-1.65	10.26	11.91	Al (OH) 3
Al2O3	-2.46	20.52	22.98	Al2O3
Al4 (OH) 10SO4	1.58	24.28	22.70	Al4 (OH) 10SO4
AlAsO4:2H2O	-6.06	-1.26	4.80	AlAsO4:2H2O
Albite	-3.51	1.13	4.64	NaAlSi3O8
Albite (low)	-2.44	1.13	3.58	NaAlSi3O8
AlOHSO4	-3.28	-6.51	-3.23	AlOHSO4
AlumK	-15.76	-21.34	-5.58	KAl (SO4) 2:12H2O
Alunite	0.75	-0.82	-1.57	KAl3 (SO4) 2 (OH) 6
Analcime	-3.06	4.95	8.01	NaAlSi2O6:H2O
Anhydrite	-3.42	-7.84	-4.42	CaSO4
Annite	-1.73	25.29	27.01	KFe3AlSi3O10 (OH) 2
Anorthite	-7.62	21.81	29.43	CaAl2Si2O8
Aragonite	-2.64	-10.87	-8.23	CaCO3
Arsenolite	-34.54	-38.15	-3.61	As4O6
Artinite	-13.07	-1.84	11.23	MgCO3:Mg (OH) 2:3H2O
As2O5	-30.05	-23.05	7.01	As2O5
B UO2 (OH) 2	-3.31	3.01	6.32	UO2 (OH) 2
Ba3 (AsO4) 2	1.83	-7.23	-9.06	Ba3 (AsO4) 2
Barite	-1.16	-11.49	-10.33	BaSO4
Birnessite	-15.19	2.90	18.09	MnO2
Bixbyite	-13.61	-13.36	0.25	Mn2O3
Boehmite	0.09	10.26	10.17	AlOOH
Brucite	-9.28	8.98	18.26	Mg (OH) 2
Bunsenite	-8.53	5.28	13.81	NiO
Ca-Nontronite	20.07	-0.82	-20.89	Fe2Al.33Si3.67O10 (OH) 2Ca0.165
Ca-Olivine	-26.72	14.03	40.75	Ca2SiO4
Ca3 (AsO4) 2:6H2O	-18.57	3.73	22.30	Ca3 (AsO4) 2:6H2O
Ca3SiO5	-56.94	22.96	79.89	Ca3SiO5
Calcite	-2.48	-10.87	-8.39	CaCO3
Celestine	-3.97	-10.41	-6.44	SrSO4
CH4 (g)	-52.88	-96.43	-43.56	CH4
Chalcedony	-0.03	-3.82	-3.78	SiO2
Chrysotile	-15.87	19.30	35.16	Mg3Si2O5 (OH) 4
Claudetite	-34.33	-38.15	-3.82	As4O6
Clinoenstatite	-7.31	5.16	12.47	MgSiO3
CO2 (g)	-1.61	-19.80	-18.19	CO2
Cristobalite	0.08	-3.82	-3.90	SiO2
Diaspore	1.99	10.26	8.27	AlOOH
Diopside	-11.45	10.27	21.72	CaMgSi2O6
Dolomite	-5.16	-21.69	-16.53	CaMg (CO3) 2
Epsomite	-5.49	-7.79	-2.30	MgSO4:7H2O
Fe (OH) 2.7Cl0.3	4.06	1.02	-3.04	Fe (OH) 2.7Cl0.3
Fe2 (SO4) 3	-48.91	-41.97	6.93	Fe2 (SO4) 3
Fe3 (OH) 8	-3.71	16.51	20.22	Fe3 (OH) 8
FeAsO4:2H2O	-7.76	-7.36	0.40	FeAsO4:2H2O
Ferrihydrite	-0.73	4.16	4.89	Fe (OH) 3
FeS (ppt)	-44.24	-48.15	-3.92	FeS
Forsterite	-16.91	14.14	31.05	Mg2SiO4
Gehlenite	-28.85	34.55	63.40	Ca2Al2SiO7
Gibbsite (C)	0.20	10.26	10.06	Al (OH) 3
Goethite	2.84	4.16	1.32	FeOOH
Greenalite	-3.90	16.91	20.81	Fe3Si2O5 (OH) 4
Greigite	-163.80	-208.83	-45.03	Fe3S4

Gummite	-8.70	3.01	11.71	UO3
Gypsum	-3.22	-7.84	-4.62	CaSO4:2H2O
Halite	-9.68	-8.15	1.53	NaCl
Halloysite	1.64	12.89	11.25	Al2Si2O5 (OH) 4
Hausmannite	-23.55	42.53	66.08	Mn3O4
Hematite	10.59	8.33	-2.26	Fe2O3
Hercynite	-2.90	28.70	31.60	FeAl2O4
Huntite	-14.83	-43.34	-28.51	CaMg3 (CO3) 4
Hydromagnesite	-28.50	-34.31	-5.81	Mg5 (CO3) 4 (OH) 2:4H2O
Jarosite-H	-12.07	-21.04	-8.98	(H3O) Fe3 (SO4) 2 (OH) 6
Jarosite-K	-6.09	-19.12	-13.03	KFe3 (SO4) 2 (OH) 6
Jarosite-Na	-9.57	-18.72	-9.15	NaFe3 (SO4) 2 (OH) 6
K-Nontronite	13.89	-1.66	-15.55	Fe2Al.33Si3.67O10 (OH) 2K0.33
Kalsilite	-6.10	8.37	14.48	KAlSiO4
Kaolinite	5.16	12.89	7.73	Al2Si2O5 (OH) 4
Larnite	-28.35	14.03	42.39	Ca2SiO4
Laumontite	-3.14	14.18	17.32	CaAl2Si4O12:4H2O
Leonhardite	7.03	28.36	21.33	Ca2Al4Si8O24:7H2O
Lepidocrocite	2.79	4.16	1.37	FeOOH
Leucite	-3.12	4.56	7.68	KAlSi2O6
Lime	-26.49	8.92	35.42	CaO
Mackinawite	-43.50	-48.15	-4.65	FeS
Magadiite	-10.10	-24.39	-14.30	NaSi7O13 (OH) 3:3H2O
Maghemite	1.94	8.33	6.39	Fe2O3
Magnesite	-3.14	-10.82	-7.68	MgCO3
Magnetite	9.91	16.51	6.60	Fe3O4
Manganite	-6.44	-6.68	-0.24	MnOOH
Melanterite	-5.95	-8.58	-2.63	FeSO4:7H2O
Merwinite	-46.50	28.12	74.61	Ca3MgSi2O8
Mg-Ferrite	-3.24	17.30	20.54	MgFe2O4
Mg-Nontronite	19.77	-0.81	-20.59	Fe2Al.33Si3.67O10 (OH) 2Mg0.165
Microcline	-0.58	0.74	1.31	KAlSi3O8
Millerite	-42.87	-51.06	-8.18	NiS
Mirabilite	-9.92	-12.12	-2.19	Na2SO4:10H2O
Mn2 (SO4) 3	-60.16	-63.66	-3.50	Mn2 (SO4) 3
Mn3 (AsO4) 2:8H2O	-12.17	0.32	12.50	Mn3 (AsO4) 2:8H2O
MnCl2:4H2O	-14.88	-13.15	1.72	MnCl2:4H2O
MnS (Green)	-52.67	-48.54	4.13	MnS
MnSO4	-12.52	-8.98	3.55	MnSO4
Monticellite	-18.99	14.08	33.07	CaMgSiO4
Montmorillonite	5.60	8.27	2.67	Mg0.485Fe.22Al1.71Si3.81O10 (OH) 2
Morenosite	-8.96	-11.49	-2.53	NiSO4:7H2O
Muscovite	4.91	21.26	16.35	KAl3Si3O10 (OH) 2
Na-Nontronite	12.98	-1.53	-14.50	Fe2Al.33Si3.67O10 (OH) 2Na0.33
Natron	-12.94	-15.15	-2.21	Na2CO3:10H2O
Nepheline	-7.33	8.77	16.10	NaAlSiO4
Nesquehonite	-5.53	-10.82	-5.29	MgCO3:3H2O
Ni (OH) 2	-3.79	5.28	9.07	Ni (OH) 2
Ni2SiO4	-9.69	6.74	16.43	Ni2SiO4
Ni3 (AsO4) 2:8H2O	-22.91	-7.21	15.70	Ni3 (AsO4) 2:8H2O
Ni4 (OH) 6SO4	-27.65	4.35	32.00	Ni4 (OH) 6SO4
NiCO3	-8.24	-14.52	-6.28	NiCO3
Nsutite	-14.60	2.90	17.50	MnO2
O2 (g)	-52.39	38.32	90.70	O2
Oripment	-122.41	-188.08	-65.67	As2S3
P-Wollstanite	-9.93	5.11	15.04	CaSiO3
Periclase	-14.58	8.98	23.56	MgO
Phlogopite	-43.53	27.67	71.19	KMg3AlSi3O10 (OH) 2
Portlandite	-15.49	8.92	24.41	Ca (OH) 2
Pyrite	-66.21	-85.33	-19.12	FeS2
Pyrocroite	-8.58	7.79	16.37	Mn (OH) 2
Pyrolusite	-14.61	2.90	17.51	MnO2
Pyrophyllite	6.85	5.25	-1.60	Al2Si4O10 (OH) 2
Quartz	0.54	-3.82	-4.36	SiO2
Realgar	-53.97	-75.45	-21.48	AsS
Retgersite	-9.38	-11.49	-2.10	NiSO4:6H2O
Rhodochrosite	-1.72	-12.01	-10.29	MnCO3
Rutherfordine	-2.33	-16.79	-14.46	UO2CO3
Sanidine (H)	-1.13	0.74	1.87	KAlSi3O8
Schoepite	-3.08	3.01	6.09	UO2 (OH) 2:H2O
Sepiolite(a)	-12.28	6.50	18.78	Mg2Si3O7.5OH:3H2O
Sepiolite(c)	-10.96	6.50	17.46	Mg2Si3O7.5OH:3H2O
Siderite	-1.37	-11.61	-10.25	FeCO3
SiO2 (a)	-0.55	-3.82	-3.27	SiO2
SiO2 (am)	-0.89	-3.82	-2.93	SiO2
Spinel	-11.88	29.50	41.38	MgAl2O4
Strontianite	-4.23	-13.44	-9.21	SrCO3
Sulfur	-35.30	-37.18	-1.87	S
Talc	-13.38	11.66	25.04	Mg3Si4O10 (OH) 2
Thenardite	-11.97	-12.12	-0.15	Na2SO4
Thermonatrite	-15.43	-15.15	0.28	Na2CO3:H2O
Tremolite	-29.83	32.20	62.02	Ca2Mg5Si8O22 (OH) 2
U3O8 (C)	-4.31	23.37	27.68	U3O8
U4O9 (C)	-3.12	-0.77	2.35	U4O9
UO2 (am)	-7.40	-4.98	2.42	UO2
UO2 (NO3) 2	-114.01	-100.50	13.51	UO2 (NO3) 2
UO2 (NO3) 2:2H2O	-105.69	-100.50	5.19	UO2 (NO3) 2:2H2O
UO2 (NO3) 2:3H2O	-104.28	-100.50	3.78	UO2 (NO3) 2:3H2O
UO2 (NO3) 2:6H2O	-102.53	-100.50	2.03	UO2 (NO3) 2:6H2O
UO3 (C)	-5.80	3.01	8.81	UO3
Uraninite	-1.34	-4.98	-3.64	UO2
Uranophane	-10.18	7.31	17.49	Ca (UO2) 2 (SiO3OH) 2
UsiO4 (C)	-2.00	-8.80	-6.80	UsiO4
Wairakite	-8.27	14.18	22.45	CaAl2Si4O12:2H2O
Witherite	-5.92	-14.52	-8.61	BaCO3
Wollastonite	-8.99	5.11	14.10	CaSiO3

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

End of simulation.

1.4 D-pit, 13 m

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.

Using pressure 1.

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

Elements	Molality	Moles
Al	2.483e-06	2.483e+01
As	2.136e-07	2.136e+00
B	8.325e-06	8.325e+01
Ba	2.185e-07	2.185e+00
Br	6.383e-07	6.383e+00
C	2.358e-03	2.357e+04
Ca	3.528e-04	3.528e+03
Cl	1.039e-04	1.039e+03
Fe	6.520e-04	6.520e+03
K	6.294e-05	6.294e+02
Li	7.204e-07	7.204e+00
Mg	4.224e-04	4.224e+03
Mn	5.800e-05	5.800e+02
Na	1.881e-04	1.881e+03
Ni	1.193e-07	1.193e+00
S	4.063e-05	4.063e+02
Si	1.790e-04	1.790e+03
Sr	1.484e-06	1.484e+01
U	5.504e-07	5.504e+00

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

pH	=	6.650	Charge balance
pe	=	-1.769	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength (mol/kgw)	=	4.067e-03	
Mass of water (kg)	=	1.000e+07	
Total alkalinity (eq/kg)	=	1.745e-03	
Total CO2 (mol/kg)	=	2.358e-03	
Temperature (°C)	=	3.70	
Pressure (atm)	=	2.12	
Electrical balance (eq)	=	1.305e+04	
Percent error, 100*(Cat- An)/(Cat+ An)	=	25.52	
Iterations	=	3	
Total H	=	1.110162e+09	
Total O	=	5.551420e+08	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	2.380e-07	2.239e-07	-6.623	-6.650	-0.027	0.00
OH-	8.494e-09	7.939e-09	-8.071	-8.100	-0.029	(0)
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.02
Al	2.483e-06					
Al (OH) 3	2.081e-06	2.083e-06	-5.682	-5.681	0.000	(0)
Al (OH) 2+	3.951e-07	3.702e-07	-6.403	-6.432	-0.028	(0)
Al (OH) 4-	3.260e-09	3.051e-09	-8.487	-8.516	-0.029	(0)
AlOH+2	2.953e-09	2.275e-09	-8.530	-8.643	-0.113	(0)
Al+3	4.039e-10	2.332e-10	-9.394	-9.632	-0.239	(0)
AlSO4+	5.468e-12	5.117e-12	-11.262	-11.291	-0.029	(0)
Al (SO4) 2-	1.100e-14	1.030e-14	-13.959	-13.987	-0.029	(0)
As (3)	2.136e-07					
H3AsO3	2.133e-07	2.135e-07	-6.671	-6.671	0.000	(0)
H2AsO3-	2.573e-10	2.407e-10	-9.590	-9.619	-0.029	(0)
H4AsO3+	2.531e-14	2.368e-14	-13.597	-13.626	-0.029	(0)
HAsO3-2	4.117e-16	3.153e-16	-15.385	-15.501	-0.116	(0)
AsO3-3	4.510e-23	2.474e-23	-22.346	-22.607	-0.261	(0)
As (5)	5.714e-14					
H2AsO4-	3.069e-14	2.871e-14	-13.513	-13.542	-0.029	(0)
HAsO4-2	2.645e-14	2.026e-14	-13.578	-13.693	-0.116	(0)
H3AsO4	9.021e-19	9.030e-19	-18.045	-18.044	0.000	(0)
AsO4-3	2.377e-19	1.304e-19	-18.624	-18.885	-0.261	(0)
B	8.325e-06					
H3BO3	8.310e-06	8.317e-06	-5.080	-5.080	0.000	(0)
H2BO3-	1.516e-08	1.415e-08	-7.819	-7.849	-0.030	(0)
Ba	2.185e-07					
Ba+2	2.185e-07	1.680e-07	-6.661	-6.775	-0.114	(0)
BaOH+	4.954e-15	4.639e-15	-14.305	-14.334	-0.029	(0)
Br	6.383e-07					
Br-	6.383e-07	5.970e-07	-6.195	-6.224	-0.029	(0)
NiBr+	8.353e-14	7.814e-14	-13.078	-13.107	-0.029	(0)
C (4)	2.358e-03					
HCO3-	1.726e-03	1.617e-03	-2.763	-2.791	-0.028	(0)
H2CO3	6.225e-04	6.231e-04	-3.206	-3.205	0.000	(0)
MgHCO3+	5.150e-06	4.817e-06	-5.288	-5.317	-0.029	(0)
CaHCO3+	2.514e-06	2.358e-06	-5.600	-5.628	-0.028	(0)
MnHCO3+	8.116e-07	7.600e-07	-6.091	-6.119	-0.029	(0)
CO3-2	2.512e-07	1.936e-07	-6.600	-6.713	-0.113	(0)
NaHCO3	9.158e-08	9.167e-08	-7.038	-7.038	0.000	(0)
NiCO3	5.934e-08	5.940e-08	-7.227	-7.226	0.000	(0)
CaCO3	5.442e-08	5.447e-08	-7.264	-7.264	0.000	(0)
MgCO3	4.295e-08	4.299e-08	-7.367	-7.367	0.000	(0)
NiHCO3+	5.659e-09	5.294e-09	-8.247	-8.276	-0.029	(0)
UO2 (CO3) 2-2	3.289e-10	2.519e-10	-9.483	-9.599	-0.116	(0)
UO2CO3	2.567e-10	2.570e-10	-9.591	-9.590	0.000	(0)
NaCO3-	2.118e-10	1.985e-10	-9.674	-9.702	-0.028	(0)

Ni (CO ₃) 2-2	2.609e-11	1.998e-11	-10.584	-10.699	-0.116	(0)
UO ₂ (CO ₃) 3-4	1.710e-11	5.880e-12	-10.767	-11.231	-0.464	(0)
Ca	3.528e-04					
Ca+2	3.490e-04	2.702e-04	-3.457	-3.568	-0.111	(0)
CaHCO ₃ +	2.514e-06	2.358e-06	-5.600	-5.628	-0.028	(0)
CaSO ₄	1.258e-06	1.260e-06	-5.900	-5.900	0.000	(0)
CaCO ₃	5.442e-08	5.447e-08	-7.264	-7.264	0.000	(0)
CaOH+	4.923e-11	4.616e-11	-10.308	-10.336	-0.028	(0)
Cl	1.039e-04					
Cl-	1.039e-04	9.709e-05	-3.983	-4.013	-0.030	(0)
MnCl+	1.848e-08	1.730e-08	-7.733	-7.762	-0.029	(0)
NiCl+	1.077e-11	1.007e-11	-10.968	-10.997	-0.029	(0)
MnCl2	4.559e-13	4.563e-13	-12.341	-12.341	0.000	(0)
NiCl2	3.555e-15	3.558e-15	-14.449	-14.449	0.000	(0)
MnCl3-	2.133e-17	1.997e-17	-16.671	-16.700	-0.029	(0)
UO ₂ Cl+	1.571e-17	1.470e-17	-16.804	-16.833	-0.029	(0)
FeCl+2	3.998e-22	3.075e-22	-21.398	-21.512	-0.114	(0)
FeCl2+	2.947e-25	2.760e-25	-24.531	-24.559	-0.029	(0)
UCl+3	1.412e-28	7.745e-29	-27.850	-28.111	-0.261	(0)
FeCl3	2.677e-30	2.679e-30	-29.572	-29.572	0.000	(0)
Fe (2)	6.520e-04					
Fe+2	6.502e-04	5.025e-04	-3.187	-3.299	-0.112	(0)
FeSO ₄	1.626e-06	1.628e-06	-5.789	-5.788	0.000	(0)
FeOH+	1.367e-07	1.280e-07	-6.864	-6.893	-0.029	(0)
Fe (OH) 2	6.616e-13	6.622e-13	-12.179	-12.179	0.000	(0)
Fe (OH) 3-	9.376e-17	8.780e-17	-16.028	-16.057	-0.029	(0)
Fe (HS) 2	1.720e-21	1.721e-21	-20.765	-20.764	0.000	(0)
Fe (HS) 3-	1.242e-32	1.162e-32	-31.906	-31.935	-0.029	(0)
Fe (3)	1.041e-11					
Fe (OH) 2+	9.897e-12	9.273e-12	-11.004	-11.033	-0.028	(0)
Fe (OH) 3	4.866e-13	4.870e-13	-12.313	-12.312	0.000	(0)
Fe (OH) 4-	2.324e-14	2.177e-14	-13.634	-13.662	-0.028	(0)
FeOH+2	2.111e-15	1.623e-15	-14.676	-14.790	-0.114	(0)
Fe+3	3.759e-19	2.170e-19	-18.425	-18.663	-0.239	(0)
FeSO ₄ +	3.214e-20	3.010e-20	-19.493	-19.521	-0.029	(0)
FeCl+2	3.998e-22	3.075e-22	-21.398	-21.512	-0.114	(0)
Fe (SO ₄) 2-	2.577e-23	2.411e-23	-22.589	-22.618	-0.029	(0)
FeCl2+	2.947e-25	2.760e-25	-24.531	-24.559	-0.029	(0)
Fe2 (OH) 2+4	5.320e-28	1.830e-28	-27.274	-27.738	-0.464	(0)
FeCl3	2.677e-30	2.679e-30	-29.572	-29.572	0.000	(0)
Fe3 (OH) 4+5	1.694e-36	3.195e-37	-35.771	-36.495	-0.724	(0)
H (0)	3.071e-13					
H2	1.535e-13	1.537e-13	-12.814	-12.813	0.000	(0)
K	6.294e-05					
K+	6.293e-05	5.879e-05	-4.201	-4.231	-0.030	(0)
KSO ₄ -	8.186e-09	7.670e-09	-8.087	-8.115	-0.028	(0)
Li	7.204e-07					
Li+	7.203e-07	6.753e-07	-6.143	-6.170	-0.028	(0)
LiSO ₄ -	8.721e-11	8.167e-11	-10.059	-10.088	-0.029	(0)
Mg	4.224e-04					
Mg+2	4.159e-04	3.228e-04	-3.381	-3.491	-0.110	(0)
MgHCO ₃ +	5.150e-06	4.817e-06	-5.288	-5.317	-0.029	(0)
MgSO ₄	1.325e-06	1.326e-06	-5.878	-5.877	0.000	(0)
MgCO ₃	4.295e-08	4.299e-08	-7.367	-7.367	0.000	(0)
MgOH+	3.471e-10	3.256e-10	-9.460	-9.487	-0.028	(0)
Mn (2)	5.800e-05					
Mn+2	5.700e-05	4.405e-05	-4.244	-4.356	-0.112	(0)
MnHCO ₃ +	8.116e-07	7.600e-07	-6.091	-6.119	-0.029	(0)
MnSO ₄	1.674e-07	1.675e-07	-6.776	-6.776	0.000	(0)
MnCl+	1.848e-08	1.730e-08	-7.733	-7.762	-0.029	(0)
MnOH+	8.333e-10	7.804e-10	-9.079	-9.108	-0.029	(0)
MnCl2	4.559e-13	4.563e-13	-12.341	-12.341	0.000	(0)
MnCl3-	2.133e-17	1.997e-17	-16.671	-16.700	-0.029	(0)
Mn (OH) 3-	6.661e-20	6.238e-20	-19.176	-19.205	-0.029	(0)
Mn (3)	1.147e-30					
Mn+3	1.147e-30	6.621e-31	-29.940	-30.179	-0.239	(0)
Mn (6)	0.000e+00					
MnO ₄ -2	0.000e+00	0.000e+00	-85.016	-85.130	-0.114	(0)
Mn (7)	0.000e+00					
MnO ₄ -	0.000e+00	0.000e+00	-97.753	-97.782	-0.030	(0)
Na	1.881e-04					
Na+	1.880e-04	1.759e-04	-3.726	-3.755	-0.029	(0)
NaHCO ₃	9.158e-08	9.167e-08	-7.038	-7.038	0.000	(0)
NaSO ₄ -	2.254e-08	2.112e-08	-7.647	-7.675	-0.028	(0)
NaCO ₃ -	2.118e-10	1.985e-10	-9.674	-9.702	-0.028	(0)
Ni	1.193e-07					
NiCO ₃	5.934e-08	5.940e-08	-7.227	-7.226	0.000	(0)
Ni+2	5.405e-08	4.139e-08	-7.267	-7.383	-0.116	(0)
NiHCO ₃ +	5.659e-09	5.294e-09	-8.247	-8.276	-0.029	(0)
NiSO ₄	1.834e-10	1.835e-10	-9.737	-9.736	0.000	(0)
Ni (CO ₃) 2-2	2.609e-11	1.998e-11	-10.584	-10.699	-0.116	(0)
NiCl+	1.077e-11	1.007e-11	-10.968	-10.997	-0.029	(0)
NiOH+	5.443e-12	5.091e-12	-11.264	-11.293	-0.029	(0)
NiBr+	8.353e-14	7.814e-14	-13.078	-13.107	-0.029	(0)
Ni (OH) 2	8.264e-14	8.272e-14	-13.083	-13.082	0.000	(0)
NiCl2	3.555e-15	3.558e-15	-14.449	-14.449	0.000	(0)
Ni (SO ₄) 2-2	4.344e-16	3.327e-16	-15.362	-15.478	-0.116	(0)
Ni (OH) 3-	3.953e-18	3.698e-18	-17.403	-17.432	-0.029	(0)
O (0)	0.000e+00					
O2	0.000e+00	0.000e+00	-74.156	-74.155	0.000	(0)
S (-2)	3.308e-13					
H2S	2.640e-13	2.642e-13	-12.578	-12.578	0.000	(0)
HS-	6.633e-14	6.200e-14	-13.178	-13.208	-0.029	(0)
S6-2	4.756e-17	3.642e-17	-16.323	-16.439	-0.116	(0)
S5-2	2.747e-17	2.103e-17	-16.561	-16.677	-0.116	(0)
S4-2	1.521e-17	1.165e-17	-16.818	-16.934	-0.116	(0)
S-2	9.037e-21	6.950e-21	-20.044	-20.158	-0.114	(0)
S3-2	4.895e-21	3.749e-21	-20.310	-20.426	-0.116	(0)
Fe (HS) 2	1.720e-21	1.721e-21	-20.765	-20.764	0.000	(0)
S2-2	2.440e-22	1.868e-22	-21.613	-21.729	-0.116	(0)
Fe (HS) 3-	1.242e-32	1.162e-32	-31.906	-31.935	-0.029	(0)
S (6)	4.062e-05					
SO ₄ -2	3.622e-05	2.770e-05	-4.441	-4.557	-0.116	(0)

FeSO4	1.626e-06	1.628e-06	-5.789	-5.788	0.000	(0)
MgSO4	1.325e-06	1.326e-06	-5.878	-5.877	0.000	(0)
CaSO4	1.258e-06	1.260e-06	-5.900	-5.900	0.000	(0)
MnSO4	1.674e-07	1.675e-07	-6.776	-6.776	0.000	(0)
NaSO4-	2.254e-08	2.112e-08	-7.647	-7.675	-0.028	(0)
KS04-	8.186e-09	7.670e-09	-8.087	-8.115	-0.028	(0)
HS04-	3.642e-10	3.409e-10	-9.439	-9.467	-0.029	(0)
NiSO4	1.834e-10	1.835e-10	-9.737	-9.736	0.000	(0)
LiSO4-	8.721e-11	8.167e-11	-10.059	-10.088	-0.029	(0)
AlSO4+	5.468e-12	5.117e-12	-11.262	-11.291	-0.029	(0)
Al (SO4) 2-	1.100e-14	1.030e-14	-13.959	-13.987	-0.029	(0)
UO2SO4	7.820e-16	7.827e-16	-15.107	-15.106	0.000	(0)
N1 (SO4) 2-2	4.344e-16	3.327e-16	-15.362	-15.478	-0.116	(0)
UO2 (SO4) 2-2	7.407e-19	5.673e-19	-18.130	-18.246	-0.116	(0)
FeSO4+	3.214e-20	3.010e-20	-19.493	-19.521	-0.029	(0)
Fe (SO4) 2-	2.577e-23	2.411e-23	-22.589	-22.618	-0.029	(0)
USO4+2	8.606e-25	6.591e-25	-24.065	-24.181	-0.116	(0)
U (SO4) 2	2.134e-25	2.136e-25	-24.671	-24.670	0.000	(0)
Si	1.790e-04					
H4SiO4	1.790e-04	1.791e-04	-3.747	-3.747	0.000	(0)
H3SiO4-	2.968e-08	2.776e-08	-7.527	-7.557	-0.029	(0)
UO2H3SiO4+	3.646e-13	3.411e-13	-12.438	-12.467	-0.029	(0)
H2SiO4-2	1.841e-14	1.419e-14	-13.735	-13.848	-0.113	(0)
Sr	1.484e-06					
Sr+2	1.484e-06	1.141e-06	-5.829	-5.943	-0.114	(0)
SrOH+	5.506e-14	5.157e-14	-13.259	-13.288	-0.029	(0)
U (3)	9.582e-34					
U+3	9.582e-34	5.257e-34	-33.019	-33.279	-0.261	(0)
U (4)	5.435e-07					
U (OH) 5-	5.367e-07	5.020e-07	-6.270	-6.299	-0.029	(0)
U (OH) 4	6.772e-09	6.779e-09	-8.169	-8.169	0.000	(0)
U (OH) 3+	7.799e-12	7.296e-12	-11.108	-11.137	-0.029	(0)
U (OH) 2+2	1.865e-15	1.428e-15	-14.729	-14.845	-0.116	(0)
UOH+3	5.826e-20	3.196e-20	-19.235	-19.495	-0.261	(0)
USO4+2	8.606e-25	6.591e-25	-24.065	-24.181	-0.116	(0)
U+4	3.869e-25	1.331e-25	-24.412	-24.876	-0.464	(0)
U (SO4) 2	2.134e-25	2.136e-25	-24.671	-24.670	0.000	(0)
UC1+3	1.412e-28	7.745e-29	-27.850	-28.111	-0.261	(0)
U6 (OH) 15+9	0.000e+00	0.000e+00	-64.383	-66.730	-2.347	(0)
U (5)	6.287e-09					
UO2+	6.287e-09	5.882e-09	-8.202	-8.231	-0.029	(0)
U (6)	6.043e-10					
UO2 (CO3) 2-2	3.289e-10	2.519e-10	-9.483	-9.599	-0.116	(0)
UO2CO3	2.567e-10	2.570e-10	-9.591	-9.590	0.000	(0)
UO2 (CO3) 3-4	1.710e-11	5.880e-12	-10.767	-11.231	-0.464	(0)
UO2OH+	1.104e-12	1.033e-12	-11.957	-11.986	-0.029	(0)
UO2H3SiO4+	3.646e-13	3.411e-13	-12.438	-12.467	-0.029	(0)
UO2+2	1.398e-13	1.071e-13	-12.854	-12.970	-0.116	(0)
UO2SO4	7.820e-16	7.827e-16	-15.107	-15.106	0.000	(0)
UO2Cl+	1.571e-17	1.470e-17	-16.804	-16.833	-0.029	(0)
UO2 (SO4) 2-2	7.407e-19	5.673e-19	-18.130	-18.246	-0.116	(0)
(UO2) 2 (OH) 2+2	1.795e-19	1.375e-19	-18.746	-18.862	-0.116	(0)
(UO2) 3 (OH) 5+	2.305e-23	2.156e-23	-22.637	-22.666	-0.029	(0)

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

Phase	SI**	log IAP	log K(276 K, 2 atm)	
Akermanite	-30.00	21.78	51.78	Ca2MgSi2O7
Al (OH) 3 (a)	-1.59	10.32	11.90	Al (OH) 3
Al2O3	-2.34	20.64	22.98	Al2O3
Al4 (OH) 10SO4	0.72	23.41	22.70	Al4 (OH) 10SO4
AlAsO4:2H2O	-12.53	-7.73	4.80	AlAsO4:2H2O
Albite	-2.66	1.97	4.64	NaAlSi3O8
Albite (low)	-1.60	1.97	3.57	NaAlSi3O8
AlOHSO4	-4.31	-7.54	-3.23	AlOHSO4
AlumK	-17.40	-22.98	-5.58	KAl (SO4) 2:12H2O
Alunite	-0.77	-2.34	-1.57	KAl3 (SO4) 2 (OH) 6
Analcime	-2.29	5.72	8.01	NaAlSi2O6:H2O
Anhydrite	-3.70	-8.13	-4.42	CaSO4
Annite	4.50	31.50	27.00	KFe3AlSi3O10 (OH) 2
Anorthite	-6.54	22.87	29.41	CaAl2Si2O8
Aragonite	-2.05	-10.28	-8.23	CaCO3
Arsenolite	-23.08	-26.68	-3.61	As4O6
Artinite	-11.61	-0.40	11.22	MgCO3:Mg (OH) 2:3H2O
As2O5	-43.09	-36.09	7.00	As2O5
B. UO2 (OH) 2	-5.99	0.33	6.32	UO2 (OH) 2
Ba3 (AsO4) 2	-7.45	-16.51	-9.06	Ba3 (AsO4) 2
Barite	-1.00	-11.33	-10.33	BaSO4
Birnessite	-23.44	-5.35	18.09	MnO2
Bixbyite	-20.71	-20.46	0.25	Mn2O3
Boehmite	0.15	10.32	10.16	AlOOH
Brucite	-8.44	9.81	18.25	Mg (OH) 2
Bunsenite	-7.88	5.92	13.80	NiO
Ca-Nontronite	14.72	-6.17	-20.89	Fe2Al1.33Si3.67O10 (OH) 2Ca0.165
Ca-Olivine	-25.02	15.72	40.73	Ca2SiO4
Ca3 (AsO4) 2:6H2O	-29.19	-6.89	22.30	Ca3 (AsO4) 2:6H2O
Ca3SiO5	-54.42	25.45	79.86	Ca3SiO5
Calcite	-1.89	-10.28	-8.39	CaCO3
Celestine	-4.06	-10.50	-6.44	SrSO4
CH4 (g)	-15.52	-59.06	-43.54	CH4
Chalcedony	0.04	-3.75	-3.78	SiO2
Chrysotile	-13.21	21.93	35.15	Mg3Si2O5 (OH) 4
Claudeteite	-22.87	-26.68	-3.81	As4O6
Clinoenstatite	-6.40	6.06	12.47	MgSiO3
CO2 (g)	-1.82	-20.01	-18.19	CO2
Cristobalite	0.15	-3.75	-3.90	SiO2
Diaspore	2.06	10.32	8.26	AlOOH
Diopside	-9.66	12.05	21.71	CaMgSi2O6
Dolomite	-3.95	-20.49	-16.53	CaMg (CO3) 2
Epsomite	-5.75	-8.05	-2.30	MgSO4:7H2O
Fe (OH) 2.7ClO.3	1.13	-1.91	-3.04	Fe (OH) 2.7ClO.3
Fe2 (SO4) 3	-57.91	-51.00	6.91	Fe2 (SO4) 3

Fe3(OH)8	-7.64	12.57	20.22	Fe3(OH)8
FeAsO4·2H2O	-17.16	-16.76	0.40	FeAsO4·2H2O
Ferrihydrite	-3.60	1.29	4.89	Fe(OH)3
FeS (ppt)	-5.94	-9.86	-3.92	FeS
Forsterite	-15.16	15.87	31.03	Mg2SiO4
Gehlenite	-27.02	36.35	63.37	Ca2Al2SiO7
Gibbsite(C)	0.26	10.32	10.05	Al(OH)3
Goethite	-0.03	1.29	1.32	FeOOH
Greenalite	1.70	22.51	20.81	Fe3Si2O5(OH)4
Greigite	-21.82	-66.86	-45.03	Fe3S4
Gummitz	-11.37	0.33	11.70	UO3
Gypsum	-3.50	-8.13	-4.62	CaSO4·2H2O
Halite	-9.30	-7.77	1.53	NaCl
Halloysite	1.91	13.14	11.23	Al2Si2O5(OH)4
Hausmannite	-29.46	36.59	66.06	Mn3O4
Hematite	4.84	2.57	-2.27	Fe2O3
Hercynite	-0.94	30.64	31.58	FeAl2O4
Huntite	-12.38	-40.89	-28.52	CaMg3(CO3)4
Hydromagnesite	-25.18	-31.01	-5.82	Mg5(CO3)4(OH)2·4H2O
Jarosite-H	-22.86	-31.86	-8.99	(H3O)Fe3(SO4)2(OH)6
Jarosite-K	-16.40	-29.44	-13.04	KFe3(SO4)2(OH)6
Jarosite-Na	-19.80	-28.96	-9.16	NaFe3(SO4)2(OH)6
K-Nontronite	8.57	-6.97	-15.55	Fe2Al.33Si3.67O10(OH)2K0.33
Kalsilite	-5.48	8.99	14.47	KAlSiO4
Kaolinite	5.43	13.14	7.72	Al2Si2O5(OH)4
Larnite	-26.65	15.72	42.37	Ca2SiO4
Laumontite	-1.93	15.38	17.31	CaAl2Si4O12·4H2O
Leonhardtite	9.46	30.76	21.30	Ca2Al4Si8O24·7H2O
Lepidocrocite	-0.08	1.29	1.37	FeOOH
Leucite	-2.43	5.24	7.67	KAlSi2O6
Lime	-25.67	9.73	35.41	CaO
Mackinawite	-5.21	-9.86	-4.65	FeS
Magadiite	-9.04	-23.33	-14.30	NaSi7O13(OH)3·3H2O
Maghemite	-3.81	2.57	6.38	Fe2O3
Magnesite	-2.52	-10.20	-7.68	MgCO3
Magnetite	5.99	12.57	6.58	Fe3O4
Manganite	-9.99	-10.23	-0.24	MnOOH
Melanterite	-5.22	-7.86	-2.63	FeSO4·7H2O
Merwinite	-43.07	31.51	74.58	Ca3MgSi2O8
Mg-Ferrite	-8.14	12.38	20.52	MgFe2O4
Mg-Nontronite	14.43	-6.15	-20.59	Fe2Al.33Si3.67O10(OH)2Mg0.165
Microcline	0.19	1.50	1.31	KAlSi3O8
Millerite	-5.76	-13.94	-8.18	NiS
Mirabilite	-9.88	-12.07	-2.19	Na2SO4·10H2O
Mn2(SO4)3	-70.52	-74.03	-3.51	Mn2(SO4)3
Mn3(AsO4)2·8H2O	-21.75	-9.26	12.50	Mn3(AsO4)2·8H2O
MnCl2·4H2O	-14.11	-12.38	1.73	MnCl2·4H2O
MnS(Green)	-15.04	-10.91	4.13	MnS
MnSO4	-12.46	-8.91	3.54	MnSO4
Monticellite	-17.27	15.79	33.06	CaMgSiO4
Montmorillonite	5.74	8.41	2.67	Mg0.485Fe.22Al1.71Si3.81O10(OH)2
Morenosite	-9.41	-11.94	-2.53	NiSO4·7H2O
Muscovite	5.80	22.13	16.34	KAl3Si3O10(OH)2
Na-Nontronite	7.69	-6.82	-14.50	Fe2Al.33Si3.67O10(OH)2Na0.33
Natron	-12.02	-14.22	-2.20	Na2CO3·10H2O
Nepheline	-6.62	9.47	16.09	NaAlSiO4
Nesquehonite	-4.91	-10.20	-5.30	MgCO3·3H2O
Ni(OH)2	-3.17	5.92	9.08	Ni(OH)2
Ni2SiO4	-8.33	8.09	16.42	Ni2SiO4
Ni3(AsO4)2·8H2O	-34.04	-18.34	15.70	Ni3(AsO4)2·8H2O
Ni4(OH)6SO4	-26.19	5.81	32.00	Ni4(OH)6SO4
NiCO3	-7.82	-14.10	-6.28	NiCO3
Nsutite	-22.85	-5.35	17.50	MnO2
O2(g)	-71.14	19.53	90.67	O2
Oripment	-7.27	-72.91	-65.64	As2S3
P-Wollstanite	-9.05	5.98	15.03	CaSiO3
Periclase	-13.74	9.81	23.55	MgO
Phlogopite	-40.25	30.92	71.17	KMg3AlSi3O10(OH)2
Portlandite	-14.67	9.73	24.40	Ca(OH)2
Pyrite	-0.84	-19.95	-19.12	FeS2
Pyrochroite	-7.42	8.94	16.36	Mn(OH)2
Pyrolusite	-22.85	-5.35	17.51	MnO2
Pyrophyllite	7.24	5.65	-1.60	Al2Si4O10(OH)2
Quartz	0.61	-3.75	-4.36	SiO2
Realgar	-9.94	-31.41	-21.47	AsS
Retgersite	-9.84	-11.94	-2.10	NiSO4·6H2O
Rhodochrosite	-0.78	-11.07	-10.29	MnCO3
Rutherfordine	-5.23	-19.68	-14.46	UO2CO3
Sanidine(H)	-0.37	1.50	1.87	KAlSi3O8
Schoepite	-5.75	0.33	6.08	UO2(OH)2·H2O
Sepiolite(a)	-10.40	8.38	18.78	Mg2Si3O7·5OH·3H2O
Sepiolite(c)	-9.07	8.38	17.45	Mg2Si3O7·5OH·3H2O
Siderite	0.24	-10.01	-10.25	FeCO3
SiO2(a)	-0.48	-3.75	-3.27	SiO2
SiO2(am)	-0.82	-3.75	-2.93	SiO2
Spinel	-10.91	30.44	41.36	MgAl2O4
Strontianite	-3.44	-12.66	-9.21	SrCO3
Sulfur	-8.22	-10.10	-1.87	S
Talc	-10.59	14.44	25.03	Mg3Si4O10(OH)2
Thenardite	-11.92	-12.07	-0.15	Na2SO4
Thermonatrite	-14.51	-14.22	0.28	Na2CO3·H2O
Tremolite	-23.46	38.53	62.00	Ca2Mg5Si8O22(OH)2
U3O8(C)	-2.95	24.70	27.65	U3O8
U4O9(C)	14.34	16.66	2.32	U4O9
UO2(am)	-0.69	1.72	2.41	UO2
UO3(C)	-8.48	0.33	8.81	UO3
Uraninite	5.37	1.72	-3.65	UO2
Uranophane	-14.59	2.90	17.49	Ca(UO2)2(SiO3OH)2
USiO4(C)	4.78	-2.02	-6.80	USiO4
Wairakite	-7.05	15.38	22.43	CaAl2Si4O12·2H2O
Witherite	-4.88	-13.49	-8.61	BaCO3
Wollastonite	-8.11	5.98	14.10	CaSiO3

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

End of simulation.

1.5 D-pit, 20 m

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.

Using pressure 1.

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

Elements	Molality	Moles
Al	2.446e-06	2.446e+01
As	1.014e-06	1.014e+01
B	1.156e-05	1.156e+02
Ba	4.733e-07	4.733e+00
Br	8.886e-07	8.886e+00
C	2.592e-03	2.592e+04
Ca	4.489e-04	4.489e+03
Cl	1.693e-04	1.693e+03
Fe	8.541e-04	8.541e+03
K	6.793e-05	6.793e+02
Li	7.204e-07	7.204e+00
Mg	4.562e-04	4.562e+03
Mn	5.876e-05	5.876e+02
Na	2.630e-04	2.630e+03
Ni	3.408e-08	3.408e-01
S	7.188e-06	7.188e+01
Si	1.383e-04	1.383e+03
Sr	1.952e-06	1.952e+01
U	3.781e-07	3.781e+00

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

pH	=	7.880	Charge balance
pe	=	-5.237	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength (mol/kgw)	=	5.129e-03	
Mass of water (kg)	=	1.000e+07	
Total alkalinity (eq/kg)	=	2.567e-03	
Total CO2 (mol/kg)	=	2.592e-03	
Temperature (°C)	=	3.90	
Pressure (atm)	=	2.73	
Electrical balance (eq)	=	1.244e+04	
Percent error, 100*(Cat- An)/(Cat+ An)	=	18.71	
Iterations	=	3	
Total H	=	1.110157e+09	
Total O	=	5.551460e+08	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	1.480e-07	1.373e-07	-6.830	-6.862	-0.033	(0)
H+	1.410e-08	1.318e-08	-7.851	-7.880	-0.029	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.01
Al	2.446e-06					
Al(OH)3	2.353e-06	2.356e-06	-5.628	-5.628	0.001	(0)
Al(OH)4-	6.684e-08	6.209e-08	-7.175	-7.207	-0.032	(0)
Al(OH)2+	2.648e-08	2.464e-08	-7.577	-7.608	-0.031	(0)
AlOH+2	1.209e-11	9.053e-12	-10.918	-11.043	-0.126	(0)
Al+3	9.850e-14	5.377e-14	-13.007	-13.269	-0.263	(0)
AlSO4+	9.156e-25	8.506e-25	-24.038	-24.070	-0.032	(0)
Al(SO4)2-	1.326e-36	1.232e-36	-35.878	-35.910	-0.032	(0)
As(3)	1.014e-06					
H3AsO3	9.937e-07	9.949e-07	-6.003	-6.002	0.001	(0)
H2AsO3-	2.069e-08	1.921e-08	-7.684	-7.716	-0.032	(0)
HAsO3-2	5.807e-13	4.316e-13	-12.236	-12.365	-0.129	(0)
H4AsO3+	6.999e-15	6.498e-15	-14.155	-14.187	-0.032	(0)
AsO3-3	1.130e-18	5.798e-19	-17.947	-18.237	-0.290	(0)
As(5)	1.355e-15					
HAsO4-2	1.270e-15	9.441e-16	-14.896	-15.025	-0.129	(0)
H2AsO4-	8.477e-17	7.871e-17	-16.072	-16.104	-0.032	(0)
AsO4-3	2.024e-19	1.038e-19	-18.694	-18.984	-0.290	(0)
H3AsO4	1.460e-22	1.461e-22	-21.836	-21.835	0.001	(0)
B	1.156e-05					
H3BO3	1.121e-05	1.122e-05	-4.950	-4.950	0.001	(0)
H2BO3-	3.516e-07	3.256e-07	-6.454	-6.487	-0.033	(0)
Ba	4.733e-07					
Ba+2	4.733e-07	3.536e-07	-6.325	-6.451	-0.127	(0)
BaOH+	1.820e-13	1.692e-13	-12.740	-12.772	-0.032	(0)
Br	8.886e-07					
Br-	8.886e-07	8.249e-07	-6.051	-6.084	-0.032	(0)
NiBr+	2.560e-15	2.377e-15	-14.592	-14.624	-0.032	(0)
C(4)	2.592e-03					
HCO3-	2.515e-03	2.340e-03	-2.599	-2.631	-0.031	(0)
H2CO3	5.322e-05	5.329e-05	-4.274	-4.273	0.001	(0)
MgHCO3+	7.887e-06	7.321e-06	-5.103	-5.135	-0.032	(0)
CO3-2	6.393e-06	4.788e-06	-5.194	-5.320	-0.126	(0)
CaHCO3+	4.549e-06	4.236e-06	-5.342	-5.373	-0.031	(0)
CaCO3	1.663e-06	1.664e-06	-5.779	-5.779	0.001	(0)

	MnHCO3+	1.169e-06	1.087e-06	-5.932	-5.964	-0.032	(0)
	MgCO3	1.115e-06	1.116e-06	-5.953	-5.952	0.001	(0)
	NaHCO3	1.851e-07	1.853e-07	-6.733	-6.732	0.001	(0)
	NiCO3	3.230e-08	3.234e-08	-7.491	-7.490	0.001	(0)
	NaCO3-	7.409e-09	6.892e-09	-8.130	-8.162	-0.031	(0)
	Ni (CO3) 2-2	3.620e-10	2.691e-10	-9.441	-9.570	-0.129	(0)
	NiHCO3+	1.828e-10	1.697e-10	-9.738	-9.770	-0.032	(0)
	UO2 (CO3) 3-4	1.383e-15	4.220e-16	-14.859	-15.375	-0.515	(0)
	UO2 (CO3) 2-2	9.990e-16	7.425e-16	-15.000	-15.129	-0.129	(0)
	UO2CO3	3.042e-17	3.046e-17	-16.517	-16.516	0.001	(0)
Ca		4.489e-04					
	Ca+2	4.427e-04	3.334e-04	-3.354	-3.477	-0.123	(0)
	CaHCO3+	4.549e-06	4.236e-06	-5.342	-5.373	-0.031	(0)
	CaCO3	1.663e-06	1.664e-06	-5.779	-5.779	0.001	(0)
	CaOH+	1.059e-09	9.865e-10	-8.975	-9.006	-0.031	(0)
	CaSO4	1.118e-15	1.120e-15	-14.951	-14.951	0.001	(0)
Cl		1.693e-04					
	Cl-	1.693e-04	1.569e-04	-3.771	-3.804	-0.033	(0)
	MnCl+	2.953e-08	2.746e-08	-7.530	-7.561	-0.032	(0)
	MnCl2	1.169e-12	1.170e-12	-11.932	-11.932	0.001	(0)
	NiCl+	3.859e-13	3.583e-13	-12.414	-12.446	-0.032	(0)
	NiCl2	2.043e-16	2.046e-16	-15.690	-15.689	0.001	(0)
	MnCl3-	8.903e-17	8.277e-17	-16.050	-16.082	-0.032	(0)
	FeCl+2	2.932e-25	2.191e-25	-24.533	-24.659	-0.127	(0)
	UO2Cl+	1.230e-25	1.142e-25	-24.910	-24.942	-0.032	(0)
	FeCl2+	3.392e-28	3.154e-28	-27.470	-27.501	-0.032	(0)
	FeCl3	4.942e-33	4.948e-33	-32.306	-32.306	0.001	(0)
	UCl+3	1.177e-34	6.038e-35	-33.929	-34.219	-0.290	(0)
Fe (2)		8.541e-04					
	Fe+2	8.489e-04	6.380e-04	-3.071	-3.195	-0.124	(0)
	FeOH+	3.021e-06	2.809e-06	-5.520	-5.551	-0.032	(0)
	Fe (HS) 2	2.164e-06	2.167e-06	-5.665	-5.664	0.001	(0)
	Fe (HS) 3-	4.961e-10	4.606e-10	-9.304	-9.337	-0.032	(0)
	Fe (OH) 2	2.516e-10	2.519e-10	-9.599	-9.599	0.001	(0)
	Fe (OH) 3-	6.118e-13	5.688e-13	-12.213	-12.245	-0.032	(0)
	FeSO4	1.490e-15	1.492e-15	-14.827	-14.826	0.001	(0)
Fe (3)		3.156e-12					
	Fe (OH) 2+	1.259e-12	1.171e-12	-11.900	-11.931	-0.031	(0)
	Fe (OH) 3	1.044e-12	1.045e-12	-11.981	-11.981	0.001	(0)
	Fe (OH) 4-	8.533e-13	7.938e-13	-12.069	-12.100	-0.031	(0)
	FeOH+2	1.638e-17	1.224e-17	-16.786	-16.912	-0.127	(0)
	Fe+3	1.740e-22	9.497e-23	-21.759	-22.022	-0.263	(0)
	FeCl+2	2.932e-25	2.191e-25	-24.533	-24.659	-0.127	(0)
	FeCl2+	3.392e-28	3.154e-28	-27.470	-27.501	-0.032	(0)
	Fe2 (OH) 2+4	3.374e-32	1.030e-32	-31.472	-31.987	-0.515	(0)
	FeSO4+	1.024e-32	9.519e-33	-31.990	-32.021	-0.032	(0)
	FeCl3	4.942e-33	4.948e-33	-32.306	-32.306	0.001	(0)
	Fe3 (OH) 4+5	0.000e+00	0.000e+00	-40.838	-41.643	-0.805	(0)
	Fe (SO4) 2-	0.000e+00	0.000e+00	-44.228	-44.261	-0.032	(0)
H (0)		9.178e-09					
	H2	4.589e-09	4.595e-09	-8.338	-8.338	0.001	(0)
K		6.793e-05					
	K+	6.793e-05	6.296e-05	-4.168	-4.201	-0.033	(0)
	KSO4-	6.374e-18	5.929e-18	-17.196	-17.227	-0.031	(0)
Li		7.204e-07					
	Li+	7.204e-07	6.707e-07	-6.142	-6.173	-0.031	(0)
	LiSO4-	6.272e-20	5.831e-20	-19.203	-19.234	-0.032	(0)
Mg		4.562e-04					
	Mg+2	4.472e-04	3.379e-04	-3.350	-3.471	-0.122	(0)
	MgHCO3+	7.887e-06	7.321e-06	-5.103	-5.135	-0.032	(0)
	MgCO3	1.115e-06	1.116e-06	-5.953	-5.952	0.001	(0)
	MgOH+	6.340e-09	5.908e-09	-8.198	-8.229	-0.031	(0)
	MgSO4	9.986e-16	9.997e-16	-15.001	-15.000	0.001	(0)
Mn (2)		5.876e-05					
	Mn+2	5.755e-05	4.325e-05	-4.240	-4.364	-0.124	(0)
	MnHCO3+	1.169e-06	1.087e-06	-5.932	-5.964	-0.032	(0)
	MnCl+	2.953e-08	2.746e-08	-7.530	-7.561	-0.032	(0)
	MnOH+	1.427e-08	1.327e-08	-7.846	-7.877	-0.032	(0)
	MnCl2	1.169e-12	1.170e-12	-11.932	-11.932	0.001	(0)
	Mn (OH) 3-	3.230e-16	3.003e-16	-15.491	-15.522	-0.032	(0)
	MnSO4	1.185e-16	1.186e-16	-15.926	-15.926	0.001	(0)
	MnCl3-	8.903e-17	8.277e-17	-16.050	-16.082	-0.032	(0)
Mn (3)		3.917e-34					
	Mn+3	3.917e-34	2.138e-34	-33.407	-33.670	-0.263	(0)
Mn (6)		0.000e+00					
	MnO4-2	0.000e+00	0.000e+00	-88.958	-89.085	-0.127	(0)
Mn (7)		0.000e+00					
	MnO4-	0.000e+00	0.000e+00	-105.158	-105.191	-0.033	(0)
Na		2.630e-04					
	Na+	2.628e-04	2.442e-04	-3.580	-3.612	-0.032	(0)
	NaHCO3	1.851e-07	1.853e-07	-6.733	-6.732	0.001	(0)
	NaCO3-	7.409e-09	6.892e-09	-8.130	-8.162	-0.031	(0)
	NaSO4-	2.269e-17	2.111e-17	-16.644	-16.676	-0.031	(0)
Ni		3.408e-08					
	NiCO3	3.230e-08	3.234e-08	-7.491	-7.490	0.001	(0)
	Ni+2	1.226e-09	9.112e-10	-8.911	-9.040	-0.129	(0)
	Ni (CO3) 2-2	3.620e-10	2.691e-10	-9.441	-9.570	-0.129	(0)
	NiHCO3+	1.828e-10	1.697e-10	-9.738	-9.770	-0.032	(0)
	NiOH+	2.085e-12	1.936e-12	-11.681	-11.713	-0.032	(0)
	Ni (OH) 2	5.250e-13	5.257e-13	-12.280	-12.279	0.001	(0)
	NiCl+	3.859e-13	3.583e-13	-12.414	-12.446	-0.032	(0)
	NiBr+	2.560e-15	2.377e-15	-14.592	-14.624	-0.032	(0)
	Ni (OH) 3-	4.300e-16	3.992e-16	-15.367	-15.399	-0.032	(0)
	NiCl2	2.043e-16	2.046e-16	-15.690	-15.689	0.001	(0)
	NiSO4	2.907e-21	2.911e-21	-20.536	-20.536	0.001	(0)
	Ni (SO4) 2-2	5.093e-36	3.785e-36	-35.293	-35.422	-0.129	(0)
O (0)		0.000e+00					
	O2	0.000e+00	0.000e+00	-83.032	-83.031	0.001	(0)
S (-2)		7.188e-06					
	Fe (HS) 2	2.164e-06	2.167e-06	-5.665	-5.664	0.001	(0)
	HS-	2.105e-06	1.952e-06	-5.677	-5.710	-0.033	(0)
	H2S	4.851e-07	4.857e-07	-6.314	-6.314	0.001	(0)
	S6-2	2.620e-08	1.947e-08	-7.582	-7.711	-0.129	(0)

S5-2	1.532e-08	1.138e-08	-7.815	-7.944	-0.129	(0)
S4-2	8.489e-09	6.309e-09	-8.071	-8.200	-0.129	(0)
Fe(HS)3-	4.961e-10	4.606e-10	-9.304	-9.337	-0.032	(0)
S-2	5.054e-12	3.776e-12	-11.296	-11.423	-0.127	(0)
S3-2	2.734e-12	2.032e-12	-11.563	-11.692	-0.129	(0)
S2-2	1.364e-13	1.014e-13	-12.865	-12.994	-0.129	(0)
S(6)	3.059e-14					
SO4-2	2.684e-14	1.992e-14	-13.571	-13.701	-0.130	(0)
FeSO4	1.490e-15	1.492e-15	-14.827	-14.826	0.001	(0)
CaSO4	1.118e-15	1.120e-15	-14.951	-14.951	0.001	(0)
MgSO4	9.986e-16	9.997e-16	-15.001	-15.000	0.001	(0)
MnSO4	1.185e-16	1.186e-16	-15.926	-15.926	0.001	(0)
NaSO4-	2.269e-17	2.111e-17	-16.644	-16.676	-0.031	(0)
KSO4-	6.374e-18	5.929e-18	-17.196	-17.227	-0.031	(0)
LiSO4-	6.272e-20	5.831e-20	-19.203	-19.234	-0.032	(0)
HSO4-	1.561e-20	1.451e-20	-19.806	-19.838	-0.032	(0)
NiSO4	2.907e-21	2.911e-21	-20.536	-20.536	0.001	(0)
AlSO4+	9.156e-25	8.506e-25	-24.038	-24.070	-0.032	(0)
FeSO4+	1.024e-32	9.519e-33	-31.990	-32.021	-0.032	(0)
UO2SO4	2.715e-33	2.718e-33	-32.566	-32.566	0.001	(0)
Ni(SO4)2-2	5.093e-36	3.785e-36	-35.293	-35.422	-0.129	(0)
Al(SO4)2-	1.326e-36	1.232e-36	-35.878	-35.910	-0.032	(0)
USO4+2	3.050e-40	2.267e-40	-39.516	-39.645	-0.129	(0)
Fe(SO4)2-	0.000e+00	0.000e+00	-44.228	-44.261	-0.032	(0)
UO2(SO4)2-2	0.000e+00	0.000e+00	-44.719	-44.848	-0.129	(0)
U(SO4)2	0.000e+00	0.000e+00	-49.276	-49.275	0.001	(0)
Si	1.383e-04					
H4SiO4	1.379e-04	1.381e-04	-3.860	-3.860	0.001	(0)
H3SiO4-	3.966e-07	3.682e-07	-6.402	-6.434	-0.032	(0)
H2SiO4-2	4.400e-12	3.295e-12	-11.357	-11.482	-0.126	(0)
UO2H3SiO4+	2.307e-20	2.142e-20	-19.637	-19.669	-0.032	(0)
Sr	1.952e-06					
Sr+2	1.952e-06	1.458e-06	-5.710	-5.836	-0.127	(0)
SrOH+	1.227e-12	1.141e-12	-11.911	-11.943	-0.032	(0)
U(3)	1.481e-36					
U+3	1.481e-36	7.597e-37	-35.829	-36.119	-0.290	(0)
U(4)	3.781e-07					
U(OH)5-	3.778e-07	3.508e-07	-6.423	-6.455	-0.032	(0)
U(OH)4	2.774e-10	2.778e-10	-9.557	-9.556	0.001	(0)
U(OH)3+	1.890e-14	1.755e-14	-13.724	-13.756	-0.032	(0)
U(OH)2+2	2.704e-19	2.009e-19	-18.568	-18.697	-0.129	(0)
UOH+3	5.107e-25	2.619e-25	-24.292	-24.582	-0.290	(0)
U+4	2.076e-31	6.335e-32	-30.683	-31.198	-0.515	(0)
UCl+3	1.177e-34	6.038e-35	-33.929	-34.219	-0.290	(0)
USO4+2	3.050e-40	2.267e-40	-39.516	-39.645	-0.129	(0)
U(SO4)2	0.000e+00	0.000e+00	-49.276	-49.275	0.001	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-83.601	-86.210	-2.610	(0)
U(5)	8.896e-14					
UO2+	8.896e-14	8.260e-14	-13.051	-13.083	-0.032	(0)
U(6)	2.412e-15					
UO2(CO3)3-4	1.383e-15	4.220e-16	-14.859	-15.375	-0.515	(0)
UO2(CO3)2-2	9.990e-16	7.425e-16	-15.000	-15.129	-0.129	(0)
UO2CO3	3.042e-17	3.046e-17	-16.517	-16.516	0.001	(0)
UO2OH+	9.188e-20	8.531e-20	-19.037	-19.069	-0.032	(0)
UO2H3SiO4+	2.307e-20	2.142e-20	-19.637	-19.669	-0.032	(0)
UO2+2	6.912e-22	5.138e-22	-21.160	-21.289	-0.129	(0)
UO2Cl+	1.230e-25	1.142e-25	-24.910	-24.942	-0.032	(0)
UO2SO4	2.715e-33	2.718e-33	-32.566	-32.566	0.001	(0)
(UO2)2(OH)2+2	1.246e-33	9.258e-34	-32.905	-33.034	-0.129	(0)
(UO2)3(OH)5+	0.000e+00	0.000e+00	-41.426	-41.458	-0.032	(0)
UO2(SO4)2-2	0.000e+00	0.000e+00	-44.719	-44.848	-0.129	(0)

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

Phase	SI**	log IAP	log K(277 K,	3 atm)
Akermanite	-22.61	29.13	51.74	Ca2MgSi2O7
Al(OH)3(a)	-1.52	10.37	11.89	Al(OH)3
Al2O3	-2.24	20.74	22.98	Al2O3
Al4(OH)10SO4	-10.67	12.02	22.69	Al4(OH)10SO4
AlAsO4:2H2O	-16.26	-11.46	4.80	AlAsO4:2H2O
Albite	-1.57	3.06	4.62	NaAlSi3O8
Albite(low)	-0.51	3.06	3.57	NaAlSi3O8
AlOHSO4	-15.86	-19.09	-3.23	AlOHSO4
AlumK	-39.29	-44.87	-5.58	KAl(SO4)2:12H2O
Alunite	-22.56	-24.13	-1.57	KAl3(SO4)2(OH)6
Analcime	-1.08	6.92	7.99	NaAlSi2O6:H2O
Anhydrite	-12.75	-17.18	-4.43	CaSO4
Annite	13.21	40.16	26.96	KFe3AlSi3O10(OH)2
Anorthite	-4.07	25.30	29.37	CaAl2Si2O8
Aragonite	-0.57	-8.80	-8.23	CaCO3
Arsenolite	-20.41	-24.01	-3.60	As4O6
Artinite	-7.70	3.50	11.20	MgCO3:Mg(OH)2:3H2O
As2O5	-50.67	-43.67	7.00	As2O5
B_UO2(OH)2	-11.84	-5.53	6.31	UO2(OH)2
Ba3(AsO4)2	-6.69	-15.75	-9.06	Ba3(AsO4)2
Barite	-9.83	-20.15	-10.33	BaSO4
Birnessite	-25.48	-7.39	18.09	MnO2
Bixbyite	-20.30	-20.06	0.24	Mn2O3
Boehmite	0.22	10.37	10.15	AlOOH
Brucite	-5.94	12.29	18.23	Mg(OH)2
Bunsenite	-7.07	6.72	13.78	NiO
Ca-Nontronite	15.41	-5.48	-20.89	Fe2Al1.33Si3.67O10(OH)2Ca0.165
Ca-Olivine	-20.00	20.71	40.70	Ca2SiO4
Ca3(AsO4)2:6H2O	-29.12	-6.82	22.30	Ca3(AsO4)2:6H2O
Ca3SiO5	-46.81	32.99	79.80	Ca3SiO5
Calcite	-0.40	-8.80	-8.40	CaCO3
Celestine	-13.10	-19.54	-6.44	SrSO4
CH4(g)	1.28	-42.22	-43.50	CH4
Chalcedony	-0.08	-3.86	-3.78	SiO2
Chrysotile	-5.97	29.15	35.12	Mg3Si2O5(OH)4
Claudetite	-20.21	-24.01	-3.80	As4O6
Clinnoenstatite	-4.03	8.43	12.46	MgSiO3

CO2(g)	-2.89	-21.08	-18.19	CO2
Cristobalite	0.03	-3.86	-3.89	SiO2
Diaspore	2.12	10.37	8.25	AlOOH
Diopside	-4.84	16.85	21.69	CaMgSi2O6
Dolomite	-1.05	-17.59	-16.54	CaMg(CO3)2
Epsomite	-14.87	-17.17	-2.30	MgSO4·7H2O
Fe(OH)2·7ClO.3	1.15	-1.89	-3.04	Fe(OH)2·7ClO.3
Fe2(SO4)3	-92.03	-85.15	6.88	Fe2(SO4)3
Fe3(OH)8	-4.42	15.80	20.22	Fe3(OH)8
FeAsO4·2H2O	-20.62	-20.22	0.40	FeAsO4·2H2O
Ferrihydrite	-3.27	1.62	4.89	Fe(OH)3
FeS(ppt)	2.89	-1.02	-3.92	FeS
Forsterite	-10.29	20.72	31.01	Mg2SiO4
Gehlenite	-21.86	41.45	63.30	Ca2Al2SiO7
Gibbsite(C)	0.33	10.37	10.04	Al(OH)3
Goethite	0.31	1.62	1.31	FeOOH
Greenalite	9.17	29.97	20.81	Fe3Si2O5(OH)4
Greigite	6.48	-38.56	-45.03	Fe3S4
Gummite	-17.22	-5.53	11.69	UO3
Gypsum	-12.55	-17.18	-4.62	CaSO4·2H2O
Halite	-8.95	-7.42	1.53	NaCl
Halloysite	1.81	13.02	11.21	Al2Si2O5(OH)4
Hausmannite	-26.54	39.47	66.01	Mn3O4
Hematite	5.52	3.23	-2.29	Fe2O3
Hercynite	1.77	33.31	31.53	FeAl2O4
Huntite	-6.64	-35.17	-28.53	CaMg3(CO3)4
Hydromagnesite	-17.02	-22.88	-5.86	Mg5(CO3)4(OH)2·4H2O
Jarosite-H	-45.04	-54.07	-9.03	(H3O)Fe3(SO4)2(OH)6
Jarosite-K	-37.33	-50.39	-13.06	KFe3(SO4)2(OH)6
Jarosite-Na	-40.62	-49.80	-9.18	NaFe3(SO4)2(OH)6
K-Nontronite	9.25	-6.29	-15.55	Fe2Al.33Si3.67O10(OH)2K0.33
Kalsilite	-4.26	10.19	14.45	KAlSiO4
Kaolinite	5.33	13.02	7.69	Al2Si2O5(OH)4
Larnite	-21.63	20.71	42.34	Ca2SiO4
Laumontite	0.31	17.58	17.28	CaAl2Si4O12·4H2O
Leonhardtite	13.91	35.17	21.26	Ca2Al4Si8O24·7H2O
Lepidocrocite	0.25	1.62	1.37	FeOOH
Leucite	-1.33	6.33	7.66	KAlSi2O6
Lime	-23.10	12.28	35.38	CaO
Mackinawite	3.62	-1.02	-4.65	FeS
Magadiite	-8.46	-22.75	-14.29	NaSi7O13(OH)3·3H2O
Maghemite	-3.15	3.23	6.38	Fe2O3
Magnesite	-1.11	-8.79	-7.68	MgCO3
Magnetite	9.25	15.80	6.55	Fe3O4
Manganite	-9.79	-10.03	-0.24	MnOOH
Melanterite	-14.26	-16.90	-2.63	FeSO4·7H2O
Merwinite	-33.10	41.42	74.52	Ca3MgSi2O8
Mg-Ferrite	-4.96	15.52	20.48	MgFe2O4
Mg-Nontronite	15.11	-5.48	-20.59	Fe2Al.33Si3.67O10(OH)2Mg0.165
Microcline	1.16	2.47	1.31	KAlSi3O8
Millerite	1.31	-6.87	-8.18	NiS
Mirabilite	-18.75	-20.93	-2.18	Na2SO4·10H2O
Mn2(SO4)3	-104.91	-108.44	-3.53	Mn2(SO4)3
Mn3(AsO4)2·8H2O	-21.98	-9.48	12.50	Mn3(AsO4)2·8H2O
MnCl2·4H2O	-13.71	-11.97	1.74	MnCl2·4H2O
MnS(Green)	-6.32	-2.19	4.12	MnS
MnSO4	-21.60	-18.06	3.53	MnSO4
Monticellite	-12.32	20.71	33.03	CaMgSiO4
Montmorillonite	6.67	9.34	2.67	Mg0.485Fe.22Al1.71Si3.81O10(OH)2
Morenosite	-20.21	-22.74	-2.53	NiSO4·7H2O
Muscovite	6.91	23.21	16.30	KAl3Si3O10(OH)2
Na-Nontronite	8.40	-6.10	-14.50	Fe2Al.33Si3.67O10(OH)2Na0.33
Natron	-10.35	-12.54	-2.20	Na2CO3·10H2O
Nepheline	-5.29	10.78	16.07	NaAlSiO4
Nesquehonite	-3.49	-8.79	-5.30	MgCO3·3H2O
Ni(OH)2	-2.38	6.72	9.10	Ni(OH)2
Ni2SiO4	-6.82	9.58	16.40	Ni2SiO4
Ni3(AsO4)2·8H2O	-39.21	-23.51	15.70	Ni3(AsO4)2·8H2O
Ni4(OH)6SO4	-34.58	-2.58	32.00	Ni4(OH)6SO4
NiCO3	-8.08	-14.36	-6.29	NiCO3
Nsutite	-24.89	-7.39	17.50	MnO2
O2(g)	-80.02	10.57	90.59	O2
Oripment	12.82	-52.77	-65.59	As2S3
P-Wollstanite	-6.60	8.42	15.02	CaSiO3
Periclase	-11.24	12.29	23.53	MgO
Phlogopite	-31.78	39.34	71.12	KMg3AlSi3O10(OH)2
Portlandite	-12.10	12.28	24.39	Ca(OH)2
Pyrite	9.78	-9.33	-19.11	FeS2
Pyrocroite	-4.95	11.40	16.35	Mn(OH)2
Pyrolusite	-24.88	-7.39	17.49	MnO2
Pyrophyllite	6.90	5.30	-1.60	Al2Si4O10(OH)2
Quartz	0.49	-3.86	-4.35	SiO2
Realgar	-0.78	-22.23	-21.45	AsS
Retgersite	-20.64	-22.74	-2.10	NiSO4·6H2O
Rhodochromite	0.61	-9.68	-10.29	MnCO3
Rutherfordine	-12.15	-26.61	-14.46	UO2CO3
Sanidine(H)	0.61	2.47	1.86	KAlSi3O8
Schoepite	-11.60	-5.53	6.07	UO2(OH)2·H2O
Sepiolite(a)	-5.78	13.00	18.78	Mg2Si3O7·5OH·3H2O
Sepiolite(c)	-4.44	13.00	17.44	Mg2Si3O7·5OH·3H2O
Siderite	1.74	-8.52	-10.25	FeCO3
SiO2(a)	-0.60	-3.86	-3.26	SiO2
SiO2(am)	-0.93	-3.86	-2.93	SiO2
Spinel	-8.27	33.03	41.30	MgAl2O4
Strontianite	-1.94	-11.16	-9.21	SrCO3
Sulfur	-6.43	-8.30	-1.88	S
Talc	-3.58	21.43	25.01	Mg3Si4O10(OH)2
Thenardite	-20.78	-20.93	-0.15	Na2SO4
Thermonatrite	-12.83	-12.54	0.28	Na2CO3·H2O
Tremolite	-6.81	55.13	61.94	Ca2Mg5Si8O22(OH)2
U3O8(C)	-16.04	11.54	27.58	U3O8
U4O9(C)	4.31	6.57	2.26	U4O9
UO2(am)	-2.08	0.32	2.40	UO2

UO3(C)	-14.33	-5.53	8.80	UO3
Uraninite	3.98	0.32	-3.66	UO2
Uranophane	-23.99	-6.50	17.49	Ca(UO2)2(SiO3OH)2
USiO4(C)	3.27	-3.54	-6.81	USiO4
Wairakite	-4.81	17.58	22.40	CaAl2Si4O12:2H2O
Witherite	-3.17	-11.77	-8.61	BaCO3
Wollastonite	-5.66	8.42	14.09	CaSiO3

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

End of simulation.

1.6 DJX-pit, 0.5 m

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
Al	2.706e-06	2.706e+01
As	1.067e-08	1.067e-01
B	2.090e-05	2.090e+02
Ba	5.825e-08	5.825e-01
Br	2.879e-07	2.879e+00
C	5.435e-04	5.435e+03
Ca	1.190e-03	1.190e+04
Cl	1.130e-04	1.130e+03
Cu	1.574e-08	1.574e-01
Fe	1.611e-07	1.611e+00
K	6.719e-05	6.719e+02
Li	4.034e-06	4.034e+01
Mg	1.259e-03	1.259e+04
Mn	7.286e-08	7.286e-01
Na	4.465e-04	4.465e+03
Ni	1.738e-06	1.738e+01
S	2.184e-03	2.184e+04
Si	6.559e-05	6.559e+02
Sr	3.436e-06	3.436e+01
U	6.344e-07	6.344e+00
Zn	4.588e-08	4.588e-01

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

pH	=	7.170	Charge balance
pe	=	2.746	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength (mol/kgw)	=	8.472e-03	
Mass of water (kg)	=	1.000e+07	
Total alkalinity (eq/kg)	=	4.937e-04	
Total CO2 (mol/kg)	=	5.435e-04	
Temperature (°C)	=	18.50	
Pressure (atm)	=	1.04	
Electrical balance (eq)	=	4.606e+03	
Percent error, 100*(Cat- An)/(Cat+ An)	=	5.10	
Iterations	=	3	
Total H	=	1.110134e+09	
Total O	=	5.551692e+08	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm ³ /mol
OH-	9.908e-08	8.994e-08	-7.004	-7.046	-0.042	(0)
H+	7.354e-08	6.761e-08	-7.133	-7.170	-0.037	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.04
Al	2.706e-06					
Al(OH)3	1.975e-06	1.979e-06	-5.704	-5.704	0.001	(0)
Al(OH)4-	6.131e-07	5.580e-07	-6.212	-6.253	-0.041	(0)
Al(OH)2+	1.165e-07	1.063e-07	-6.934	-6.974	-0.040	(0)
AlOH+2	8.548e-10	5.917e-10	-9.068	-9.228	-0.160	(0)
Al+3	1.304e-11	6.117e-12	-10.885	-11.213	-0.329	(0)
AlSO4+	8.174e-12	7.440e-12	-11.088	-11.128	-0.041	(0)
Al(SO4)2-	7.968e-13	7.252e-13	-12.099	-12.140	-0.041	(0)
As(3)	3.168e-14					
H3AsO3	3.144e-14	3.150e-14	-13.503	-13.502	0.001	(0)
H2AsO3-	2.368e-16	2.154e-16	-15.626	-15.667	-0.041	(0)
HAsO3-2	2.763e-21	1.890e-21	-20.559	-20.724	-0.165	(0)
H4AsO3+	1.160e-21	1.055e-21	-20.935	-20.977	-0.041	(0)
AsO3-3	2.017e-27	8.581e-28	-26.695	-27.066	-0.371	(0)
As(5)	1.067e-08					
HAsO4-2	8.208e-09	5.614e-09	-8.086	-8.251	-0.165	(0)
H2AsO4-	2.461e-09	2.238e-09	-8.609	-8.650	-0.041	(0)
AsO4-3	4.202e-13	1.787e-13	-12.377	-12.748	-0.371	(0)
H3AsO4	2.480e-14	2.485e-14	-13.606	-13.605	0.001	(0)
B	2.090e-05					
H3BO3	2.073e-05	2.077e-05	-4.683	-4.683	0.001	(0)
H2BO3-	1.728e-07	1.564e-07	-6.763	-6.806	-0.043	(0)
Ba	5.825e-08					
Ba+2	5.825e-08	4.017e-08	-7.235	-7.396	-0.161	(0)
BaOH+	1.620e-14	1.477e-14	-13.790	-13.831	-0.040	(0)

Br	2.879e-07					
Br-	2.879e-07	2.617e-07	-6.541	-6.582	-0.041	(0)
NiBr+	4.315e-13	3.924e-13	-12.365	-12.406	-0.041	(0)
ZnBr+	1.892e-15	1.721e-15	-14.723	-14.764	-0.041	(0)
ZnBr2	1.789e-22	1.793e-22	-21.747	-21.746	0.001	(0)
C(4)	5.435e-04					
HCO3-	4.722e-04	4.307e-04	-3.326	-3.366	-0.040	(0)
H2CO3	6.153e-05	6.165e-05	-4.211	-4.210	0.001	(0)
MgHCO3+	4.054e-06	3.685e-06	-5.392	-5.434	-0.041	(0)
CaHCO3+	2.838e-06	2.592e-06	-5.547	-5.586	-0.039	(0)
NiCO3	9.065e-07	9.083e-07	-6.043	-6.042	0.001	(0)
UO2(CO3)2-2	4.488e-07	3.070e-07	-6.348	-6.513	-0.165	(0)
CO3-2	3.732e-07	2.583e-07	-6.428	-6.588	-0.160	(0)
CaCO3	2.274e-07	2.279e-07	-6.643	-6.642	0.001	(0)
MgCO3	1.707e-07	1.710e-07	-6.768	-6.767	0.001	(0)
UO2CO3	1.663e-07	1.666e-07	-6.779	-6.778	0.001	(0)
NaHCO3	8.467e-08	8.483e-08	-7.072	-7.071	0.001	(0)
NiHCO3+	2.688e-08	2.445e-08	-7.571	-7.612	-0.041	(0)
UO2(CO3)3-4	1.402e-08	3.068e-09	-7.853	-8.513	-0.660	(0)
CuCO3	2.417e-09	2.421e-09	-8.617	-8.616	0.001	(0)
NaCO3-	1.517e-09	1.384e-09	-8.819	-8.859	-0.040	(0)
ZnCO3	1.286e-09	1.289e-09	-8.891	-8.890	0.001	(0)
ZnHCO3+	1.206e-09	1.097e-09	-8.919	-8.960	-0.041	(0)
Ni(CO3)2-2	5.962e-10	4.078e-10	-9.225	-9.390	-0.165	(0)
MnHCO3+	3.358e-10	3.060e-10	-9.474	-9.514	-0.040	(0)
CuHCO3+	3.352e-10	3.048e-10	-9.475	-9.516	-0.041	(0)
Zn(CO3)2-2	1.041e-11	7.119e-12	-10.983	-11.148	-0.165	(0)
Cu(CO3)2-2	1.151e-12	7.875e-13	-11.939	-12.104	-0.165	(0)
Ca	1.190e-03					
Ca+2	1.015e-03	7.089e-04	-2.994	-3.149	-0.156	(0)
CaSO4	1.717e-04	1.721e-04	-3.765	-3.764	0.001	(0)
CaHCO3+	2.838e-06	2.592e-06	-5.547	-5.586	-0.039	(0)
CaCO3	2.274e-07	2.279e-07	-6.643	-6.642	0.001	(0)
CaOH+	1.677e-09	1.531e-09	-8.776	-8.815	-0.039	(0)
Cl	1.130e-04					
Cl-	1.130e-04	1.024e-04	-3.947	-3.990	-0.042	(0)
NiCl+	1.339e-10	1.217e-10	-9.873	-9.915	-0.041	(0)
MnCl+	2.001e-11	1.824e-11	-10.699	-10.739	-0.040	(0)
CuCl2-	5.734e-12	5.212e-12	-11.242	-11.283	-0.041	(0)
ZnCl+	5.658e-12	5.143e-12	-11.247	-11.289	-0.041	(0)
ZnOHCl	1.252e-12	1.254e-12	-11.902	-11.902	0.001	(0)
CuCl+	3.823e-13	3.475e-13	-12.418	-12.459	-0.041	(0)
NiCl2	4.530e-14	4.539e-14	-13.344	-13.343	0.001	(0)
UO2Cl+	9.429e-15	8.575e-15	-14.026	-14.067	-0.041	(0)
CuCl3-2	1.196e-15	8.248e-16	-14.922	-15.084	-0.161	(0)
ZnCl2	5.361e-16	5.371e-16	-15.271	-15.270	0.001	(0)
MnCl2	5.065e-16	5.075e-16	-15.295	-15.295	0.001	(0)
CuCl2	1.776e-17	1.779e-17	-16.751	-16.750	0.001	(0)
ZnCl3-	6.526e-20	5.932e-20	-19.185	-19.227	-0.041	(0)
MnCl3-	2.572e-20	2.344e-20	-19.590	-19.630	-0.040	(0)
FeCl+2	1.253e-20	8.642e-21	-19.902	-20.063	-0.161	(0)
CuCl3-	6.324e-24	5.749e-24	-23.199	-23.240	-0.041	(0)
FeCl2+	5.357e-24	4.881e-24	-23.271	-23.311	-0.040	(0)
ZnCl4-2	4.181e-24	2.883e-24	-23.379	-23.540	-0.161	(0)
FeCl3	4.991e-29	5.000e-29	-28.302	-28.301	0.001	(0)
CuCl4-2	5.346e-30	3.686e-30	-29.272	-29.433	-0.161	(0)
UCl+3	7.717e-38	3.283e-38	-37.113	-37.484	-0.371	(0)
Cu(1)	1.713e-09					
Cu+	1.708e-09	1.546e-09	-8.768	-8.811	-0.043	(0)
CuCl2-	5.734e-12	5.212e-12	-11.242	-11.283	-0.041	(0)
CuCl3-2	1.196e-15	8.248e-16	-14.922	-15.084	-0.161	(0)
Cu(S4)2-3	0.000e+00	0.000e+00	-100.339	-100.586	-0.247	(0)
CuS4S5-3	0.000e+00	0.000e+00	-101.077	-101.316	-0.238	(0)
Cu(2)	1.402e-08					
Cu(OH)2	7.960e-09	7.976e-09	-8.099	-8.098	0.001	(0)
Cu+2	2.598e-09	1.745e-09	-8.585	-8.758	-0.173	(0)
CuCO3	2.417e-09	2.421e-09	-8.617	-8.616	0.001	(0)
CuSO4	4.278e-10	4.286e-10	-9.369	-9.368	0.001	(0)
CuHCO3+	3.352e-10	3.048e-10	-9.475	-9.516	-0.041	(0)
CuOH+	2.840e-10	2.581e-10	-9.547	-9.588	-0.041	(0)
Cu(CO3)2-2	1.151e-12	7.875e-13	-11.939	-12.104	-0.165	(0)
CuCl+	3.823e-13	3.475e-13	-12.418	-12.459	-0.041	(0)
Cu2(OH)2+2	2.204e-14	1.507e-14	-13.657	-13.822	-0.165	(0)
Cu(OH)3-	7.834e-15	7.125e-15	-14.106	-14.147	-0.041	(0)
CuCl2	1.776e-17	1.779e-17	-16.751	-16.750	0.001	(0)
Cu(OH)4-2	3.067e-20	2.098e-20	-19.513	-19.678	-0.165	(0)
CuCl3-	6.324e-24	5.749e-24	-23.199	-23.240	-0.041	(0)
CuCl4-2	5.346e-30	3.686e-30	-29.272	-29.433	-0.161	(0)
Cu(HS)3-	0.000e+00	0.000e+00	-147.075	-147.117	-0.041	(0)
Fe(2)	1.591e-07					
Fe+2	1.395e-07	9.713e-08	-6.855	-7.013	-0.157	(0)
FeSO4	1.923e-08	1.926e-08	-7.716	-7.715	0.001	(0)
FeOH+	3.034e-10	2.765e-10	-9.518	-9.558	-0.040	(0)
Fe(OH)2	1.949e-14	1.953e-14	-13.710	-13.709	0.001	(0)
Fe(OH)3-	1.103e-17	1.005e-17	-16.957	-16.998	-0.040	(0)
Fe(HS)2	0.000e+00	0.000e+00	-107.568	-107.568	0.001	(0)
Fe(HS)3-	0.000e+00	0.000e+00	-160.242	-160.283	-0.041	(0)
Fe(3)	2.094e-09					
Fe(OH)2+	1.768e-09	1.613e-09	-8.752	-8.792	-0.040	(0)
Fe(OH)3	2.797e-10	2.802e-10	-9.553	-9.552	0.001	(0)
Fe(OH)4-	4.544e-11	4.145e-11	-10.343	-10.382	-0.040	(0)
FeOH+2	3.230e-13	2.227e-13	-12.491	-12.652	-0.161	(0)
FeSO4+	3.422e-17	3.118e-17	-16.466	-16.506	-0.040	(0)
Fe+3	7.352e-18	3.448e-18	-17.134	-17.462	-0.329	(0)
Fe(SO4)2-	1.331e-18	1.210e-18	-17.876	-17.917	-0.041	(0)
FeCl+2	1.253e-20	8.642e-21	-19.902	-20.063	-0.161	(0)
Fe2(OH)2+4	8.027e-24	1.757e-24	-23.095	-23.755	-0.660	(0)
FeCl2+	5.357e-24	4.881e-24	-23.271	-23.311	-0.040	(0)
FeCl3	4.991e-29	5.000e-29	-28.302	-28.301	0.001	(0)
Fe3(OH)4+5	6.169e-30	5.743e-31	-29.210	-30.241	-1.031	(0)
H(0)	2.226e-23					
H2	1.113e-23	1.115e-23	-22.953	-22.953	0.001	(0)
K	6.719e-05					

K+	6.666e-05	6.046e-05	-4.176	-4.219	-0.042	(0)
KS04-	5.223e-07	4.764e-07	-6.282	-6.322	-0.040	(0)
Li	4.034e-06					
Li+	4.012e-06	3.665e-06	-5.397	-5.436	-0.039	(0)
LiSO4-	2.211e-08	2.015e-08	-7.655	-7.696	-0.040	(0)
Mg	1.259e-03					
Mg+2	1.092e-03	7.666e-04	-2.962	-3.115	-0.154	(0)
MgSO4	1.626e-04	1.629e-04	-3.789	-3.788	0.001	(0)
MgHCO3+	4.054e-06	3.685e-06	-5.392	-5.434	-0.041	(0)
MgCO3	1.707e-07	1.710e-07	-6.768	-6.767	0.001	(0)
MgOH+	1.141e-08	1.044e-08	-7.943	-7.981	-0.039	(0)
Mn (2)	7.286e-08					
Mn+2	6.322e-08	4.401e-08	-7.199	-7.356	-0.157	(0)
MnSO4	9.277e-09	9.295e-09	-8.033	-8.032	0.001	(0)
MnHCO3+	3.358e-10	3.060e-10	-9.474	-9.514	-0.040	(0)
MnCl+	2.001e-11	1.824e-11	-10.699	-10.739	-0.040	(0)
MnOH+	1.068e-11	9.734e-12	-10.971	-11.012	-0.040	(0)
MnCl2	5.065e-16	5.075e-16	-15.295	-15.295	0.001	(0)
MnCl3-	2.572e-20	2.344e-20	-19.590	-19.630	-0.040	(0)
Mn (OH) 3-	2.476e-21	2.257e-21	-20.606	-20.647	-0.040	(0)
Mn (3)	4.283e-30					
Mn+3	4.283e-30	2.009e-30	-29.368	-29.697	-0.329	(0)
Mn (6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-59.743	-59.905	-0.161	(0)
Mn (7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-66.935	-66.978	-0.043	(0)
Na	4.465e-04					
Na+	4.438e-04	4.040e-04	-3.353	-3.394	-0.041	(0)
NaSO4-	2.680e-06	2.445e-06	-5.572	-5.612	-0.040	(0)
NaHCO3	8.467e-08	8.483e-08	-7.072	-7.071	0.001	(0)
NaCO3-	1.517e-09	1.384e-09	-8.819	-8.859	-0.040	(0)
Ni	1.738e-06					
NiCO3	9.065e-07	9.083e-07	-6.043	-6.042	0.001	(0)
Ni+2	6.934e-07	4.743e-07	-6.159	-6.324	-0.165	(0)
NiSO4	1.098e-07	1.100e-07	-6.960	-6.959	0.001	(0)
NiHCO3+	2.688e-08	2.445e-08	-7.571	-7.612	-0.041	(0)
NiOH+	6.673e-10	6.069e-10	-9.176	-9.217	-0.041	(0)
Ni (CO3) 2-2	5.962e-10	4.078e-10	-9.225	-9.390	-0.165	(0)
NiCl+	1.339e-10	1.217e-10	-9.873	-9.915	-0.041	(0)
Ni (SO4) 2-2	1.152e-11	7.876e-12	-10.939	-11.104	-0.165	(0)
Ni (OH) 2	1.035e-11	1.037e-11	-10.985	-10.984	0.001	(0)
NiBr+	4.315e-13	3.924e-13	-12.365	-12.406	-0.041	(0)
NiCl2	4.530e-14	4.539e-14	-13.344	-13.343	0.001	(0)
Ni (OH) 3-	1.687e-15	1.534e-15	-14.773	-14.814	-0.041	(0)
O (0)	0.000e+00					
O2	0.000e+00	0.000e+00	-48.620	-48.619	0.001	(0)
S (-2)	0.000e+00					
HS-	0.000e+00	0.000e+00	-54.710	-54.752	-0.042	(0)
H2S	0.000e+00	0.000e+00	-54.892	-54.891	0.001	(0)
S5-2	0.000e+00	0.000e+00	-57.164	-57.329	-0.165	(0)
S6-2	0.000e+00	0.000e+00	-57.299	-57.463	-0.165	(0)
S4-2	0.000e+00	0.000e+00	-57.405	-57.570	-0.165	(0)
S-2	0.000e+00	0.000e+00	-60.537	-60.698	-0.161	(0)
S3-2	0.000e+00	0.000e+00	-60.869	-61.034	-0.165	(0)
S2-2	0.000e+00	0.000e+00	-62.132	-62.297	-0.165	(0)
Cu (S4) 2-3	0.000e+00	0.000e+00	-100.339	-100.586	-0.247	(0)
CuS4S5-3	0.000e+00	0.000e+00	-101.077	-101.316	-0.238	(0)
Zn (HS) 2	0.000e+00	0.000e+00	-102.168	-102.167	0.001	(0)
Fe (HS) 2	0.000e+00	0.000e+00	-107.568	-107.568	0.001	(0)
Cu (HS) 3-	0.000e+00	0.000e+00	-147.075	-147.117	-0.041	(0)
Zn (HS) 3-	0.000e+00	0.000e+00	-155.718	-155.759	-0.041	(0)
Fe (HS) 3-	0.000e+00	0.000e+00	-160.242	-160.283	-0.041	(0)
S (6)	2.184e-03					
SO4-2	1.846e-03	1.259e-03	-2.734	-2.900	-0.166	(0)
CaSO4	1.717e-04	1.721e-04	-3.765	-3.764	0.001	(0)
MgSO4	1.626e-04	1.629e-04	-3.789	-3.788	0.001	(0)
NaSO4-	2.680e-06	2.445e-06	-5.572	-5.612	-0.040	(0)
KS04-	5.223e-07	4.764e-07	-6.282	-6.322	-0.040	(0)
NiSO4	1.098e-07	1.100e-07	-6.960	-6.959	0.001	(0)
LiSO4-	2.211e-08	2.015e-08	-7.655	-7.696	-0.040	(0)
FeSO4	1.923e-08	1.926e-08	-7.716	-7.715	0.001	(0)
MnSO4	9.277e-09	9.295e-09	-8.033	-8.032	0.001	(0)
HSO4-	7.593e-09	6.911e-09	-8.120	-8.160	-0.041	(0)
ZnSO4	7.000e-09	7.014e-09	-8.155	-8.154	0.001	(0)
CuSO4	4.278e-10	4.286e-10	-9.369	-9.368	0.001	(0)
Zn (SO4) 2-2	1.105e-10	7.557e-11	-9.957	-10.122	-0.165	(0)
UO2SO4	2.805e-11	2.810e-11	-10.552	-10.551	0.001	(0)
Ni (SO4) 2-2	1.152e-11	7.876e-12	-10.939	-11.104	-0.165	(0)
AlSO4+	8.174e-12	7.440e-12	-11.088	-11.128	-0.041	(0)
UO2 (SO4) 2-2	1.484e-12	1.015e-12	-11.828	-11.993	-0.165	(0)
Al (SO4) 2-	7.968e-13	7.252e-13	-12.099	-12.140	-0.041	(0)
FeSO4+	3.422e-17	3.118e-17	-16.466	-16.506	-0.040	(0)
Fe (SO4) 2-	1.331e-18	1.210e-18	-17.876	-17.917	-0.041	(0)
U (SO4) 2	1.427e-31	1.430e-31	-30.846	-30.845	0.001	(0)
USO4+2	9.904e-33	6.774e-33	-32.004	-32.169	-0.165	(0)
Si	6.559e-05					
H4SiO4	6.550e-05	6.563e-05	-4.184	-4.183	0.001	(0)
H3SiO4-	8.936e-08	8.123e-08	-7.049	-7.090	-0.041	(0)
UO2H3SiO4+	2.245e-10	2.042e-10	-9.649	-9.690	-0.041	(0)
H2SiO4-2	1.601e-12	1.108e-12	-11.796	-11.955	-0.160	(0)
Sr	3.436e-06					
Sr+2	3.436e-06	2.369e-06	-5.464	-5.625	-0.161	(0)
SrOH+	1.480e-12	1.348e-12	-11.830	-11.870	-0.040	(0)
U (3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-46.239	-46.610	-0.371	(0)
U (4)	4.487e-13					
U (OH) 5-	4.475e-13	4.069e-13	-12.349	-12.390	-0.041	(0)
U (OH) 4	1.278e-15	1.281e-15	-14.893	-14.892	0.001	(0)
U (OH) 3+	3.770e-19	3.428e-19	-18.424	-18.465	-0.041	(0)
U (OH) 2+2	1.885e-23	1.289e-23	-22.725	-22.890	-0.165	(0)
UOH+3	1.055e-28	4.489e-29	-27.977	-28.348	-0.371	(0)
U (SO4) 2	1.427e-31	1.430e-31	-30.846	-30.845	0.001	(0)
USO4+2	9.904e-33	6.774e-33	-32.004	-32.169	-0.165	(0)

U+4	9.772e-35	2.139e-35	-34.010	-34.670	-0.660	(0)
UCl+3	7.717e-38	3.283e-38	-37.113	-37.484	-0.371	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-114.358	-117.699	-3.341	(0)
U(5)	7.201e-11					
UO2+	7.201e-11	6.549e-11	-10.143	-10.184	-0.041	(0)
U(6)	6.343e-07					
UO2(CO3)2-2	4.488e-07	3.070e-07	-6.348	-6.513	-0.165	(0)
UO2CO3	1.663e-07	1.666e-07	-6.779	-6.778	0.001	(0)
UO2(CO3)3-4	1.402e-08	3.068e-09	-7.853	-8.513	-0.660	(0)
UO2OH+	4.756e-09	4.325e-09	-8.323	-8.364	-0.041	(0)
UO2H3SiO4+	2.245e-10	2.042e-10	-9.649	-9.690	-0.041	(0)
UO2+2	7.724e-11	5.283e-11	-10.112	-10.277	-0.165	(0)
UO2SO4	2.805e-11	2.810e-11	-10.552	-10.551	0.001	(0)
(UO2)3(OH)5+	1.141e-11	1.037e-11	-10.943	-10.984	-0.041	(0)
UO2(SO4)2-2	1.484e-12	1.015e-12	-11.828	-11.993	-0.165	(0)
(UO2)2(OH)2+2	1.376e-12	9.411e-13	-11.861	-12.026	-0.165	(0)
UO2Cl+	9.429e-15	8.575e-15	-14.026	-14.067	-0.041	(0)
Zn	4.588e-08					
Zn+2	3.592e-08	2.500e-08	-7.445	-7.602	-0.157	(0)
ZnSO4	7.000e-09	7.014e-09	-8.155	-8.154	0.001	(0)
ZnCO3	1.286e-09	1.289e-09	-8.891	-8.890	0.001	(0)
ZnHCO3+	1.206e-09	1.097e-09	-8.919	-8.960	-0.041	(0)
ZnOH+	2.694e-10	2.450e-10	-9.570	-9.611	-0.041	(0)
Zn(SO4)2-2	1.105e-10	7.557e-11	-9.957	-10.122	-0.165	(0)
Zn(OH)2	6.888e-11	6.902e-11	-10.162	-10.161	0.001	(0)
Zn(CO3)2-2	1.041e-11	7.119e-12	-10.983	-11.148	-0.165	(0)
ZnCl+	5.658e-12	5.143e-12	-11.247	-11.289	-0.041	(0)
ZnOHCl	1.252e-12	1.254e-12	-11.902	-11.902	0.001	(0)
Zn(OH)3-	3.550e-15	3.228e-15	-14.450	-14.491	-0.041	(0)
ZnBr+	1.892e-15	1.721e-15	-14.723	-14.764	-0.041	(0)
ZnCl2	5.361e-16	5.371e-16	-15.271	-15.270	0.001	(0)
ZnCl3-	6.526e-20	5.932e-20	-19.185	-19.227	-0.041	(0)
Zn(OH)4-2	1.106e-20	7.567e-21	-19.956	-20.121	-0.165	(0)
ZnBr2	1.789e-22	1.793e-22	-21.747	-21.746	0.001	(0)
ZnCl4-2	4.181e-24	2.883e-24	-23.379	-23.540	-0.161	(0)
Zn(HS)2	0.000e+00	0.000e+00	-102.168	-102.167	0.001	(0)
Zn(HS)3-	0.000e+00	0.000e+00	-155.718	-155.759	-0.041	(0)

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

Phase	SI**	log IAP	log K(291 K, 1 atm)	
Akermanite	-23.48	25.24	48.72	Ca2MgSi2O7
Al(OH)3(a)	-0.53	10.30	10.82	Al(OH)3
Al2O3	-2.39	20.59	22.98	Al2O3
Al4(OH)10SO4	1.25	23.95	22.70	Al4(OH)10SO4
AlAsO4·2H2O	-8.11	-3.31	4.80	AlAsO4·2H2O
Albite	-2.31	1.52	3.83	NaAlSi3O8
Albite(low)	-1.35	1.52	2.88	NaAlSi3O8
AlOHSO4	-3.71	-6.94	-3.23	AlOHSO4
AlumK	-15.94	-21.23	-5.29	KAl(SO4)2·12H2O
Alunite	0.77	-0.64	-1.41	KAl3(SO4)2(OH)6
Analcime	-1.39	5.71	7.09	NaAlSi2O6·H2O
Anhydrite	-1.47	-6.05	-4.58	CaSO4
Anilite	-30.40	-62.99	-32.59	Cu0.25Cu1.5S
Annite	-1.68	22.68	24.36	KFe3AlSi3O10(OH)2
Anorthite	-3.17	23.42	26.58	CaAl2Si2O8
Antlerite	-8.78	-0.49	8.29	Cu3(OH)4SO4
Aragonite	-1.44	-9.74	-8.30	CaCO3
Arsenolite	-50.97	-54.01	-3.04	As4O6
Artinite	-8.55	1.52	10.07	MgCO3:Mg(OH)2:3H2O
As2O5	-34.00	-27.21	6.79	As2O5
Atacamite	-7.64	0.00	7.65	Cu2(OH)3Cl
Azurite	-8.58	-25.11	-16.53	Cu3(OH)2(CO3)2
B_UO2(OH)2	-1.71	4.06	5.77	UO2(OH)2
Ba3(AsO4)2	2.58	-6.38	-8.95	Ba3(AsO4)2
Barite	-0.22	-10.30	-10.08	BaSO4
Bianchite	-8.74	-10.50	-1.76	ZnSO4·6H2O
Birnessite	-16.36	1.73	18.09	MnO2
Bixbyite	-16.01	-16.37	-0.36	Mn2O3
BlaubleiI	-33.06	-57.23	-24.16	Cu0.9Cu0.2S
BlaubleiII	-32.61	-59.89	-27.28	Cu0.6Cu0.8S
Boehmite	1.26	10.30	9.04	AlOOH
Brochantite	-10.25	5.09	15.34	Cu4(OH)6SO4
Brucite	-5.99	11.22	17.21	Mg(OH)2
Bunsenite	-4.82	8.02	12.84	NiO
Ca-Nontronite	18.88	-2.01	-20.89	Fe2Al.33Si3.67O10(OH)2Ca0.165
Ca-Olivine	-20.34	18.20	38.54	Ca2SiO4
Ca3(AsO4)2·6H2O	-15.94	6.36	22.30	Ca3(AsO4)2·6H2O
Ca3SiO5	-46.22	29.39	75.60	Ca3SiO5
Calcite	-1.30	-9.74	-8.44	CaCO3
Celestine	-2.07	-8.53	-6.46	SrSO4
CH4(g)	-59.16	-100.25	-41.10	CH4
Chalcanthite	-8.99	-11.66	-2.66	CuSO4·5H2O
Chalcedony	-0.58	-4.18	-3.60	SiO2
Chalcocite	-29.78	-65.20	-35.43	Cu2S
Chalcocypirite	-75.09	-110.94	-35.85	CuFeS2
Chrysotile	-7.74	25.31	33.05	Mg3Si2O5(OH)4
Claudetite	-50.72	-54.01	-3.28	As4O6
Clinoenstatite	-4.62	7.04	11.66	MgSiO3
CO2(g)	-2.76	-20.93	-18.17	CO2
Covellite	-32.91	-56.34	-23.43	CuS
Cristobalite	-0.51	-4.18	-3.68	SiO2
Cu(OH)2	-3.31	5.58	8.89	Cu(OH)2
Cu2SO4	-18.65	-20.52	-1.88	Cu2SO4
Cu3(AsO4)2·6H2O	-16.56	-10.46	6.10	Cu3(AsO4)2·6H2O
CuBr	-6.97	-15.39	-8.42	CuBr
CuCO3	-5.72	-15.35	-9.63	CuCO3
CuMetal	-2.52	-11.56	-9.04	Cu
CuOCuSO4	-18.19	-6.08	12.11	CuO:CuSO4
CupricFerrite	7.16	13.68	6.51	CuFe2O4
Cuprite	-1.63	-3.28	-1.65	Cu2O
CuprousFerrite	11.26	2.41	-8.86	CuFeO2

CuSO4	-14.96	-11.66	3.31	CuSO4
Diaspore	3.02	10.30	7.28	AlOOH
Diopside	-6.36	14.05	20.41	CaMgSi2O6
Diopside	-5.25	1.40	6.65	CuSiO3:H2O
Djurleite	-29.92	-64.62	-34.70	Cu0.066Cu1.868S
Dolomite	-2.58	-19.44	-16.86	CaMg(CO3)2
Epsomite	-3.83	-6.02	-2.19	MgSO4:7H2O
Fe(OH)2.7Cl0.3	3.74	0.70	-3.04	Fe(OH)2.7Cl0.3
Fe2(SO4)3	-48.17	-43.62	4.55	Fe2(SO4)3
Fe3(OH)8	-4.80	15.42	20.22	Fe3(OH)8
FeAsO4:2H2O	-9.96	-9.56	0.40	FeAsO4:2H2O
Ferrihydrite	-0.84	4.05	4.89	Fe(OH)3
FeS(ppt)	-50.68	-54.60	-3.92	FeS
Forsterite	-10.82	18.27	29.09	Mg2SiO4
Gehlenite	-19.93	38.79	58.72	Ca2Al2SiO7
Gibbsite(C)	1.15	10.30	9.14	Al(OH)3
Goethite	3.31	4.05	0.74	FeOOH
Goslarite	-8.49	-10.50	-2.01	ZnSO4:7H2O
Greenalite	-7.19	13.62	20.81	Fe3Si2O5(OH)4
Greigite	-187.23	-232.27	-45.03	Fe3S4
Gummite	-6.72	4.06	10.78	UO3
Gypsum	-1.44	-6.05	-4.61	CaSO4:2H2O
Halite	-8.95	-7.38	1.57	NaCl
Halloysite	2.58	12.23	9.64	Al2Si2O5(OH)4
Hausmannite	-22.07	40.78	62.85	Mn3O4
Hematite	11.60	8.10	-3.50	Fe2O3
Hercynite	-0.52	27.92	28.44	FeAl2O4
Huntite	-9.30	-38.85	-29.55	CaMg3(CO3)4
Hydromagnesite	-19.68	-27.59	-7.91	Mg5(CO3)4(OH)2:4H2O
Jarosite-H	-11.14	-22.34	-11.20	(H3O)Fe3(SO4)2(OH)6
Jarosite-K	-5.10	-19.39	-14.29	KFe3(SO4)2(OH)6
Jarosite-Na	-7.95	-18.56	-10.61	NaFe3(SO4)2(OH)6
K-Nontronite	12.66	-2.88	-15.55	Fe2Al.33Si3.67O10(OH)2K0.33
Kalsilite	-4.25	9.07	13.31	KAlSiO4
Kaolinite	5.92	12.23	6.30	Al2Si2O5(OH)4
Langite	-12.35	5.09	17.44	Cu4(OH)6SO4:H2O
Larnite	-21.88	18.20	40.08	Ca2SiO4
Laumontite	-0.23	15.05	15.28	CaAl2Si4O12:4H2O
Leonhardtite	12.22	30.10	17.88	Ca2Al4Si8O24:7H2O
Lepidocrocite	2.68	4.05	1.37	FeOOH
Leucite	-1.90	4.88	6.78	KAlSi2O6
Lime	-22.36	11.19	33.55	CaO
Mackinawite	-49.95	-54.60	-4.65	FeS
Magadiite	-11.20	-25.50	-14.30	NaSi7O13(OH)3:3H2O
Maghemite	1.71	8.10	6.39	Fe2O3
Magnesite	-1.78	-9.70	-7.93	MgCO3
Magnetite	10.86	15.42	4.56	Fe3O4
Malachite	-4.84	-9.76	-4.93	Cu2(OH)2CO3
Manganite	-7.95	-8.19	-0.24	MnOOH
Melanothallite	-20.67	-16.74	3.93	CuCl2
Melanterite	-7.40	-9.91	-2.52	FeSO4:7H2O
Merwinite	-33.86	36.43	70.29	Ca3MgSi2O8
Mg-Ferrite	1.47	19.32	17.85	MgFe2O4
Mg-Nontronite	18.58	-2.01	-20.59	Fe2Al.33Si3.67O10(OH)2Mg0.165
Microcline	-0.12	0.70	0.82	KAlSi3O8
Millerite	-45.82	-53.91	-8.08	NiS
Mirabilite	-8.26	-9.69	-1.42	Na2SO4:10H2O
Mn2(SO4)3	-63.02	-68.09	-5.07	Mn2(SO4)3
Mn3(AsO4)2:8H2O	-18.76	-6.26	12.50	Mn3(AsO4)2:8H2O
MnCl2:4H2O	-17.76	-15.34	2.43	MnCl2:4H2O
MnS(Green)	-58.83	-54.94	3.89	MnS
MnSO4	-13.18	-10.26	2.92	MnSO4
Monticellite	-12.85	18.23	31.08	CaMgSiO4
Montmorillonite	5.33	8.00	2.67	Mg0.485Fe.22Al1.71Si3.81O10(OH)2
Morenosite	-6.82	-9.22	-2.41	NiSO4:7H2O
Muscovite	7.33	21.29	13.96	KAl3Si3O10(OH)2
Na-Nontronite	11.89	-2.61	-14.50	Fe2Al.33Si3.67O10(OH)2Na0.33
Nantokite	-5.88	-12.80	-6.92	CuCl
Natron	-11.81	-13.38	-1.57	Na2CO3:10H2O
Nepheline	-4.87	9.89	14.76	NaAlSiO4
Nesquehonite	-4.18	-9.70	-5.53	MgCO3:3H2O
Ni(OH)2	-2.29	8.02	10.30	Ni(OH)2
Ni2SiO4	-3.24	11.85	15.08	Ni2SiO4
Ni3(AsO4)2:8H2O	-18.86	-3.16	15.70	Ni3(AsO4)2:8H2O
Ni4(OH)6SO4	-17.18	14.82	32.00	Ni4(OH)6SO4
NiCO3	-6.23	-12.91	-6.68	NiCO3
Nsutite	-15.78	1.73	17.50	MnO2
O2(g)	-45.64	39.66	85.31	O2
Oripment	-150.45	-212.77	-62.33	As2S3
P-Wollstanite	-7.18	7.01	14.19	CaSiO3
Periclase	-10.88	11.22	22.10	MgO
Phlogopite	-33.34	34.37	67.71	KMg3AlSi3O10(OH)2
Portlandite	-11.99	11.19	23.18	Ca(OH)2
Pyrite	-78.02	-96.69	-18.66	FeS2
Pyrocroite	-8.47	6.98	15.46	Mn(OH)2
Pyrolusite	-14.61	1.73	16.34	MnO2
Pyrophyllite	5.46	3.86	-1.60	Al2Si4O10(OH)2
Quartz	-0.08	-4.18	-4.11	SiO2
Realgar	-65.09	-85.34	-20.25	AsS
Retgersite	-7.17	-9.22	-2.06	NiSO4:6H2O
Rhodochrosite	-3.57	-13.94	-10.38	MnCO3
Rutherfordine	-2.42	-16.86	-14.45	UO2CO3
Sanidine(H)	-0.60	0.70	1.29	KAlSi3O8
Schoepite	-1.54	4.06	5.60	UO2(OH)2:H2O
Sepiolite(a)	-8.88	9.90	18.78	Mg2Si3O7.5OH:3H2O
Sepiolite(c)	-6.46	9.90	16.36	Mg2Si3O7.5OH:3H2O
Siderite	-3.14	-13.60	-10.46	FeCO3
SiO2(a)	-1.09	-4.18	-3.09	SiO2
SiO2(am)	-1.41	-4.18	-2.77	SiO2
Smithsonite	-4.26	-14.19	-9.93	ZnCO3
Sphalerite	-43.43	-55.18	-11.75	ZnS
Spinel	-5.97	31.82	37.79	MgAl2O4
Strontianite	-2.97	-12.21	-9.24	SrCO3

Sulfur	-40.05	-42.09	-2.04	S
Talc	-6.68	16.94	23.63	Mg3Si4O10(OH)2
Tenorite	-2.29	5.58	7.87	CuO
Thenardite	-9.52	-9.69	-0.17	Na2SO4
Thermonatrite	-13.55	-13.38	0.17	Na2CO3:H2O
Tremolite	-13.08	45.04	58.12	Ca2Mg5Si8O22(OH)2
U3O8(C)	-1.31	21.69	23.00	U3O8
U4O9(C)	-2.40	-4.13	-1.73	U4O9
UO2(am)	-7.35	-5.99	1.36	UO2
UO3(C)	-3.97	4.06	8.03	UO3
Uraninite	-1.59	-5.99	-4.40	UO2
Uranophane	-6.54	10.95	17.49	Ca(UO2)2(SiO3OH)2
USiO4(C)	-2.79	-10.17	-7.38	USiO4
Wairakite	-4.85	15.05	19.90	CaAl2Si4O12:2H2O
Willemite	-6.58	9.29	15.88	Zn2SiO4
Witherite	-5.39	-13.98	-8.59	BaCO3
Wollastonite	-6.31	7.01	13.31	CaSiO3
Wurtzite	-45.42	-55.18	-9.76	ZnS
Zincite	-4.76	6.74	11.50	ZnO
Zincosite	-13.83	-10.50	3.32	ZnSO4
Zn(BO2)2	-10.92	-2.63	8.29	Zn(BO2)2
Zn(OH)2(A)	-5.71	6.74	12.45	Zn(OH)2
Zn(OH)2(B)	-5.01	6.74	11.75	Zn(OH)2
Zn(OH)2(C)	-5.46	6.74	12.20	Zn(OH)2
Zn(OH)2(E)	-4.76	6.74	11.50	Zn(OH)2
Zn(OH)2(G)	-4.97	6.74	11.71	Zn(OH)2
Zn2(OH)2SO4	-11.26	-3.76	7.50	Zn2(OH)2SO4
Zn2(OH)3Cl	-12.88	2.32	15.20	Zn2(OH)3Cl
Zn3(AsO4)2:2.5H2O	-20.65	-7.00	13.65	Zn3(AsO4)2:2.5H2O
Zn3O(SO4)2	-34.30	-14.27	20.03	Zn3O(SO4)2
Zn4(OH)6SO4	-18.69	9.71	28.40	Zn4(OH)6SO4
Zn5(OH)8Cl2	-27.13	11.37	38.50	Zn5(OH)8Cl2
ZnBr2:2H2O	-26.10	-20.77	5.33	ZnBr2:2H2O
ZnCl2	-22.90	-15.58	7.32	ZnCl2
ZnCO3:H2O	-3.93	-14.19	-10.26	ZnCO3:H2O
ZnMetal	-39.45	-13.09	26.36	Zn
ZnO(Active)	-4.57	6.74	11.31	ZnO
ZnS(A)	-46.07	-55.18	-9.11	ZnS
ZnSiO3	-0.67	2.56	3.23	ZnSiO3
ZnSO4:H2O	-10.11	-10.50	-0.40	ZnSO4:H2O

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

End of simulation.

1.7 DJX-pit, 50 m

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.
Using pressure 1.

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

Elements	Molality	Moles
Al	1.134e-05	1.134e+02
As	5.333e-09	5.333e-02
B	5.827e-05	5.827e+02
Ba	5.825e-08	5.825e-01
Br	6.508e-07	6.508e+00
C	6.287e-04	6.287e+03
Ca	2.677e-03	2.677e+04
Cl	2.113e-04	2.113e+03
Cu	1.574e-07	1.574e+00
Fe	3.581e-08	3.581e-01
K	9.059e-05	9.059e+02
Li	1.052e-05	1.052e+02
Mg	3.043e-03	3.043e+04
Mn	4.013e-05	4.013e+02
N	2.714e-05	2.714e+02
Na	1.093e-03	1.093e+04
Ni	2.159e-05	2.159e+02
S	5.474e-03	5.474e+04
Si	1.774e-04	1.774e+03
Sr	8.801e-06	8.801e+01
U	1.340e-06	1.340e+01
Zn	5.383e-06	5.383e+01

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

pH	=	5.550	Charge balance
pe	=	4.792	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength (mol/kgw)	=	1.870e-02	
Mass of water (kg)	=	1.000e+07	
Total alkalinity (eq/kg)	=	1.381e-04	
Total CO2 (mol/kg)	=	6.287e-04	
Temperature (°C)	=	4.23	
Pressure (atm)	=	5.34	
Electrical balance (eq)	=	1.554e+04	
Percent error, 100*(Cat- An)/(Cat+ An)	=	7.98	
Iterations	=	3	
Total H	=	1.110146e+09	
Total O	=	5.553090e+08	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm ³ /mol
H+	3.150e-06	2.819e-06	-5.502	-5.550	-0.048	0.00
OH-	7.572e-10	6.619e-10	-9.121	-9.179	-0.058	(0)
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.01
Al	1.134e-05					
Al(OH)2+	5.703e-06	5.032e-06	-5.244	-5.298	-0.054	(0)
Al(OH)3	2.244e-06	2.254e-06	-5.649	-5.647	0.002	(0)
Al+3	1.358e-06	5.003e-07	-5.867	-6.301	-0.434	(0)
AlSO4+	1.153e-06	1.013e-06	-5.938	-5.994	-0.056	(0)
AlOH+2	6.685e-07	4.049e-07	-6.175	-6.393	-0.218	(0)
Al(SO4)2-	2.130e-07	1.871e-07	-6.672	-6.728	-0.056	(0)
Al(OH)4-	3.485e-10	3.062e-10	-9.458	-9.514	-0.056	(0)
As(3)	4.374e-12					
H3AsO3	4.373e-12	4.392e-12	-11.359	-11.357	0.002	(0)
H2AsO3-	4.582e-16	4.022e-16	-15.339	-15.396	-0.057	(0)
H4AsO3+	6.989e-18	6.135e-18	-17.156	-17.212	-0.057	(0)
HAsO3-2	7.235e-23	4.296e-23	-22.141	-22.367	-0.226	(0)
AsO3-3	8.836e-31	2.734e-31	-30.054	-30.563	-0.509	(0)
As(5)	5.329e-09					
H2AsO4-	4.918e-09	4.317e-09	-8.308	-8.365	-0.057	(0)
HAsO4-2	4.085e-10	2.425e-10	-9.389	-9.615	-0.226	(0)
H3AsO4	1.713e-12	1.720e-12	-11.766	-11.764	0.002	(0)
AsO4-3	4.068e-16	1.259e-16	-15.391	-15.900	-0.509	(0)
B	5.827e-05					
H3BO3	5.826e-05	5.852e-05	-4.235	-4.233	0.002	(0)
H2BO3-	9.191e-09	7.991e-09	-8.037	-8.097	-0.061	(0)
Ba	5.825e-08					
Ba+2	5.825e-08	3.503e-08	-7.235	-7.456	-0.221	(0)
BaOH+	9.213e-17	8.113e-17	-16.036	-16.091	-0.055	(0)
Br	6.508e-07					
Br-	6.508e-07	5.703e-07	-6.187	-6.244	-0.057	(0)
NiBr+	2.104e-11	1.847e-11	-10.677	-10.734	-0.057	(0)
ZnBr+	4.256e-13	3.736e-13	-12.371	-12.428	-0.057	(0)
ZnBr2	8.447e-20	8.483e-20	-19.073	-19.071	0.002	(0)
C(4)	6.287e-04					
H2CO3	5.070e-04	5.092e-04	-3.295	-3.293	0.002	(0)
HCO3-	1.178e-04	1.040e-04	-3.929	-3.983	-0.054	(0)
MgHCO3+	1.694e-06	1.485e-06	-5.771	-5.828	-0.057	(0)
UO2CO3	1.027e-06	1.031e-06	-5.989	-5.987	0.002	(0)
CaHCO3+	8.418e-07	7.446e-07	-6.075	-6.128	-0.053	(0)
NiHCO3+	9.755e-08	8.563e-08	-7.011	-7.067	-0.057	(0)
NiCO3	7.596e-08	7.629e-08	-7.119	-7.118	0.002	(0)
NaHCO3	3.224e-08	3.238e-08	-7.492	-7.490	0.002	(0)
MnHCO3+	2.590e-08	2.281e-08	-7.587	-7.642	-0.055	(0)
ZnHCO3+	2.020e-08	1.773e-08	-7.695	-7.751	-0.057	(0)
UO2(CO3)2-2	8.966e-09	5.323e-09	-8.047	-8.274	-0.226	(0)
CuHCO3+	2.264e-09	1.987e-09	-8.645	-8.702	-0.057	(0)
CO3-2	1.659e-09	1.005e-09	-8.780	-8.998	-0.218	(0)
CaCO3	1.366e-09	1.372e-09	-8.865	-8.863	0.002	(0)
MgCO3	1.065e-09	1.070e-09	-8.973	-8.971	0.002	(0)
ZnCO3	4.973e-10	4.995e-10	-9.303	-9.301	0.002	(0)
CuCO3	3.768e-10	3.785e-10	-9.424	-9.422	0.002	(0)
NaCO3-	6.508e-12	5.741e-12	-11.187	-11.241	-0.054	(0)
UO2(CO3)3-4	4.980e-12	6.187e-13	-11.303	-12.209	-0.906	(0)
Ni(CO3)2-2	2.245e-13	1.333e-13	-12.649	-12.875	-0.226	(0)
Zn(CO3)2-2	1.808e-14	1.073e-14	-13.743	-13.969	-0.226	(0)
Cu(CO3)2-2	8.067e-16	4.789e-16	-15.093	-15.320	-0.226	(0)
Ca	2.677e-03					
Ca+2	2.118e-03	1.306e-03	-2.674	-2.884	-0.210	(0)
CaSO4	5.582e-04	5.606e-04	-3.253	-3.251	0.002	(0)
CaHCO3+	8.418e-07	7.446e-07	-6.075	-6.128	-0.053	(0)
CaCO3	1.366e-09	1.372e-09	-8.865	-8.863	0.002	(0)
CaOH+	2.112e-11	1.868e-11	-10.675	-10.729	-0.053	(0)
Cl	2.113e-04					
Cl-	2.112e-04	1.843e-04	-3.675	-3.734	-0.059	(0)
MnCl+	1.712e-08	1.507e-08	-7.767	-7.822	-0.055	(0)
NiCl+	5.387e-09	4.729e-09	-8.269	-8.325	-0.057	(0)
ZnCl+	5.267e-10	4.616e-10	-9.278	-9.336	-0.057	(0)
UO2Cl+	2.474e-11	2.171e-11	-10.607	-10.663	-0.057	(0)
CuCl+	1.330e-11	1.166e-11	-10.876	-10.933	-0.057	(0)
CuCl2-	6.237e-12	5.466e-12	-11.205	-11.262	-0.057	(0)
ZnOHCl	5.385e-12	5.408e-12	-11.269	-11.267	0.002	(0)
NiCl2	3.158e-12	3.172e-12	-11.501	-11.499	0.002	(0)
MnCl2	7.513e-13	7.546e-13	-12.124	-12.122	0.002	(0)
ZnCl2	8.108e-14	8.143e-14	-13.091	-13.089	0.002	(0)
CuCl3-2	2.436e-15	1.465e-15	-14.613	-14.834	-0.221	(0)
CuCl2	9.023e-16	9.062e-16	-15.045	-15.043	0.002	(0)
MnCl3-	7.119e-17	6.269e-17	-16.148	-16.203	-0.055	(0)
ZnCl3-	1.680e-17	1.473e-17	-16.775	-16.832	-0.057	(0)
FeCl+2	1.373e-19	8.256e-20	-18.862	-19.083	-0.221	(0)
ZnCl4-2	1.891e-21	1.137e-21	-20.723	-20.944	-0.221	(0)
CuCl3-	4.553e-22	3.990e-22	-21.342	-21.399	-0.057	(0)
FeCl2+	1.566e-22	1.379e-22	-21.805	-21.860	-0.055	(0)
FeCl3	2.531e-27	2.542e-27	-26.597	-26.595	0.002	(0)
CuCl4-2	1.293e-27	7.778e-28	-26.888	-27.109	-0.221	(0)
UCl+3	6.411e-31	1.984e-31	-30.193	-30.703	-0.509	(0)
Cu(1)	5.613e-10					
Cu+	5.551e-10	4.826e-10	-9.256	-9.316	-0.061	(0)
CuCl2-	6.237e-12	5.466e-12	-11.205	-11.262	-0.057	(0)
CuCl3-2	2.436e-15	1.465e-15	-14.613	-14.834	-0.221	(0)
Cu(S4)2-3	0.000e+00	0.000e+00	-102.370	-102.671	-0.300	(0)
CuS4S5-3	0.000e+00	0.000e+00	-103.113	-103.401	-0.288	(0)
Cu(2)	1.568e-07					
Cu+2	1.227e-07	7.011e-08	-6.911	-7.154	-0.243	(0)
CuSO4	3.100e-08	3.114e-08	-7.509	-7.507	0.002	(0)
CuHCO3+	2.264e-09	1.987e-09	-8.645	-8.702	-0.057	(0)
CuCO3	3.768e-10	3.785e-10	-9.424	-9.422	0.002	(0)
CuOH+	2.847e-10	2.495e-10	-9.546	-9.603	-0.057	(0)

Cu(OH) 2	1.847e-10	1.855e-10	-9.734	-9.732	0.002	(0)
CuCl+	1.330e-11	1.166e-11	-10.876	-10.933	-0.057	(0)
Cu2(OH) 2+2	5.000e-15	2.968e-15	-14.301	-14.527	-0.226	(0)
CuCl2	9.023e-16	9.062e-16	-15.045	-15.043	0.002	(0)
Cu(CO3) 2-2	8.067e-16	4.789e-16	-15.093	-15.320	-0.226	(0)
Cu(OH) 3-	4.541e-18	3.986e-18	-17.343	-17.399	-0.057	(0)
CuCl3-	4.553e-22	3.990e-22	-21.342	-21.399	-0.057	(0)
Cu(OH) 4-2	4.756e-25	2.823e-25	-24.323	-24.549	-0.226	(0)
CuCl4-2	1.293e-27	7.778e-28	-26.888	-27.109	-0.221	(0)
Cu(HS) 3-	0.000e+00	0.000e+00	-142.965	-143.021	-0.057	(0)
Fe (2)	3.580e-08					
Fe+2	3.027e-08	1.853e-08	-7.519	-7.732	-0.213	(0)
FeSO4	5.535e-09	5.559e-09	-8.257	-8.255	0.002	(0)
FeOH+	4.465e-13	3.932e-13	-12.350	-12.405	-0.055	(0)
Fe(OH) 2	1.701e-19	1.708e-19	-18.769	-18.767	0.002	(0)
Fe(OH) 3-	2.060e-24	1.814e-24	-23.686	-23.741	-0.055	(0)
Fe(HS) 2	0.000e+00	0.000e+00	-106.628	-106.626	0.002	(0)
Fe(HS) 3-	0.000e+00	0.000e+00	-158.454	-158.511	-0.057	(0)
Fe (3)	9.302e-12					
Fe(OH) 2+	9.237e-12	8.149e-12	-11.034	-11.089	-0.054	(0)
Fe(OH) 3	3.392e-14	3.407e-14	-13.470	-13.468	0.002	(0)
FeOH+2	3.090e-14	1.858e-14	-13.510	-13.731	-0.221	(0)
FeSO4+	4.402e-16	3.876e-16	-15.356	-15.412	-0.055	(0)
Fe(OH) 4-	1.374e-16	1.212e-16	-15.862	-15.916	-0.054	(0)
Fe+3	8.174e-17	3.010e-17	-16.088	-16.521	-0.434	(0)
Fe(SO4) 2-	3.248e-17	2.851e-17	-16.488	-16.545	-0.057	(0)
FeCl+2	1.373e-19	8.256e-20	-18.862	-19.083	-0.221	(0)
FeCl2+	1.566e-22	1.379e-22	-21.805	-21.860	-0.055	(0)
Fe2(OH) 2+4	1.881e-25	2.337e-26	-24.726	-25.631	-0.906	(0)
FeCl3	2.531e-27	2.542e-27	-26.597	-26.595	0.002	(0)
Fe3(OH) 4+5	9.357e-34	3.597e-35	-33.029	-34.444	-1.415	(0)
H (0)	3.654e-24					
H2	1.827e-24	1.835e-24	-23.738	-23.736	0.002	(0)
K	9.059e-05					
K+	8.952e-05	7.810e-05	-4.048	-4.107	-0.059	(0)
KSO4-	1.069e-06	9.433e-07	-5.971	-6.025	-0.054	(0)
Li	1.052e-05					
Li+	1.040e-05	9.201e-06	-4.983	-5.036	-0.053	(0)
LiSO4-	1.157e-07	1.019e-07	-6.937	-6.992	-0.055	(0)
Mg	3.043e-03					
Mg+2	2.464e-03	1.534e-03	-2.608	-2.814	-0.206	(0)
MgSO4	5.777e-04	5.802e-04	-3.238	-3.236	0.002	(0)
MgHCO3+	1.694e-06	1.485e-06	-5.771	-5.828	-0.057	(0)
MgCO3	1.065e-09	1.070e-09	-8.973	-8.971	0.002	(0)
MgOH+	1.465e-10	1.299e-10	-9.834	-9.886	-0.052	(0)
Mn (2)	4.013e-05					
Mn+2	3.302e-05	2.021e-05	-4.481	-4.694	-0.213	(0)
MnSO4	7.065e-06	7.095e-06	-5.151	-5.149	0.002	(0)
MnHCO3+	2.590e-08	2.281e-08	-7.587	-7.642	-0.055	(0)
MnCl+	1.712e-08	1.507e-08	-7.767	-7.822	-0.055	(0)
MnOH+	3.403e-11	2.996e-11	-10.468	-10.523	-0.055	(0)
MnCl2	7.513e-13	7.546e-13	-12.124	-12.122	0.002	(0)
MnCl3-	7.119e-17	6.269e-17	-16.148	-16.203	-0.055	(0)
Mn(OH) 3-	1.639e-23	1.443e-23	-22.785	-22.841	-0.055	(0)
Mn(NO3) 2	0.000e+00	0.000e+00	-84.372	-84.370	0.002	(0)
Mn (3)	2.741e-24					
Mn+3	2.741e-24	1.010e-24	-23.562	-23.996	-0.434	(0)
Mn (6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-67.577	-67.797	-0.221	(0)
Mn (7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-73.790	-73.850	-0.060	(0)
N (-3)	2.714e-05					
NH4+	2.629e-05	2.286e-05	-4.580	-4.641	-0.061	(0)
NH4SO4-	8.487e-07	7.473e-07	-6.071	-6.126	-0.055	(0)
NH3	9.465e-10	9.506e-10	-9.024	-9.022	0.002	(0)
N (3)	1.568e-30					
NO2-	1.568e-30	1.376e-30	-29.805	-29.861	-0.057	(0)
N (5)	0.000e+00					
NO3-	0.000e+00	0.000e+00	-40.089	-40.149	-0.060	(0)
Mn(NO3) 2	0.000e+00	0.000e+00	-84.372	-84.370	0.002	(0)
Na	1.093e-03					
Na+	1.081e-03	9.503e-04	-2.966	-3.022	-0.056	(0)
NaSO4-	1.189e-05	1.049e-05	-4.925	-4.979	-0.054	(0)
NaHCO3	3.224e-08	3.238e-08	-7.492	-7.490	0.002	(0)
NaCO3-	6.508e-12	5.741e-12	-11.187	-11.241	-0.054	(0)
Ni	2.159e-05					
Ni+2	1.725e-05	1.024e-05	-4.763	-4.990	-0.226	(0)
NiSO4	4.163e-06	4.181e-06	-5.381	-5.379	0.002	(0)
NiHCO3+	9.755e-08	8.563e-08	-7.011	-7.067	-0.057	(0)
NiCO3	7.596e-08	7.629e-08	-7.119	-7.118	0.002	(0)
NiCl+	5.387e-09	4.729e-09	-8.269	-8.325	-0.057	(0)
Ni(SO4) 2-2	1.163e-09	6.904e-10	-8.934	-9.161	-0.226	(0)
NiOH+	1.192e-10	1.047e-10	-9.924	-9.980	-0.057	(0)
NiBr+	2.104e-11	1.847e-11	-10.677	-10.734	-0.057	(0)
NiCl2	3.158e-12	3.172e-12	-11.501	-11.499	0.002	(0)
Ni(CO3) 2-2	2.245e-13	1.333e-13	-12.649	-12.875	-0.226	(0)
Ni(OH) 2	1.291e-13	1.296e-13	-12.889	-12.887	0.002	(0)
Ni(OH) 3-	5.255e-19	4.613e-19	-18.279	-18.336	-0.057	(0)
O (0)	0.000e+00					
O2	0.000e+00	0.000e+00	-52.111	-52.109	0.002	(0)
S (-2)	0.000e+00					
H2S	0.000e+00	0.000e+00	-52.204	-52.202	0.002	(0)
HS-	0.000e+00	0.000e+00	-53.864	-53.922	-0.058	(0)
S6-2	0.000e+00	0.000e+00	-58.027	-58.253	-0.226	(0)
S5-2	0.000e+00	0.000e+00	-58.251	-58.478	-0.226	(0)
S4-2	0.000e+00	0.000e+00	-58.507	-58.734	-0.226	(0)
S-2	0.000e+00	0.000e+00	-61.733	-61.954	-0.221	(0)
S3-2	0.000e+00	0.000e+00	-61.998	-62.225	-0.226	(0)
S2-2	0.000e+00	0.000e+00	-63.299	-63.526	-0.226	(0)
Zn(HS) 2	0.000e+00	0.000e+00	-98.510	-98.508	0.002	(0)
Cu(S4) 2-3	0.000e+00	0.000e+00	-102.370	-102.671	-0.300	(0)
CuS4S5-3	0.000e+00	0.000e+00	-103.113	-103.401	-0.288	(0)
Fe(HS) 2	0.000e+00	0.000e+00	-106.628	-106.626	0.002	(0)

Cu (HS) 3-	0.000e+00	0.000e+00	-142.965	-143.021	-0.057	(0)
Zn (HS) 3-	0.000e+00	0.000e+00	-151.213	-151.270	-0.057	(0)
Fe (HS) 3-	0.000e+00	0.000e+00	-158.454	-158.511	-0.057	(0)
S (6)	5.474e-03					
SO4-2	4.309e-03	2.538e-03	-2.366	-2.596	-0.230	(0)
MgSO4	5.777e-04	5.802e-04	-3.238	-3.236	0.002	(0)
CaSO4	5.582e-04	5.606e-04	-3.253	-3.251	0.002	(0)
NaSO4-	1.189e-05	1.049e-05	-4.925	-4.979	-0.054	(0)
MnSO4	7.065e-06	7.095e-06	-5.151	-5.149	0.002	(0)
NiSO4	4.163e-06	4.181e-06	-5.381	-5.379	0.002	(0)
ZnSO4	1.242e-06	1.248e-06	-5.906	-5.904	0.002	(0)
AlSO4+	1.153e-06	1.013e-06	-5.938	-5.994	-0.056	(0)
KSO4-	1.069e-06	9.433e-07	-5.971	-6.025	-0.054	(0)
NH4SO4-	8.487e-07	7.473e-07	-6.071	-6.126	-0.055	(0)
HSO4-	4.537e-07	3.986e-07	-6.343	-6.399	-0.056	(0)
Al (SO4) 2-	2.130e-07	1.871e-07	-6.672	-6.728	-0.056	(0)
LiSO4-	1.157e-07	1.019e-07	-6.937	-6.992	-0.055	(0)
UO2SO4	5.630e-08	5.654e-08	-7.250	-7.248	0.002	(0)
Zn (SO4) 2-2	5.147e-08	3.056e-08	-7.288	-7.515	-0.226	(0)
CuSO4	3.100e-08	3.114e-08	-7.509	-7.507	0.002	(0)
UO2 (SO4) 2-2	6.344e-09	3.766e-09	-8.198	-8.424	-0.226	(0)
FeSO4	5.535e-09	5.559e-09	-8.257	-8.255	0.002	(0)
Ni (SO4) 2-2	1.163e-09	6.904e-10	-8.934	-9.161	-0.226	(0)
FeSO4+	4.402e-16	3.876e-16	-15.356	-15.412	-0.055	(0)
Fe (SO4) 2-	3.248e-17	2.851e-17	-16.488	-16.545	-0.057	(0)
U (SO4) 2	2.388e-24	2.398e-24	-23.622	-23.620	0.002	(0)
USO4+2	1.343e-25	7.970e-26	-24.872	-25.099	-0.226	(0)
Si	1.774e-04					
H4SiO4	1.774e-04	1.782e-04	-3.751	-3.749	0.002	(0)
UO2H3SiO4+	2.378e-08	2.087e-08	-7.624	-7.680	-0.057	(0)
H3SiO4-	2.589e-09	2.269e-09	-8.587	-8.644	-0.057	(0)
H2SiO4-2	1.649e-16	9.990e-17	-15.783	-16.000	-0.218	(0)
Sr	8.801e-06					
Sr+2	8.801e-06	5.293e-06	-5.055	-5.276	-0.221	(0)
SrOH+	2.273e-14	2.002e-14	-13.643	-13.699	-0.055	(0)
U (3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-42.178	-42.688	-0.509	(0)
U (4)	3.012e-15					
U (OH) 5-	2.621e-15	2.301e-15	-14.581	-14.638	-0.057	(0)
U (OH) 4	3.848e-16	3.865e-16	-15.415	-15.413	0.002	(0)
U (OH) 3+	5.910e-18	5.188e-18	-17.228	-17.285	-0.057	(0)
U (OH) 2+2	2.113e-20	1.255e-20	-19.675	-19.901	-0.226	(0)
UOH+3	1.110e-23	3.433e-24	-22.955	-23.464	-0.509	(0)
U (SO4) 2	2.388e-24	2.398e-24	-23.622	-23.620	0.002	(0)
USO4+2	1.343e-25	7.970e-26	-24.872	-25.099	-0.226	(0)
U+4	1.396e-27	1.734e-28	-26.855	-27.761	-0.906	(0)
UCl+3	6.411e-31	1.984e-31	-30.193	-30.703	-0.509	(0)
U6 (OH) 15+9	0.000e+00	0.000e+00	-95.940	-100.526	-4.585	(0)
U (5)	1.412e-09					
UO2+	1.412e-09	1.240e-09	-8.850	-8.907	-0.057	(0)
U (6)	1.339e-06					
UO2CO3	1.027e-06	1.031e-06	-5.989	-5.987	0.002	(0)
UO2+2	1.397e-07	8.296e-08	-6.855	-7.081	-0.226	(0)
UO2OH+	7.516e-08	6.598e-08	-7.124	-7.181	-0.057	(0)
UO2SO4	5.630e-08	5.654e-08	-7.250	-7.248	0.002	(0)
UO2H3SiO4+	2.378e-08	2.087e-08	-7.624	-7.680	-0.057	(0)
UO2 (CO3) 2-2	8.966e-09	5.323e-09	-8.047	-8.274	-0.226	(0)
UO2 (SO4) 2-2	6.344e-09	3.766e-09	-8.198	-8.424	-0.226	(0)
(UO2) 2 (OH) 2+2	9.124e-10	5.417e-10	-9.040	-9.266	-0.226	(0)
(UO2) 3 (OH) 5+	3.983e-11	3.496e-11	-10.400	-10.456	-0.057	(0)
UO2Cl+	2.474e-11	2.171e-11	-10.607	-10.663	-0.057	(0)
UO2 (CO3) 3-4	4.980e-12	6.187e-13	-11.303	-12.209	-0.906	(0)
Zn	5.383e-06					
Zn+2	4.068e-06	2.490e-06	-5.391	-5.604	-0.213	(0)
ZnSO4	1.242e-06	1.248e-06	-5.906	-5.904	0.002	(0)
Zn (SO4) 2-2	5.147e-08	3.056e-08	-7.288	-7.515	-0.226	(0)
ZnHCO3+	2.020e-08	1.773e-08	-7.695	-7.751	-0.057	(0)
ZnCl+	5.267e-10	4.616e-10	-9.278	-9.336	-0.057	(0)
ZnCO3	4.973e-10	4.995e-10	-9.303	-9.301	0.002	(0)
ZnOH+	2.036e-10	1.787e-10	-9.691	-9.748	-0.057	(0)
ZnOHCl	5.385e-12	5.408e-12	-11.269	-11.267	0.002	(0)
Zn (OH) 2	3.962e-12	3.979e-12	-11.402	-11.400	0.002	(0)
ZnBr+	4.256e-13	3.736e-13	-12.371	-12.428	-0.057	(0)
ZnCl2	8.108e-14	8.143e-14	-13.091	-13.089	0.002	(0)
Zn (CO3) 2-2	1.808e-14	1.073e-14	-13.743	-13.969	-0.226	(0)
ZnCl3-	1.680e-17	1.473e-17	-16.775	-16.832	-0.057	(0)
Zn (OH) 3-	5.101e-18	4.477e-18	-17.292	-17.349	-0.057	(0)
ZnBr2	8.447e-20	8.483e-20	-19.073	-19.071	0.002	(0)
ZnCl4-2	1.891e-21	1.137e-21	-20.723	-20.944	-0.221	(0)
Zn (OH) 4-2	4.253e-25	2.525e-25	-24.371	-24.598	-0.226	(0)
Zn (HS) 2	0.000e+00	0.000e+00	-98.510	-98.508	0.002	(0)
Zn (HS) 3-	0.000e+00	0.000e+00	-151.213	-151.270	-0.057	(0)

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

Phase	SI**	log IAP	log K(277 K,	5 atm)
Akerminite	-34.45	17.22	51.67	Ca2MgSi2O7
Al (OH) 3 (a)	-1.51	10.35	11.86	Al (OH) 3
Al2O3	-2.28	20.70	22.98	Al2O3
Al4 (OH) 10SO4	5.01	27.70	22.69	Al4 (OH) 10SO4
AlAsO4:2H2O	-6.21	-1.42	4.80	AlAsO4:2H2O
Albite	-2.98	1.63	4.61	NaAlSi3O8
Albite (low)	-1.92	1.63	3.55	NaAlSi3O8
AlOHSO4	-0.12	-3.35	-3.23	AlOHSO4
AlumK	-10.02	-15.60	-5.58	KAl (SO4) 2:12H2O
Alunite	6.67	5.10	-1.57	KAl3 (SO4) 2 (OH) 6
Analcime	-2.60	5.38	7.97	NaAlSi2O6:H2O
Anhydrite	-1.05	-5.48	-4.43	CaSO4
Anilite	-29.87	-64.14	-34.27	Cu0.25Cu1.5S
Annite	-16.25	10.65	26.90	KFe3AlSi3O10 (OH) 2
Anorthite	-7.89	21.41	29.31	CaAl2Si2O8
Antlerite	-10.14	-1.86	8.28	Cu3 (OH) 4SO4

Aragonite	-3.65	-11.88	-8.23	CaCO ₃
Arsenolite	-41.85	-45.43	-3.58	As ₄ O ₆
Artinite	-14.70	-3.53	11.17	MgCO ₃ :Mg(OH) ₂ :3H ₂ O
As ₂ O ₅	-30.53	-23.53	7.00	As ₂ O ₅
Atacamite	-9.75	-1.39	8.36	Cu ₂ (OH) ₂ 3Cl
Azurite	-12.74	-28.36	-15.62	Cu ₃ (OH) ₂ (CO ₃) ₂
B ₂ UO ₂ (OH) ₂	-2.28	4.02	6.29	UO ₂ (OH) ₂
Ba ₃ (AsO ₄) ₂	-3.54	-12.60	-9.05	Ba ₃ (AsO ₄) ₂
Barite	0.27	-10.05	-10.32	BaSO ₄
Bianchite	-6.43	-8.20	-1.77	ZnSO ₄ :6H ₂ O
Birnessite	-15.09	2.99	18.09	MnO ₂
Bixbyite	-14.91	-14.69	0.22	Mn ₂ O ₃
BlaubleiI	-32.51	-56.67	-24.16	Cu _{0.9} Cu _{0.2} S
BlaubleiIII	-32.84	-60.12	-27.28	Cu _{0.6} Cu _{0.8} S
Boehmite	0.23	10.35	10.12	AlOOH
Brochantite	-13.24	2.09	15.33	Cu ₄ (OH) ₆ SO ₄
Brucite	-9.92	8.29	18.21	Mg(OH) ₂
Bunsenite	-7.65	6.11	13.76	NiO
Ca-Nontronite	12.15	-8.73	-20.89	Fe ₂ Al _{1.33} Si _{3.67} O ₁₀ (OH) ₂ Ca _{0.165}
Ca-Olivine	-27.97	12.68	40.65	Ca ₂ SiO ₄
Ca ₃ (AsO ₄) ₂ :6H ₂ O	-21.17	1.12	22.29	Ca ₃ (AsO ₄) ₂ :6H ₂ O
Ca ₃ SiO ₅	-58.80	20.90	79.70	Ca ₃ SiO ₅
Calcite	-3.49	-11.88	-8.40	CaCO ₃
Celestine	-1.43	-7.87	-6.44	SrSO ₄
CH ₄ (g)	-59.39	-102.83	-43.44	CH ₄
Chalcanthite	-7.02	-9.75	-2.73	CuSO ₄ :5H ₂ O
Chalcedony	0.02	-3.75	-3.77	SiO ₂
Chalcocite	-29.68	-67.00	-37.33	Cu ₂ S
Chalcopyrite	-74.41	-111.63	-37.22	CuFeS ₂
Chrysotile	-17.71	17.36	35.07	Mg ₃ Si ₂ O ₅ (OH) ₄
Claudetite	-41.64	-45.43	-3.79	As ₄ O ₆
Clinoenstatite	-7.90	4.54	12.44	MgSiO ₃
CO ₂ (g)	-1.91	-20.10	-18.19	CO ₂
Covellite	-31.17	-55.53	-24.36	CuS
Cristobalite	0.14	-3.75	-3.89	SiO ₂
Cu(OH) ₂	-5.53	3.95	9.47	Cu(OH) ₂
Cu ₂ (OH) ₂ 3NO ₃	-48.00	-37.81	10.19	Cu ₂ (OH) ₂ 3NO ₃
Cu ₂ SO ₄	-19.53	-21.23	-1.70	Cu ₂ SO ₄
Cu ₃ (AsO ₄) ₂ :6H ₂ O	-17.78	-11.69	6.09	Cu ₃ (AsO ₄) ₂ :6H ₂ O
CuBr	-6.63	-15.56	-8.93	CuBr
CuCO ₃	-6.52	-16.15	-9.63	CuCO ₃
CuMetal	-4.41	-14.11	-9.70	Cu
CuO:CuSO ₄	-19.29	-5.80	13.48	CuO:CuSO ₄
CupricFerrite	-3.80	4.20	8.00	CuFe ₂ O ₄
Cuprite	-5.64	-7.53	-1.89	Cu ₂ O
CuprousFerrite	5.08	-3.64	-8.71	CuFeO ₂
CuSO ₄	-13.76	-9.75	4.01	CuSO ₄
Diaspore	2.13	10.35	8.22	AlOOH
Diopside	-12.66	9.00	21.66	CaMgSi ₂ O ₆
Diopside	-6.80	0.20	6.99	CuSiO ₃ :H ₂ O
Djurleite	-29.70	-66.25	-36.55	Cu _{0.066} Cu _{1.868} S
Dolomite	-7.15	-23.69	-16.55	CaMg(CO ₃) ₂
Epsomite	-3.11	-5.41	-2.31	MgSO ₄ :7H ₂ O
Fe(OH) ₂ :7ClO ₃	0.39	-2.66	-3.04	Fe(OH) ₂ :7ClO ₃
Fe ₂ (SO ₄) ₃	-47.65	-40.83	6.82	Fe ₂ (SO ₄) ₃
Fe ₃ (OH) ₈	-16.59	3.62	20.21	Fe ₃ (OH) ₈
FeAsO ₄ :2H ₂ O	-12.03	-11.64	0.40	FeAsO ₄ :2H ₂ O
Ferrihydrite	-4.76	0.13	4.89	Fe(OH) ₃
FeS(ppt)	-52.19	-56.10	-3.92	FeS
Forsterite	-18.14	12.82	30.96	Mg ₂ SiO ₄
Gehlenite	-29.81	33.38	63.19	Ca ₂ Al ₂ SiO ₇
Gibbsite(C)	0.33	10.35	10.02	Al(OH) ₃
Goethite	-1.16	0.13	1.29	FeOOH
Goslarite	-6.05	-8.20	-2.15	ZnSO ₄ :7H ₂ O
Greenalite	-18.20	2.60	20.81	Fe ₃ Si ₂ O ₅ (OH) ₄
Greigite	-189.23	-234.26	-45.03	Fe ₃ S ₄
Gummite	-7.65	4.02	11.66	UO ₃
Gypsum	-0.85	-5.48	-4.63	CaSO ₄ :2H ₂ O
Halite	-8.29	-6.76	1.53	NaCl
Halloysite	2.03	13.20	11.17	Al ₂ Si ₂ O ₅ (OH) ₄
Hausmannite	-26.03	39.90	65.93	Mn ₃ O ₄
Hematite	2.58	0.26	-2.32	Fe ₂ O ₃
Hercynite	-7.39	24.06	31.46	FeAl ₂ O ₄
Huntite	-18.76	-47.32	-28.55	CaMg ₃ (CO ₃) ₄
Hydromagnesite	-33.05	-38.96	-5.91	Mg ₅ (CO ₃) ₄ (OH) ₂ :4H ₂ O
Jarosite-H	-17.92	-27.01	-9.08	(H ₃ O)Fe ₃ (SO ₄) ₂ (OH) ₆
Jarosite-K	-12.47	-25.56	-13.09	KFe ₃ (SO ₄) ₂ (OH) ₆
Jarosite-Na	-15.26	-24.48	-9.22	NaFe ₃ (SO ₄) ₂ (OH) ₆
K-Nontronite	5.93	-9.61	-15.55	Fe ₂ Al _{1.33} Si _{3.67} O ₁₀ (OH) ₂ K _{0.33}
Kalsilite	-6.38	8.04	14.43	KAlSiO ₄
Kaolinite	5.54	13.20	7.66	Al ₂ Si ₂ O ₅ (OH) ₄
Langite	-16.87	2.09	18.95	Cu ₄ (OH) ₆ SO ₄ :H ₂ O
Larnite	-29.60	12.68	42.28	Ca ₂ SiO ₄
Laumontite	-3.31	13.92	17.23	CaAl ₂ Si ₄ O ₁₂ :4H ₂ O
Leonhardtite	6.66	27.83	21.18	Ca ₂ Al ₄ Si ₈ O ₂₄ :7H ₂ O
Lepidocrocite	-1.24	0.13	1.37	FeOOH
Leucite	-3.34	4.29	7.64	KAlSi ₂ O ₆
Lime	-27.12	8.22	35.33	CaO
Mackinawite	-51.46	-56.10	-4.65	FeS
Magadiite	-9.43	-23.72	-14.29	NaSi ₇ O ₁₃ (OH) ₃ :3H ₂ O
Maghemite	-6.13	0.26	6.38	Fe ₂ O ₃
Magnesite	-4.12	-11.81	-7.69	MgCO ₃
Magnetite	-2.88	3.62	6.50	Fe ₃ O ₄
Malachite	-7.88	-12.21	-4.33	Cu ₂ (OH) ₂ CO ₃
Manganite	-7.11	-7.35	-0.24	MnOOH
Melanothallite	-19.03	-14.62	4.41	CuCl ₂
Melanterite	-7.69	-10.33	-2.64	FeSO ₄ :7H ₂ O
Merwinite	-48.99	25.43	74.42	Ca ₃ MgSi ₂ O ₈
Mg-Ferrite	-11.88	8.54	20.42	MgFe ₂ O ₄
Mg-Nontronite	11.86	-8.72	-20.59	Fe ₂ Al _{1.33} Si _{3.67} O ₁₀ (OH) ₂ Mg _{0.165}
Microcline	-0.75	0.54	1.30	KAlSi ₃ O ₈
Millerite	-45.18	-53.36	-8.18	NiS
Mirabilite	-6.47	-8.64	-2.17	Na ₂ SO ₄ :10H ₂ O

Mn2(SO4)3	-52.21	-55.78	-3.57	Mn2(SO4)3
Mn3(AsO4)2:8H2O	-16.80	-4.31	12.49	Mn3(AsO4)2:8H2O
MnCl2:4H2O	-13.91	-12.16	1.75	MnCl2:4H2O
MnS(Green)	-57.18	-53.07	4.12	MnS
MnSO4	-10.81	-7.29	3.52	MnSO4
Monticellite	-20.23	12.75	32.98	CaMgSiO4
Montmorillonite	4.78	7.46	2.67	Mg0.485Fe.22Al1.71Si3.81O10(OH)2
Morenosite	-5.05	-7.59	-2.53	NiSO4:7H2O
Muscovite	4.99	21.24	16.25	KAl3Si3O10(OH)2
Na-Nontronite	5.25	-9.25	-14.50	Fe2Al.33Si3.67O10(OH)2Na0.33
Nantokite	-5.74	-13.05	-7.31	CuCl
Natron	-12.85	-15.04	-2.19	Na2CO3:10H2O
Nepheline	-6.91	9.13	16.04	NaAlSiO4
Nesquehonite	-6.50	-11.81	-5.31	MgCO3:3H2O
Ni(OH)2	-3.02	6.11	9.13	Ni(OH)2
Ni2SiO4	-7.90	8.47	16.37	Ni2SiO4
Ni3(AsO4)2:8H2O	-20.89	-5.20	15.69	Ni3(AsO4)2:8H2O
Ni4(OH)6SO4	-21.25	10.74	31.99	Ni4(OH)6SO4
NiCO3	-7.69	-13.99	-6.29	NiCO3
Nsutite	-14.51	2.99	17.50	MnO2
O2(g)	-49.10	41.37	90.46	O2
Oripment	-135.62	-201.13	-65.51	As2S3
P-Wollstanite	-10.54	4.47	15.00	CaSiO3
Periclase	-15.21	8.29	23.49	MgO
Phlogopite	-45.64	25.40	71.04	KMg3AlSi3O10(OH)2
Portlandite	-16.14	8.22	24.36	Ca(OH)2
Pyrite	-75.79	-94.89	-19.10	FeS2
Pyrocroite	-9.92	6.41	16.32	Mn(OH)2
Pyrolusite	-14.46	2.99	17.46	MnO2
Pyrophyllite	7.29	5.70	-1.59	Al2Si4O10(OH)2
Quartz	0.60	-3.75	-4.34	SiO2
Realgar	-59.75	-81.17	-21.42	AsS
Retgersite	-5.48	-7.59	-2.11	NiSO4:6H2O
Rhodochrosite	-3.40	-13.69	-10.30	MnCO3
Rutherfordine	-1.62	-16.08	-14.46	UO2CO3
Sanidine(H)	-1.31	0.54	1.85	KAlSi3O8
Schoepite	-2.04	4.02	6.06	UO2(OH)2:2H2O
Sepiolite(a)	-13.46	5.32	18.78	Mg2Si3O7.5OH:3H2O
Sepiolite(c)	-12.09	5.32	17.41	Mg2Si3O7.5OH:3H2O
Siderite	-6.47	-16.73	-10.26	FeCO3
SiO2(a)	-0.49	-3.75	-3.26	SiO2
SiO2(am)	-0.83	-3.75	-2.92	SiO2
Smithsonite	-4.84	-14.60	-9.76	ZnCO3
Sphalerite	-41.91	-53.98	-12.07	ZnS
Spinel	-12.23	28.98	41.22	MgAl2O4
Strontianite	-5.06	-14.27	-9.21	SrCO3
Sulfur	-36.91	-38.79	-1.88	S
Talc	-15.12	9.86	24.98	Mg3Si4O10(OH)2
Tenorite	-4.51	3.95	8.45	CuO
Thenardite	-8.49	-8.64	-0.15	Na2SO4
Thermonatrite	-15.32	-15.04	0.28	Na2CO3:H2O
Tremolite	-33.99	27.87	61.86	Ca2Mg5Si8O22(OH)2
U3O8(C)	-2.78	24.68	27.46	U3O8
U4O9(C)	-3.72	-1.56	2.16	U4O9
UO2(am)	-7.93	-5.56	2.37	UO2
UO2(NO3)2	-100.85	-87.38	13.47	UO2(NO3)2
UO2(NO3)2:2H2O	-92.56	-87.38	5.18	UO2(NO3)2:2H2O
UO2(NO3)2:3H2O	-91.15	-87.38	3.77	UO2(NO3)2:3H2O
UO2(NO3)2:6H2O	-89.41	-87.38	2.03	UO2(NO3)2:6H2O
UO3(C)	-4.76	4.02	8.78	UO3
Uraninite	-1.88	-5.56	-3.68	UO2
Uranophane	-8.74	8.75	17.49	Ca(UO2)2(SiO3OH)2
USiO4(C)	-2.49	-9.31	-6.82	USiO4
Wairakite	-8.42	13.92	22.34	CaAl2Si4O12:2H2O
Willemite	-9.92	7.24	17.16	Zn2SiO4
Witherite	-7.85	-16.45	-8.60	BaCO3
Wollastonite	-9.60	4.47	14.07	CaSiO3
Wurtzite	-44.02	-53.98	-9.96	ZnS
Zincite	-6.84	5.50	12.34	ZnO
Zincosite	-12.26	-8.20	4.06	ZnSO4
Zn(BO2)2	-11.26	-2.97	8.29	Zn(BO2)2
Zn(NO3)2:6H2O	-89.03	-85.90	3.13	Zn(NO3)2:6H2O
Zn(OH)2(A)	-6.95	5.50	12.45	Zn(OH)2
Zn(OH)2(B)	-6.25	5.50	11.75	Zn(OH)2
Zn(OH)2(C)	-6.70	5.50	12.20	Zn(OH)2
Zn(OH)2(E)	-6.00	5.50	11.50	Zn(OH)2
Zn(OH)2(G)	-6.21	5.50	11.71	Zn(OH)2
Zn2(OH)2SO4	-10.20	-2.70	7.50	Zn2(OH)2SO4
Zn2(OH)3Cl	-13.49	1.71	15.20	Zn2(OH)3Cl
Zn3(AsO4)2:2.5H2O	-20.69	-7.04	13.65	Zn3(AsO4)2:2.5H2O
Zn3O(SO4)2	-33.32	-10.90	22.42	Zn3O(SO4)2
Zn4(OH)6SO4	-20.10	8.29	28.39	Zn4(OH)6SO4
Zn5(OH)8Cl2	-29.58	8.91	38.49	Zn5(OH)8Cl2
ZnBr2:2H2O	-23.71	-18.09	5.62	ZnBr2:2H2O
ZnCl2	-21.06	-13.07	7.99	ZnCl2
ZnCO3:H2O	-4.34	-14.60	-10.26	ZnCO3:H2O
ZnMetal	-42.96	-15.19	27.78	Zn
ZnO(Active)	-5.81	5.50	11.31	ZnO
ZnS(A)	-44.72	-53.98	-9.25	ZnS
ZnSiO3	-2.19	1.75	3.93	ZnSiO3
ZnSO4:H2O	-8.21	-8.20	0.01	ZnSO4:H2O

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

End of simulation.

1.8 DJX-pit, 80 m

Beginning of batch-reaction calculations.

Reaction step 1.

Using solution 1.

Using pressure 1.

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

Elements	Molality	Moles
Al	1.394e-05	1.394e+01
As	1.973e-08	1.973e-02
B	1.483e-04	1.483e+02
Ba	1.165e-07	1.165e-01
Br	3.680e-06	3.680e+00
C	2.766e-04	2.766e+02
Ca	7.229e-03	7.229e+03
Cl	8.566e-04	8.566e+02
Cu	3.305e-07	3.305e-01
Fe	8.953e-08	8.953e-02
K	2.682e-04	2.682e+02
Li	1.138e-05	1.138e+01
Mg	6.406e-03	6.406e+03
Mn	7.723e-05	7.723e+01
N	1.114e-04	1.114e+02
Na	5.589e-03	5.589e+03
Ni	3.561e-05	3.561e+01
S	1.479e-02	1.479e+04
Si	1.865e-04	1.865e+02
Sr	2.913e-05	2.913e+01
U	7.327e-06	7.327e+00
Zn	9.573e-06	9.573e+00

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

pH	=	5.609	Charge balance
pe	=	4.475	Adjusted to redox equilibrium
Activity of water	=	0.999	
Ionic strength (mol/kgw)	=	4.434e-02	
Mass of water (kg)	=	1.000e+06	
Total alkalinity (eq/kg)	=	8.919e-05	
Total CO2 (mol/kg)	=	2.766e-04	
Temperature (°C)	=	4.00	
Pressure (atm)	=	7.92	
Electrical balance (eq)	=	3.086e+03	
Percent error, 100*(Cat- An)/(Cat+ An)	=	6.46	
Iterations	=	3	
Total H	=	1.110146e+08	
Total O	=	5.556743e+07	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	2.850e-06	2.458e-06	-5.545	-5.609	-0.064	0.00
OH-	9.041e-10	7.455e-10	-9.044	-9.128	-0.084	(0)
H2O	5.551e+01	9.995e-01	1.744	-0.000	0.000	18.01
Al	1.394e-05					
Al(OH)2+	6.346e-06	5.329e-06	-5.197	-5.273	-0.076	(0)
Al(OH)3	2.715e-06	2.743e-06	-5.566	-5.562	0.004	(0)
AlSO4+	1.918e-06	1.597e-06	-5.717	-5.797	-0.079	(0)
Al+3	1.520e-06	4.013e-07	-5.818	-6.397	-0.578	(0)
AlOH+2	7.372e-07	3.666e-07	-6.132	-6.436	-0.303	(0)
Al(SO4)2-	6.980e-07	5.814e-07	-6.156	-6.236	-0.079	(0)
Al(OH)4-	4.811e-10	4.007e-10	-9.318	-9.397	-0.079	(0)
As(3)	4.403e-11					
H3AsO3	4.402e-11	4.448e-11	-10.356	-10.352	0.004	(0)
H2AsO3-	5.553e-15	4.626e-15	-14.256	-14.335	-0.079	(0)
H4AsO3+	6.500e-17	5.416e-17	-16.187	-16.266	-0.079	(0)
HAsO3-2	1.163e-21	5.603e-22	-20.935	-21.252	-0.317	(0)
AsO3-3	2.095e-29	4.053e-30	-28.679	-29.392	-0.713	(0)
As(5)	1.969e-08					
H2AsO4-	1.771e-08	1.476e-08	-7.752	-7.831	-0.079	(0)
HAsO4-2	1.971e-09	9.498e-10	-8.705	-9.022	-0.317	(0)
H3AsO4	5.061e-12	5.113e-12	-11.296	-11.291	0.004	(0)
AsO4-3	2.903e-15	5.617e-16	-14.537	-15.250	-0.713	(0)
B	1.483e-04					
H3BO3	1.482e-04	1.498e-04	-3.829	-3.825	0.004	(0)
H2BO3-	2.864e-08	2.335e-08	-7.543	-7.632	-0.089	(0)
Ba	1.165e-07					
Ba+2	1.165e-07	5.712e-08	-6.934	-7.243	-0.310	(0)
BaOH+	1.776e-16	1.486e-16	-15.751	-15.828	-0.077	(0)
Br	3.680e-06					
Br-	3.679e-06	3.050e-06	-5.434	-5.516	-0.082	(0)
NiBr+	1.430e-10	1.192e-10	-9.845	-9.924	-0.079	(0)
ZnBr+	3.021e-12	2.517e-12	-11.520	-11.599	-0.079	(0)
ZnBr2	3.025e-18	3.056e-18	-17.519	-17.515	0.004	(0)
C(4)	2.766e-04					
H2CO3	2.106e-04	2.127e-04	-3.677	-3.672	0.004	(0)
HCO3-	5.957e-05	5.002e-05	-4.225	-4.301	-0.076	(0)
UO2CO3	3.978e-06	4.019e-06	-5.400	-5.396	0.004	(0)
MgHCO3+	1.360e-06	1.127e-06	-5.866	-5.948	-0.082	(0)
CaHCO3+	8.412e-07	7.100e-07	-6.075	-6.149	-0.074	(0)
NaHCO3	7.361e-08	7.436e-08	-7.133	-7.129	0.004	(0)
NiHCO3+	5.925e-08	4.936e-08	-7.227	-7.307	-0.079	(0)
NiCO3	4.994e-08	5.045e-08	-7.302	-7.297	0.004	(0)
UO2(CO3)2-2	2.344e-08	1.130e-08	-7.630	-7.947	-0.317	(0)
MnHCO3+	1.872e-08	1.566e-08	-7.728	-7.805	-0.077	(0)
ZnHCO3+	1.281e-08	1.067e-08	-7.893	-7.972	-0.079	(0)
CuHCO3+	1.690e-09	1.408e-09	-8.772	-8.851	-0.079	(0)

CaCO3	1.482e-09	1.498e-09	-8.829	-8.825	0.004	(0)
CO3-2	1.107e-09	5.507e-10	-8.956	-9.259	-0.303	(0)
MgCO3	9.154e-10	9.248e-10	-9.038	-9.034	0.004	(0)
ZnCO3	3.414e-10	3.449e-10	-9.467	-9.462	0.004	(0)
CuCO3	3.045e-10	3.076e-10	-9.516	-9.512	0.004	(0)
NaCO3-	1.777e-11	1.492e-11	-10.750	-10.826	-0.076	(0)
UO2 (CO3) 3-4	1.358e-11	7.328e-13	-10.867	-12.135	-1.268	(0)
Ni (CO3) 2-2	1.002e-13	4.828e-14	-12.999	-13.316	-0.317	(0)
Zn (CO3) 2-2	8.426e-15	4.061e-15	-14.074	-14.391	-0.317	(0)
Cu (CO3) 2-2	4.425e-16	2.133e-16	-15.354	-15.671	-0.317	(0)
Ca	7.229e-03					
Ca+2	5.049e-03	2.606e-03	-2.297	-2.584	-0.287	(0)
CaSO4	2.179e-03	2.201e-03	-2.662	-2.657	0.004	(0)
CaHCO3+	8.412e-07	7.100e-07	-6.075	-6.149	-0.074	(0)
CaCO3	1.482e-09	1.498e-09	-8.829	-8.825	0.004	(0)
CaOH+	4.966e-11	4.191e-11	-10.304	-10.378	-0.074	(0)
Cl	8.566e-04					
Cl-	8.565e-04	7.034e-04	-3.067	-3.153	-0.086	(0)
MnCl+	9.884e-08	8.271e-08	-7.005	-7.082	-0.077	(0)
NiCl+	2.614e-08	2.178e-08	-7.583	-7.662	-0.079	(0)
ZnCl+	2.647e-09	2.194e-09	-8.577	-8.659	-0.082	(0)
UO2Cl+	7.055e-10	5.878e-10	-9.152	-9.231	-0.079	(0)
CuCl2-	2.947e-10	2.443e-10	-9.531	-9.612	-0.082	(0)
CuCl+	7.859e-11	6.514e-11	-10.105	-10.186	-0.082	(0)
NiCl2	5.519e-11	5.576e-11	-10.258	-10.254	0.004	(0)
ZnOHCl	2.959e-11	2.989e-11	-10.529	-10.524	0.004	(0)
MnCl2	1.564e-11	1.580e-11	-10.806	-10.801	0.004	(0)
ZnCl2	1.461e-12	1.476e-12	-11.835	-11.831	0.004	(0)
CuCl3-2	5.092e-13	2.497e-13	-12.293	-12.603	-0.310	(0)
CuCl2	1.908e-14	1.927e-14	-13.719	-13.715	0.004	(0)
MnCl3-	5.989e-15	5.011e-15	-14.223	-14.300	-0.077	(0)
ZnCl3-	1.227e-15	1.017e-15	-14.911	-14.993	-0.082	(0)
ZnCl4-2	6.101e-19	2.991e-19	-18.215	-18.524	-0.310	(0)
FeCl+2	5.733e-19	2.811e-19	-18.242	-18.551	-0.310	(0)
CuCl3-	3.889e-20	3.223e-20	-19.410	-19.492	-0.082	(0)
FeCl2+	2.160e-21	1.807e-21	-20.666	-20.743	-0.077	(0)
CuCl4-2	4.935e-25	2.420e-25	-24.307	-24.616	-0.310	(0)
FeCl3	1.258e-25	1.271e-25	-24.900	-24.896	0.004	(0)
UCl+3	7.128e-29	1.379e-29	-28.147	-28.860	-0.713	(0)
Cu (1)	2.110e-09					
Cu+	1.815e-09	1.480e-09	-8.741	-8.830	-0.089	(0)
CuCl2-	2.947e-10	2.443e-10	-9.531	-9.612	-0.082	(0)
CuCl3-2	5.092e-13	2.497e-13	-12.293	-12.603	-0.310	(0)
Cu (S4) 2-3	0.000e+00	0.000e+00	-97.050	-97.413	-0.363	(0)
CuS4S5-3	0.000e+00	0.000e+00	-97.798	-98.143	-0.345	(0)
Cu (2)	3.284e-07					
Cu+2	2.354e-07	1.040e-07	-6.628	-6.983	-0.355	(0)
CuSO4	8.999e-08	9.092e-08	-7.046	-7.041	0.004	(0)
CuHCO3+	1.690e-09	1.408e-09	-8.772	-8.851	-0.079	(0)
CuOH+	5.131e-10	4.252e-10	-9.290	-9.371	-0.082	(0)
Cu (OH) 2	3.596e-10	3.633e-10	-9.444	-9.440	0.004	(0)
CuCO3	3.045e-10	3.076e-10	-9.516	-9.512	0.004	(0)
CuCl+	7.859e-11	6.514e-11	-10.105	-10.186	-0.082	(0)
CuCl2	1.908e-14	1.927e-14	-13.719	-13.715	0.004	(0)
Cu2 (OH) 2+2	1.743e-14	8.399e-15	-13.759	-14.076	-0.317	(0)
Cu (CO3) 2-2	4.425e-16	2.133e-16	-15.354	-15.671	-0.317	(0)
Cu (OH) 3-	1.077e-17	8.971e-18	-16.968	-17.047	-0.079	(0)
CuCl3-	3.889e-20	3.223e-20	-19.410	-19.492	-0.082	(0)
Cu (OH) 4-2	1.515e-24	7.302e-25	-23.820	-24.137	-0.317	(0)
CuCl4-2	4.935e-25	2.420e-25	-24.307	-24.616	-0.310	(0)
Cu (HS) 3-	0.000e+00	0.000e+00	-135.793	-135.872	-0.079	(0)
Fe (2)	8.951e-08					
Fe+2	6.908e-08	3.506e-08	-7.161	-7.455	-0.295	(0)
FeSO4	2.043e-08	2.064e-08	-7.690	-7.685	0.004	(0)
FeOH+	1.002e-12	8.382e-13	-11.999	-12.077	-0.077	(0)
Fe (OH) 2	4.047e-19	4.088e-19	-18.393	-18.388	0.004	(0)
Fe (OH) 3-	5.945e-24	4.975e-24	-23.226	-23.303	-0.077	(0)
Fe (HS) 2	0.000e+00	0.000e+00	-101.702	-101.697	0.004	(0)
Fe (HS) 3-	0.000e+00	0.000e+00	-151.177	-151.256	-0.079	(0)
Fe (3)	1.161e-11					
Fe (OH) 2+	1.153e-11	9.680e-12	-10.938	-11.014	-0.076	(0)
Fe (OH) 3	4.603e-14	4.650e-14	-13.337	-13.333	0.004	(0)
FeOH+2	3.857e-14	1.891e-14	-13.414	-13.723	-0.310	(0)
FeSO4+	8.171e-16	6.837e-16	-15.088	-15.165	-0.077	(0)
Fe (OH) 4-	2.264e-16	1.901e-16	-15.645	-15.721	-0.076	(0)
Fe (SO4) 2-	1.189e-16	9.906e-17	-15.925	-16.004	-0.079	(0)
Fe+3	1.026e-16	2.708e-17	-15.989	-16.567	-0.578	(0)
FeCl+2	5.733e-19	2.811e-19	-18.242	-18.551	-0.310	(0)
FeCl2+	2.160e-21	1.807e-21	-20.666	-20.743	-0.077	(0)
Fe2 (OH) 2+4	4.538e-25	2.448e-26	-24.343	-25.611	-1.268	(0)
FeCl3	1.258e-25	1.271e-25	-24.900	-24.896	0.004	(0)
Fe3 (OH) 4+5	4.281e-33	4.469e-35	-32.368	-34.350	-1.981	(0)
H (0)	1.188e-23					
H2	5.941e-24	6.002e-24	-23.226	-23.222	0.004	(0)
K	2.682e-04					
K+	2.622e-04	2.153e-04	-3.581	-3.667	-0.086	(0)
KSO4-	6.078e-06	5.104e-06	-5.216	-5.292	-0.076	(0)
Li	1.138e-05					
Li+	1.114e-05	9.399e-06	-4.953	-5.027	-0.074	(0)
LiSO4-	2.454e-07	2.053e-07	-6.610	-6.688	-0.077	(0)
Mg	6.406e-03					
Mg+2	4.615e-03	2.430e-03	-2.336	-2.614	-0.279	(0)
MgSO4	1.790e-03	1.808e-03	-2.747	-2.743	0.004	(0)
MgHCO3+	1.360e-06	1.127e-06	-5.866	-5.948	-0.082	(0)
MgCO3	9.154e-10	9.248e-10	-9.038	-9.034	0.004	(0)
MgOH+	2.726e-10	2.310e-10	-9.565	-9.636	-0.072	(0)
Mn (2)	7.723e-05					
Mn+2	5.726e-05	2.906e-05	-4.242	-4.537	-0.295	(0)
MnSO4	1.985e-05	2.005e-05	-4.702	-4.698	0.004	(0)
MnCl+	9.884e-08	8.271e-08	-7.005	-7.082	-0.077	(0)
MnHCO3+	1.872e-08	1.566e-08	-7.728	-7.805	-0.077	(0)
MnOH+	5.789e-11	4.844e-11	-10.237	-10.315	-0.077	(0)
MnCl2	1.564e-11	1.580e-11	-10.806	-10.801	0.004	(0)

MnCl3-	5.989e-15	5.011e-15	-14.223	-14.300	-0.077	(0)
Mn(OH) 3-	3.763e-23	3.149e-23	-22.424	-22.502	-0.077	(0)
Mn(NO3) 2	0.000e+00	0.000e+00	-87.181	-87.177	0.004	(0)
Mn(3)	2.759e-24					
Mn+3	2.759e-24	7.282e-25	-23.559	-24.138	-0.578	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-68.214	-68.523	-0.310	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-74.823	-74.910	-0.086	(0)
N(-3)	1.114e-04					
NH4+	1.048e-04	8.547e-05	-3.979	-4.068	-0.089	(0)
NH4SO4-	6.585e-06	5.510e-06	-5.181	-5.259	-0.077	(0)
NH3	3.960e-09	4.000e-09	-8.402	-8.398	0.004	(0)
N(3)	1.892e-31					
NO2-	1.892e-31	1.577e-31	-30.723	-30.802	-0.079	(0)
N(5)	0.000e+00					
NO3-	0.000e+00	0.000e+00	-41.545	-41.631	-0.086	(0)
Mn(NO3) 2	0.000e+00	0.000e+00	-87.181	-87.177	0.004	(0)
Na	5.589e-03					
Na+	5.471e-03	4.569e-03	-2.262	-2.340	-0.078	(0)
NaSO4-	1.183e-04	9.931e-05	-3.927	-4.003	-0.076	(0)
NaHCO3	7.361e-08	7.436e-08	-7.133	-7.129	0.004	(0)
NaCO3-	1.777e-11	1.492e-11	-10.750	-10.826	-0.076	(0)
Ni	3.561e-05					
Ni+2	2.564e-05	1.236e-05	-4.591	-4.908	-0.317	(0)
NiSO4	9.827e-06	9.928e-06	-5.008	-5.003	0.004	(0)
NiHCO3+	5.925e-08	4.936e-08	-7.227	-7.307	-0.079	(0)
NiCO3	4.994e-08	5.045e-08	-7.302	-7.297	0.004	(0)
NiCl+	2.614e-08	2.178e-08	-7.583	-7.662	-0.079	(0)
Ni(SO4) 2-2	6.724e-09	3.241e-09	-8.172	-8.489	-0.317	(0)
NiOH+	1.710e-10	1.425e-10	-9.767	-9.846	-0.079	(0)
NiBr+	1.430e-10	1.192e-10	-9.845	-9.924	-0.079	(0)
NiCl2	5.519e-11	5.576e-11	-10.258	-10.254	0.004	(0)
Ni(OH) 2	2.045e-13	2.066e-13	-12.689	-12.685	0.004	(0)
Ni(CO3) 2-2	1.002e-13	4.828e-14	-12.999	-13.316	-0.317	(0)
Ni(OH) 3-	1.014e-18	8.447e-19	-17.994	-18.073	-0.079	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-53.227	-53.223	0.004	(0)
S(-2)	0.000e+00					
H2S	0.000e+00	0.000e+00	-49.936	-49.932	0.004	(0)
HS-	0.000e+00	0.000e+00	-51.512	-51.596	-0.084	(0)
S6-2	0.000e+00	0.000e+00	-55.551	-55.868	-0.317	(0)
S5-2	0.000e+00	0.000e+00	-55.781	-56.098	-0.317	(0)
S4-2	0.000e+00	0.000e+00	-56.037	-56.354	-0.317	(0)
S-2	0.000e+00	0.000e+00	-59.267	-59.577	-0.310	(0)
S3-2	0.000e+00	0.000e+00	-59.529	-59.846	-0.317	(0)
S2-2	0.000e+00	0.000e+00	-60.831	-61.148	-0.317	(0)
Zn(HS) 2	0.000e+00	0.000e+00	-93.760	-93.755	0.004	(0)
Cu(S4) 2-3	0.000e+00	0.000e+00	-97.050	-97.413	-0.363	(0)
CuS4S5-3	0.000e+00	0.000e+00	-97.798	-98.143	-0.345	(0)
Fe(HS) 2	0.000e+00	0.000e+00	-101.702	-101.697	0.004	(0)
Cu(HS) 3-	0.000e+00	0.000e+00	-135.793	-135.872	-0.079	(0)
Zn(HS) 3-	0.000e+00	0.000e+00	-144.112	-144.192	-0.079	(0)
Fe(HS) 3-	0.000e+00	0.000e+00	-151.177	-151.256	-0.079	(0)
S(6)	1.479e-02					
SO4-2	1.065e-02	5.004e-03	-1.973	-2.301	-0.328	(0)
CaSO4	2.179e-03	2.201e-03	-2.662	-2.657	0.004	(0)
MgSO4	1.790e-03	1.808e-03	-2.747	-2.743	0.004	(0)
NaSO4-	1.183e-04	9.931e-05	-3.927	-4.003	-0.076	(0)
MnSO4	1.985e-05	2.005e-05	-4.702	-4.698	0.004	(0)
NiSO4	9.827e-06	9.928e-06	-5.008	-5.003	0.004	(0)
NH4SO4-	6.585e-06	5.510e-06	-5.181	-5.259	-0.077	(0)
KSO4-	6.078e-06	5.104e-06	-5.216	-5.292	-0.076	(0)
ZnSO4	3.063e-06	3.094e-06	-5.514	-5.509	0.004	(0)
AlSO4+	1.918e-06	1.597e-06	-5.717	-5.797	-0.079	(0)
HSO4-	8.179e-07	6.812e-07	-6.087	-6.167	-0.079	(0)
UO2SO4	7.783e-07	7.863e-07	-6.109	-6.104	0.004	(0)
Al(SO4) 2-	6.980e-07	5.814e-07	-6.156	-6.236	-0.079	(0)
Zn(SO4) 2-2	3.108e-07	1.498e-07	-6.508	-6.825	-0.317	(0)
LiSO4-	2.454e-07	2.053e-07	-6.610	-6.688	-0.077	(0)
UO2(SO4) 2-2	2.140e-07	1.031e-07	-6.670	-6.987	-0.317	(0)
CuSO4	8.999e-08	9.092e-08	-7.046	-7.041	0.004	(0)
FeSO4	2.043e-08	2.064e-08	-7.690	-7.685	0.004	(0)
Ni(SO4) 2-2	6.724e-09	3.241e-09	-8.172	-8.489	-0.317	(0)
FeSO4+	8.171e-16	6.837e-16	-15.088	-15.165	-0.077	(0)
Fe(SO4) 2-	1.189e-16	9.906e-17	-15.925	-16.004	-0.079	(0)
U(SO4) 2	1.688e-22	1.705e-22	-21.773	-21.768	0.004	(0)
USO4+2	5.998e-24	2.891e-24	-23.222	-23.539	-0.317	(0)
Si	1.865e-04					
H4SiO4	1.863e-04	1.882e-04	-3.730	-3.725	0.004	(0)
UO2H3SiO4+	2.157e-07	1.797e-07	-6.666	-6.745	-0.079	(0)
H3SiO4-	3.269e-09	2.709e-09	-8.486	-8.567	-0.082	(0)
H2SiO4-2	2.656e-16	1.321e-16	-15.576	-15.879	-0.303	(0)
Sr	2.913e-05					
Sr+2	2.913e-05	1.428e-05	-4.536	-4.845	-0.310	(0)
SrOH+	7.257e-14	6.073e-14	-13.139	-13.217	-0.077	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-40.407	-41.120	-0.713	(0)
U(4)	1.102e-13					
U(OH) 5-	9.815e-14	8.178e-14	-13.008	-13.087	-0.079	(0)
U(OH) 4	1.188e-14	1.201e-14	-13.925	-13.921	0.004	(0)
U(OH) 3+	1.688e-16	1.407e-16	-15.773	-15.852	-0.079	(0)
U(OH) 2+2	6.189e-19	2.983e-19	-18.208	-18.525	-0.317	(0)
UOH+3	3.714e-22	7.186e-23	-21.430	-22.144	-0.713	(0)
U(SO4) 2	1.688e-22	1.705e-22	-21.773	-21.768	0.004	(0)
USO4+2	5.998e-24	2.891e-24	-23.222	-23.539	-0.317	(0)
U+4	5.946e-26	3.207e-27	-25.226	-26.494	-1.268	(0)
UC1+3	7.128e-29	1.379e-29	-28.147	-28.860	-0.713	(0)
U6(OH) 15+9	0.000e+00	0.000e+00	-85.599	-92.018	-6.420	(0)
U(5)	2.202e-08					
UO2+	2.202e-08	1.835e-08	-7.657	-7.736	-0.079	(0)
U(6)	7.305e-06					
UO2CO3	3.978e-06	4.019e-06	-5.400	-5.396	0.004	(0)

UO2+2	1.223e-06	5.895e-07	-5.912	-6.230	-0.317	(0)
UO2SO4	7.783e-07	7.863e-07	-6.109	-6.104	0.004	(0)
UO2OH+	6.367e-07	5.305e-07	-6.196	-6.275	-0.079	(0)
UO2H3SiO4+	2.157e-07	1.797e-07	-6.666	-6.745	-0.079	(0)
UO2(SO4)2-2	2.140e-07	1.031e-07	-6.670	-6.987	-0.317	(0)
(UO2)2(OH)2+2	7.380e-08	3.557e-08	-7.132	-7.449	-0.317	(0)
(UO2)3(OH)5+	2.905e-08	2.420e-08	-7.537	-7.616	-0.079	(0)
UO2(CO3)2-2	2.344e-08	1.130e-08	-7.630	-7.947	-0.317	(0)
UO2Cl+	7.055e-10	5.878e-10	-9.152	-9.231	-0.079	(0)
UO2(CO3)3-4	1.358e-11	7.328e-13	-10.867	-12.135	-1.268	(0)
Zn	9.573e-06					
Zn+2	6.184e-06	3.138e-06	-5.209	-5.503	-0.295	(0)
ZnSO4	3.063e-06	3.094e-06	-5.514	-5.509	0.004	(0)
Zn(SO4)2-2	3.108e-07	1.498e-07	-6.508	-6.825	-0.317	(0)
ZnHCO3+	1.281e-08	1.067e-08	-7.893	-7.972	-0.079	(0)
ZnCl+	2.647e-09	2.194e-09	-8.577	-8.659	-0.082	(0)
ZnCO3	3.414e-10	3.449e-10	-9.467	-9.462	0.004	(0)
ZnOH+	3.044e-10	2.536e-10	-9.517	-9.596	-0.079	(0)
ZnOHCl	2.959e-11	2.989e-11	-10.529	-10.524	0.004	(0)
Zn(OH)2	6.554e-12	6.621e-12	-11.184	-11.179	0.004	(0)
ZnBr+	3.021e-12	2.517e-12	-11.520	-11.599	-0.079	(0)
ZnCl2	1.461e-12	1.476e-12	-11.835	-11.831	0.004	(0)
Zn(CO3)2-2	8.426e-15	4.061e-15	-14.074	-14.391	-0.317	(0)
ZnCl3-	1.227e-15	1.017e-15	-14.911	-14.993	-0.082	(0)
Zn(OH)3-	1.027e-17	8.561e-18	-16.988	-17.067	-0.079	(0)
ZnBr2	3.025e-18	3.056e-18	-17.519	-17.515	0.004	(0)
ZnCl4-2	6.101e-19	2.991e-19	-18.215	-18.524	-0.310	(0)
Zn(OH)4-2	1.151e-24	5.548e-25	-23.939	-24.256	-0.317	(0)
Zn(HS)2	0.000e+00	0.000e+00	-93.760	-93.755	0.004	(0)
Zn(HS)3-	0.000e+00	0.000e+00	-144.112	-144.192	-0.079	(0)

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

Phase	SI**	log IAP	log K(277 K, 8 atm)	
Akerminite	-33.30	18.42	51.72	Ca2MgSi2O7
Al(OH)3(a)	-1.44	10.43	11.87	Al(OH)3
Al2O3	-2.11	20.86	22.97	Al2O3
Al4(OH)10SO4	5.53	28.21	22.68	Al4(OH)10SO4
AlAsO4:2H2O	-5.66	-0.86	4.80	AlAsO4:2H2O
Albite	-2.10	2.53	4.63	NaAlSi3O8
Albite(low)	-1.04	2.53	3.57	NaAlSi3O8
AlOHSO4	0.14	-3.09	-3.23	AlOHSO4
AlumK	-9.07	-14.67	-5.60	KAl(SO4)2:12H2O
Alunite	7.78	6.20	-1.58	KAl3(SO4)2(OH)6
Analcime	-1.74	6.25	7.99	NaAlSi2O6:H2O
Anhydrite	-0.46	-4.88	-4.43	CaSO4
Anilite	-26.68	-60.98	-34.30	Cu0.25Cu1.5S
Annite	-14.45	12.49	26.94	KFe3AlSi3O10(OH)2
Anorthite	-7.31	22.05	29.35	CaAl2Si2O8
Antlerite	-9.09	-0.81	8.28	Cu3(OH)4SO4
Aragonite	-3.61	-11.84	-8.23	CaCO3
Arsenolite	-37.82	-41.41	-3.58	As4O6
Artinite	-14.45	-3.27	11.18	MgCO3:Mg(OH)2:3H2O
As2O5	-29.59	-22.58	7.01	As2O5
Atacamite	-8.66	-0.29	8.37	Cu2(OH)3Cl
Azurite	-12.64	-28.25	-15.60	Cu3(OH)2(CO3)2
B_UO2(OH)2	-1.31	4.99	6.30	UO2(OH)2
Ba3(AsO4)2	-1.60	-10.66	-9.06	Ba3(AsO4)2
Barite	0.78	-9.54	-10.32	BaSO4
Bianchite	-6.03	-7.81	-1.77	ZnSO4:6H2O
Birnessite	-15.31	2.77	18.09	MnO2
Bixbyite	-14.85	-14.62	0.23	Mn2O3
BlaubleiI	-29.88	-54.04	-24.16	Cu0.9Cu0.2S
BlaubleiII	-29.96	-57.24	-27.28	Cu0.6Cu0.8S
Boehmite	0.30	10.43	10.14	AlOOH
Brochantite	-11.90	3.42	15.33	Cu4(OH)6SO4
Brucite	-9.62	8.60	18.22	Mg(OH)2
Bunsenite	-7.47	6.31	13.78	NiO
Ca-Nontronite	12.60	-8.28	-20.88	Fe2Al1.33Si3.67O10(OH)2Ca0.165
Ca-Olivine	-27.14	13.54	40.69	Ca2SiO4
Ca3(AsO4)2:6H2O	-18.97	3.32	22.29	Ca3(AsO4)2:6H2O
Ca3SiO5	-57.59	22.18	79.77	Ca3SiO5
Calcite	-3.45	-11.84	-8.40	CaCO3
Celestine	-0.71	-7.15	-6.44	SrSO4
CH4(g)	-57.67	-101.15	-43.48	CH4
Chalcanthite	-6.55	-9.28	-2.73	CuSO4:5H2O
Chalcedony	0.05	-3.72	-3.77	SiO2
Chalcocite	-26.29	-63.65	-37.36	Cu2S
Chalcocopyrite	-69.17	-106.41	-37.24	CuFeS2
Chrysotile	-16.74	18.36	35.10	Mg3Si2O5(OH)4
Claudetite	-37.62	-41.41	-3.79	As4O6
Clinoenstatite	-7.57	4.88	12.45	MgSiO3
CO2(g)	-2.29	-20.48	-18.19	CO2
Covellite	-28.60	-52.97	-24.37	CuS
Cristobalite	0.16	-3.72	-3.89	SiO2
Cu(OH)2	-5.25	4.24	9.48	Cu(OH)2
Cu2(OH)3NO3	-48.97	-38.77	10.20	Cu2(OH)3NO3
Cu2SO4	-18.26	-19.96	-1.70	Cu2SO4
Cu3(AsO4)2:6H2O	-15.96	-9.88	6.09	Cu3(AsO4)2:6H2O
CuBr	-5.41	-14.35	-8.94	CuBr
CuCO3	-6.61	-16.24	-9.63	CuCO3
CuMetal	-3.59	-13.31	-9.71	Cu
CuOCuSO4	-18.55	-5.05	13.50	CuO:CuSO4
CupricFerrite	-3.26	4.76	8.02	CuFe2O4
Cuprite	-4.54	-6.44	-1.90	Cu2O
CuprousFerrite	5.75	-2.96	-8.71	CuFeO2
CuSO4	-13.30	-9.28	4.02	CuSO4
Diaspore	2.20	10.43	8.24	AlOOH
Diopside	-11.89	9.79	21.68	CaMgSi2O6
Diopside	-6.49	0.51	7.00	CuSiO3:H2O
Djurleite	-26.36	-62.94	-36.58	Cu0.066Cu1.868S
Dolomite	-7.18	-23.72	-16.54	CaMg(CO3)2

Epsomite	-2.60	-4.92	-2.31	MgSO ₄ :7H ₂ O
Fe(OH)2.7Cl _{0.3}	0.68	-2.37	-3.05	Fe(OH)2.7Cl _{0.3}
Fe ₂ (SO ₄) ₃	-46.90	-40.04	6.86	Fe ₂ (SO ₄) ₃
Fe ₃ (OH) ₈	-15.92	4.28	20.20	Fe ₃ (OH) ₈
FeAsO ₄ :2H ₂ O	-11.43	-11.03	0.40	FeAsO ₄ :2H ₂ O
Ferrihydrite	-4.62	0.26	4.88	Fe(OH) ₃
FeS (ppt)	-49.53	-53.44	-3.92	FeS
Forsterite	-17.51	13.48	30.99	Mg ₂ SiO ₄
Gehlenite	-28.86	34.41	63.26	Ca ₂ Al ₂ SiO ₇
Gibbsite (C)	0.40	10.43	10.03	Al(OH) ₃
Goethite	-1.04	0.26	1.30	FeOOH
Goslarite	-5.65	-7.81	-2.16	ZnSO ₄ :7H ₂ O
Greenalite	-16.97	3.84	20.81	Fe ₃ Si ₂ O ₅ (OH) ₄
Greigite	-179.50	-224.54	-45.03	Fe ₃ S ₄
Gummitz	-6.69	4.99	11.68	UO ₃
Gypsum	-0.26	-4.89	-4.63	CaSO ₄ :2H ₂ O
Halite	-7.02	-5.49	1.53	NaCl
Halloysite	2.21	13.41	11.20	Al ₂ Si ₂ O ₅ (OH) ₄
Hausmannite	-25.77	40.22	65.98	Mn ₃ O ₄
Hematite	2.82	0.52	-2.30	Fe ₂ O ₃
Hercynite	-6.88	24.63	31.50	FeAl ₂ O ₄
Huntite	-18.93	-47.46	-28.54	CaMg ₃ (CO ₃) ₄
Hydromagnesite	-33.01	-38.89	-5.88	Mg ₅ (CO ₃) ₄ (OH) ₂ :4H ₂ O
Jarosite-H	-17.20	-26.26	-9.05	(H ₃ O)Fe ₃ (SO ₄) ₂ (OH) ₆
Jarosite-K	-11.24	-24.31	-13.08	KFe ₃ (SO ₄) ₂ (OH) ₆
Jarosite-Na	-13.78	-22.99	-9.20	NaFe ₃ (SO ₄) ₂ (OH) ₆
K-Nontronite	6.48	-9.07	-15.54	Fe ₂ Al _{1.33} Si _{3.67} O ₁₀ (OH) ₂ K _{0.33}
Kalsilite	-5.80	8.65	14.44	KAlSiO ₄
Kaolinite	5.73	13.41	7.68	Al ₂ Si ₂ O ₅ (OH) ₄
Langite	-15.55	3.42	18.97	Cu ₄ (OH) ₆ SO ₄ :H ₂ O
Larnite	-28.78	13.54	42.32	Ca ₂ SiO ₄
Laumontite	-2.66	14.60	17.26	CaAl ₂ Si ₄ O ₁₂ :4H ₂ O
Leonhardite	7.96	29.20	21.23	Ca ₂ Al ₄ Si ₈ O ₂₄ :7H ₂ O
Lepidocrocite	-1.11	0.26	1.37	FeOOH
Leucite	-2.73	4.92	7.65	KAlSi ₂ O ₆
Lime	-26.73	8.63	35.36	CaO
Mackinawite	-48.79	-53.44	-4.65	FeS
Magadiite	-8.53	-22.81	-14.28	NaSi ₇ O ₁₃ (OH) ₃ :3H ₂ O
Maghemite	-5.86	0.52	6.38	Fe ₂ O ₃
Magnesite	-4.19	-11.87	-7.69	MgCO ₃
Magnetite	-2.25	4.28	6.53	Fe ₃ O ₄
Malachite	-7.69	-12.01	-4.32	Cu ₂ (OH) ₂ CO ₃
Manganite	-7.07	-7.31	-0.24	MnOOH
Melanophthalite	-17.70	-13.29	4.41	CuCl ₂
Melanterite	-7.11	-9.76	-2.65	FeSO ₄ :7H ₂ O
Merwinite	-47.43	27.06	74.49	Ca ₃ MgSi ₂ O ₈
Mg-Ferrite	-11.33	9.13	20.46	MgFe ₂ O ₄
Mg-Nontronite	12.30	-8.29	-20.58	Fe ₂ Al _{1.33} Si _{3.67} O ₁₀ (OH) ₂ Mg _{0.165}
Microcline	-0.11	1.20	1.31	KAlSi ₃ O ₈
Millerite	-42.71	-50.89	-8.18	NiS
Mirabilite	-4.79	-6.98	-2.19	Na ₂ SO ₄ :10H ₂ O
Mn ₂ (SO ₄) ₃	-51.64	-55.18	-3.54	Mn ₂ (SO ₄) ₃
Mn ₃ (AsO ₄) ₂ :8H ₂ O	-15.02	-2.54	12.48	Mn ₃ (AsO ₄) ₂ :8H ₂ O
MnCl ₂ :4H ₂ O	-12.58	-10.84	1.74	MnCl ₂ :4H ₂ O
MnS (Green)	-54.64	-50.52	4.12	MnS
MnSO ₄	-10.37	-6.84	3.53	MnSO ₄
Monticellite	-19.50	13.51	33.02	CaMgSiO ₄
Montmorillonite	5.20	7.88	2.68	Mg _{0.485} Fe _{0.22} Al _{1.71} Si _{3.81} O ₁₀ (OH) ₂
Morenosite	-4.67	-7.21	-2.54	NiSO ₄ :7H ₂ O
Muscovite	5.78	22.06	16.29	KAl ₃ Si ₃ O ₁₀ (OH) ₂
Na-Nontronite	5.87	-8.63	-14.50	Fe ₂ Al _{1.33} Si _{3.67} O ₁₀ (OH) ₂ Na _{0.33}
Nantokite	-4.67	-11.98	-7.31	CuCl
Natron	-11.73	-13.94	-2.21	Na ₂ CO ₃ :10H ₂ O
Nepheline	-6.09	9.98	16.06	NaAlSiO ₄
Nesquehonite	-6.57	-11.87	-5.31	MgCO ₃ :3H ₂ O
Ni(OH) ₂	-2.79	6.31	9.10	Ni(OH) ₂
Ni ₂ SiO ₄	-7.50	8.90	16.39	Ni ₂ SiO ₄
Ni ₃ (AsO ₄) ₂ :8H ₂ O	-19.33	-3.65	15.68	Ni ₃ (AsO ₄) ₂ :8H ₂ O
Ni ₄ (OH) ₆ SO ₄	-20.26	11.72	31.99	Ni ₄ (OH) ₆ SO ₄
NiCO ₃	-7.88	-14.17	-6.29	NiCO ₃
Nsutite	-14.72	2.77	17.50	MnO ₂
O ₂ (g)	-50.21	40.34	90.55	O ₂
Oripment	-126.76	-192.32	-65.56	As ₂ S ₃
P-Wollstanite	-10.11	4.91	15.02	CaSiO ₃
Periclase	-14.91	8.60	23.51	MgO
Phlogopite	-44.08	27.01	71.10	KMg ₃ AlSi ₃ O ₁₀ (OH) ₂
Portlandite	-15.74	8.63	24.37	Ca(OH) ₂
Pyrite	-71.37	-90.48	-19.11	FeS ₂
Pyrochroite	-9.66	6.68	16.34	Mn(OH) ₂
Pyrolusite	-14.70	2.77	17.48	MnO ₂
Pyrophyllite	7.55	5.96	-1.59	Al ₂ Si ₄ O ₁₀ (OH) ₂
Quartz	0.62	-3.72	-4.35	SiO ₂
Realgar	-56.21	-77.64	-21.44	As ₂ S ₃
Retgersite	-5.09	-7.21	-2.12	NiSO ₄ :6H ₂ O
Rhodochromite	-3.50	-13.80	-10.29	MnCO ₃
Rutherfordine	-1.03	-15.49	-14.46	UO ₂ CO ₃
Sanidine (H)	-0.66	1.20	1.86	KAlSi ₃ O ₈
Schoepite	-1.08	4.99	6.07	UO ₂ (OH) ₂ :H ₂ O
Sepiolite (a)	-12.75	6.03	18.78	Mg ₂ Si ₃ O ₇ :5OH:3H ₂ O
Sepiolite (c)	-11.40	6.03	17.43	Mg ₂ Si ₃ O ₇ :5OH:3H ₂ O
Siderite	-6.46	-16.71	-10.25	FeCO ₃
SiO ₂ (a)	-0.46	-3.72	-3.26	SiO ₂
SiO ₂ (am)	-0.80	-3.72	-2.92	SiO ₂
Smithsonite	-5.00	-14.76	-9.76	ZnCO ₃
Sphalerite	-39.41	-51.49	-12.08	ZnS
Spinel	-11.80	29.47	41.27	MgAl ₂ O ₄
Strontianite	-4.89	-14.10	-9.21	SrCO ₃
Sulfur	-35.16	-37.04	-1.88	S
Talc	-14.10	10.91	25.01	Mg ₃ Si ₄ O ₁₀ (OH) ₂
Tenorite	-4.23	4.24	8.46	CuO
Thenardite	-6.83	-6.98	-0.15	Na ₂ SO ₄
Thermonatrite	-14.22	-13.94	0.28	Na ₂ CO ₃ :H ₂ O
Tremolite	-31.44	30.49	61.93	Ca ₂ Mg ₅ Si ₈ O ₂₂ (OH) ₂

U3O8(C)	0.64	28.17	27.53	U3O8
U4O9(C)	1.73	3.94	2.22	U4O9
UO2(am)	-6.44	-4.06	2.39	UO2
UO2(NO3)2	-102.98	-89.49	13.49	UO2(NO3)2
UO2(NO3)2:2H2O	-94.68	-89.49	5.18	UO2(NO3)2:2H2O
UO2(NO3)2:3H2O	-93.26	-89.49	3.77	UO2(NO3)2:3H2O
UO2(NO3)2:6H2O	-91.51	-89.49	2.02	UO2(NO3)2:6H2O
UO3(C)	-3.80	4.99	8.79	UO3
Uraninite	-0.39	-4.06	-3.67	UO2
Uranophane	-6.33	11.16	17.49	Ca(UO2)2(SiO3OH)2
USiO4(C)	-0.97	-7.78	-6.81	USiO4
Wairakite	-7.78	14.60	22.38	CaAl2Si4O12:2H2O
Willemite	-9.48	7.71	17.18	Zn2SiO4
Witherite	-7.90	-16.50	-8.60	BaCO3
Wollastonite	-9.17	4.91	14.08	CaSiO3
Wurtzite	-41.53	-51.49	-9.96	ZnS
Zincite	-6.64	5.72	12.35	ZnO
Zincosite	-11.88	-7.80	4.08	ZnSO4
Zn(BO2)2	-10.23	-1.93	8.29	Zn(BO2)2
Zn(NO3)2:6H2O	-91.89	-88.77	3.12	Zn(NO3)2:6H2O
Zn(OH)2(A)	-6.73	5.72	12.45	Zn(OH)2
Zn(OH)2(B)	-6.03	5.72	11.75	Zn(OH)2
Zn(OH)2(C)	-6.48	5.72	12.20	Zn(OH)2
Zn(OH)2(E)	-5.78	5.72	11.50	Zn(OH)2
Zn(OH)2(G)	-5.99	5.72	11.71	Zn(OH)2
Zn2(OH)2SO4	-9.58	-2.09	7.50	Zn2(OH)2SO4
Zn2(OH)3Cl	-12.52	2.67	15.19	Zn2(OH)3Cl
Zn3(AsO4)2:2.5H2O	-19.08	-5.44	13.64	Zn3(AsO4)2:2.5H2O
Zn3O(SO4)2	-32.35	-9.89	22.46	Zn3O(SO4)2
Zn4(OH)6SO4	-19.04	9.34	28.39	Zn4(OH)6SO4
Zn5(OH)8Cl2	-27.43	11.05	38.48	Zn5(OH)8Cl2
ZnBr2:2H2O	-22.16	-16.54	5.62	ZnBr2:2H2O
ZnCl2	-19.81	-11.81	8.00	ZnCl2
ZnCO3:H2O	-4.50	-14.76	-10.26	ZnCO3:H2O
ZnMetal	-42.25	-14.45	27.80	Zn
ZnO(Active)	-5.59	5.72	11.31	ZnO
ZnS(A)	-42.23	-51.49	-9.26	ZnS
ZnSiO3	-1.96	1.99	3.95	ZnSiO3
ZnSO4:H2O	-7.82	-7.80	0.02	ZnSO4:H2O

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

End of simulation.