

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

LLNL\_AQUEOUS\_MODEL\_PARAMETERS  
NAMED\_EXPRESSIONS  
SOLUTION\_MASTER\_SPECIES  
SOLUTION\_SPECIES  
PHASES  
EXCHANGE\_MASTER\_SPECIES  
EXCHANGE\_SPECIES  
SURFACE\_MASTER\_SPECIES  
SURFACE\_SPECIES  
RATES  
END

-----  
Reading input data for simulation 1.  
-----

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\llnl.dat  
SOLUTION 1 Flujo 2  
temp 25  
pH 2.80  
pe 17  
redox pe  
units mg/l  
density 1  
Cl 45.3  
S(6) 947.3  
Al 8.4  
As 0.3  
Ca 34.9  
Cu 0.1  
Fe 43.4  
K 15.8  
Mg 11.5  
Mn 6.0  
Na 14.2  
Zn 1.5  
C(4) 0  
water 1 # kg  
SOLUTION 2 AS1  
temp 25  
units mg/l  
pe 10  
pH 7.54  
Cl 24.2  
F 0.25  
N(5) 2.9  
S(6) 243  
Al 0  
As 0.0966  
Ca 86.82  
Cu 0.113  
Fe 0  
Hg 0  
K 3.07  
Mg 16.17  
Mn 0.181  
Na 43.01  
Ni 0

```

Pb      0
Zn      0.195
MIX 4
      1      1
      2      3
SELECTED_OUTPUT
file          DAM_AGUASUP
ph            true
percent_error true
totals        Al As Cu Fe Mg Mn Zn
              S(6)

```

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

Initial solution 1.      Flujo 2

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

Elements	Molality	Moles
Al	3.117e-004	3.117e-004
As	4.009e-006	4.009e-006
Ca	8.718e-004	8.718e-004
Cl	1.279e-003	1.279e-003
Cu	1.575e-006	1.575e-006
Fe	7.780e-004	7.780e-004
K	4.046e-004	4.046e-004
Mg	4.737e-004	4.737e-004
Mn	1.093e-004	1.093e-004
Na	6.184e-004	6.184e-004
S(6)	9.875e-003	9.875e-003
Zn	2.297e-005	2.297e-005

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

```

pH = 2.800
pe = 17.000
Activity of water = 1.000
Ionic strength = 2.333e-002
Mass of water (kg) = 1.000e+000
Total alkalinity (eq/kg) = -3.569e-003
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = -1.177e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -46.23
Iterations = 10
Total H = 1.110539e+002
Total O = 5.556546e+001

```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	1.790e-003	1.585e-003	-2.747	-2.800	-0.053
OH-	7.066e-012	6.077e-012	-11.151	-11.216	-0.065
H2O	5.553e+001	9.997e-001	1.744	-0.000	0.000
Al	3.117e-004				
AlSO4+	1.622e-004	1.400e-004	-3.790	-3.854	-0.064
Al+3	9.218e-005	3.030e-005	-4.035	-4.519	-0.483
Al(SO4)2-	5.687e-005	4.907e-005	-4.245	-4.309	-0.064
AlOH+2	3.842e-007	2.141e-007	-6.415	-6.669	-0.254
Al(OH)2+	3.635e-010	3.136e-010	-9.440	-9.504	-0.064
Al2(OH)2+4	7.091e-011	7.454e-012	-10.149	-11.128	-0.978
HALO2	2.880e-013	2.880e-013	-12.541	-12.541	0.000

Al3(OH)4+5	1.833e-015	5.800e-017	-14.737	-16.237	-1.500
AlO2-	7.214e-017	6.224e-017	-16.142	-16.206	-0.064
NaAlO2	6.150e-021	6.150e-021	-20.211	-20.211	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-64.935	-67.875	-2.940
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-149.965	-149.965	0.000
As(3)	1.136e-026				
HAsO2	6.062e-027	6.062e-027	-26.217	-26.217	0.000
As(OH)3	5.299e-027	5.299e-027	-26.276	-26.276	0.000
H2AsO3-	2.370e-033	2.045e-033	-32.625	-32.689	-0.064
AsO2-	2.266e-033	1.955e-033	-32.645	-32.709	-0.064
AsO2OH-2	0.000e+000	0.000e+000	-40.640	-40.899	-0.259
As(5)	4.009e-006				
H2AsO4-	3.230e-006	2.787e-006	-5.491	-5.555	-0.064
H3AsO4	7.780e-007	7.780e-007	-6.109	-6.109	0.000
HAsO4-2	5.302e-010	2.919e-010	-9.276	-9.535	-0.259
AsO4-3	1.815e-018	4.725e-019	-17.741	-18.326	-0.584
Ca	8.718e-004				
Ca+2	6.315e-004	3.641e-004	-3.200	-3.439	-0.239
CaSO4	2.402e-004	2.402e-004	-3.619	-3.619	0.000
CaCl+	9.801e-008	8.456e-008	-7.009	-7.073	-0.064
CaCl2	1.090e-010	1.090e-010	-9.963	-9.963	0.000
CaOH+	3.760e-014	3.244e-014	-13.425	-13.489	-0.064
Cl(-1)	1.279e-003				
Cl-	1.278e-003	1.096e-003	-2.893	-2.960	-0.067
HCl	3.900e-007	3.900e-007	-6.409	-6.409	0.000
MgCl+	1.634e-007	1.410e-007	-6.787	-6.851	-0.064
MnCl+	1.037e-007	8.947e-008	-6.984	-7.048	-0.064
NaCl	9.975e-008	9.975e-008	-7.001	-7.001	0.000
CaCl+	9.801e-008	8.456e-008	-7.009	-7.073	-0.064
FeCl+2	2.048e-008	1.142e-008	-7.689	-7.942	-0.254
ZnCl+	1.825e-008	1.574e-008	-7.739	-7.803	-0.064
KCl	1.231e-008	1.231e-008	-7.910	-7.910	0.000
FeCl2+	1.174e-008	1.013e-008	-7.930	-7.995	-0.064
CuCl+	1.974e-009	1.703e-009	-8.705	-8.769	-0.064
CaCl2	1.090e-010	1.090e-010	-9.963	-9.963	0.000
ZnCl2	2.015e-011	2.015e-011	-10.696	-10.696	0.000
FeCl+	6.033e-012	5.206e-012	-11.219	-11.284	-0.064
CuCl2	9.828e-013	9.828e-013	-12.008	-12.008	0.000
Zn(OH)Cl	1.698e-013	1.698e-013	-12.770	-12.770	0.000
MnCl3-	2.720e-014	2.347e-014	-13.565	-13.630	-0.064
ZnCl3-	1.413e-014	1.219e-014	-13.850	-13.914	-0.064
ZnCl4-2	1.840e-016	1.013e-016	-15.735	-15.994	-0.259
FeCl2	3.061e-017	3.061e-017	-16.514	-16.514	0.000
FeCl4-	1.694e-017	1.462e-017	-16.771	-16.835	-0.064
CuCl2-	2.868e-022	2.474e-022	-21.542	-21.607	-0.064
FeCl4-2	1.929e-022	1.062e-022	-21.715	-21.974	-0.259
CuCl4-2	4.022e-023	2.214e-023	-22.396	-22.655	-0.259
CuCl3-2	3.163e-024	1.741e-024	-23.500	-23.759	-0.259
Cl(1)	1.997e-017				
HClO	1.997e-017	1.997e-017	-16.700	-16.700	0.000
ClO-	3.937e-022	3.397e-022	-21.405	-21.469	-0.064
Cl(3)	4.701e-033				
HClO2	3.145e-033	3.145e-033	-32.502	-32.502	0.000
ClO2-	1.556e-033	1.342e-033	-32.808	-32.872	-0.064
Cl(5)	4.389e-031				
ClO3-	4.389e-031	3.775e-031	-30.358	-30.423	-0.065
Cl(7)	6.162e-033				
ClO4-	6.161e-033	5.299e-033	-32.210	-32.276	-0.065
ZnClO4+	9.934e-037	8.571e-037	-36.003	-36.067	-0.064
Cu(1)	3.896e-021				
Cu+	3.606e-021	3.111e-021	-20.443	-20.507	-0.064
CuCl2-	2.868e-022	2.474e-022	-21.542	-21.607	-0.064
CuCl3-2	3.163e-024	1.741e-024	-23.500	-23.759	-0.259
Cu(2)	1.575e-006				
Cu+2	9.856e-007	5.683e-007	-6.006	-6.245	-0.239
CuSO4	5.878e-007	5.878e-007	-6.231	-6.231	0.000

CuCl+	1.974e-009	1.703e-009	-8.705	-8.769	-0.064
CuOH+	2.143e-011	1.849e-011	-10.669	-10.733	-0.064
CuCl2	9.828e-013	9.828e-013	-12.008	-12.008	0.000
CuCl4-2	4.022e-023	2.214e-023	-22.396	-22.655	-0.259
CuO2-2	5.806e-035	3.196e-035	-34.236	-34.495	-0.259
Fe(2)	1.598e-008				
Fe+2	1.131e-008	6.521e-009	-7.947	-8.186	-0.239
FeSO4	4.667e-009	4.667e-009	-8.331	-8.331	0.000
FeCl+	6.033e-012	5.206e-012	-11.219	-11.284	-0.064
FeOH+	1.508e-015	1.301e-015	-14.822	-14.886	-0.064
FeCl2	3.061e-017	3.061e-017	-16.514	-16.514	0.000
FeCl4-2	1.929e-022	1.062e-022	-21.715	-21.974	-0.259
Fe(OH)2	6.518e-024	6.518e-024	-23.186	-23.186	0.000
Fe(OH)3-	1.897e-031	1.637e-031	-30.722	-30.786	-0.064
Fe(OH)4-2	0.000e+000	0.000e+000	-42.727	-42.986	-0.259
Fe(3)	7.780e-004				
FeOH+2	4.569e-004	2.547e-004	-3.340	-3.594	-0.254
Fe+3	1.902e-004	6.253e-005	-3.721	-4.204	-0.483
Fe(OH)2+	6.165e-005	5.319e-005	-4.210	-4.274	-0.064
FeSO4+	3.166e-005	2.732e-005	-4.499	-4.564	-0.064
Fe2(OH)2+4	1.661e-005	1.745e-006	-4.780	-5.758	-0.978
Fe(SO4)2-	2.417e-006	2.085e-006	-5.617	-5.681	-0.064
Fe3(OH)4+5	6.129e-007	1.940e-008	-6.213	-7.712	-1.500
FeCl+2	2.048e-008	1.142e-008	-7.689	-7.942	-0.254
Fe(OH)3	1.569e-008	1.569e-008	-7.804	-7.804	0.000
FeCl2+	1.174e-008	1.013e-008	-7.930	-7.995	-0.064
Fe(OH)4-	2.882e-015	2.487e-015	-14.540	-14.604	-0.064
FeCl4-	1.694e-017	1.462e-017	-16.771	-16.835	-0.064
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-42.703	-42.700	0.002
K	4.046e-004				
K+	3.904e-004	3.346e-004	-3.408	-3.475	-0.067
KSO4-	1.414e-005	1.220e-005	-4.850	-4.914	-0.064
KHSO4	1.705e-008	1.705e-008	-7.768	-7.768	0.000
KCl	1.231e-008	1.231e-008	-7.910	-7.910	0.000
KOH	7.319e-016	7.319e-016	-15.136	-15.136	0.000
Mg	4.737e-004				
Mg+2	2.748e-004	1.648e-004	-3.561	-3.783	-0.222
MgSO4	1.987e-004	1.987e-004	-3.702	-3.702	0.000
MgCl+	1.634e-007	1.410e-007	-6.787	-6.851	-0.064
Mg4(OH)4+4	0.000e+000	0.000e+000	-42.704	-43.682	-0.978
Mn(2)	1.093e-004				
Mn+2	6.651e-005	3.835e-005	-4.177	-4.416	-0.239
MnSO4	4.272e-005	4.272e-005	-4.369	-4.369	0.000
MnCl+	1.037e-007	8.947e-008	-6.984	-7.048	-0.064
MnOH+	7.206e-013	6.218e-013	-12.142	-12.206	-0.064
MnCl3-	2.720e-014	2.347e-014	-13.565	-13.630	-0.064
Mn2OH+3	9.297e-017	2.555e-017	-16.032	-16.593	-0.561
Mn(OH)2	9.628e-022	9.628e-022	-21.016	-21.016	0.000
Mn2(OH)3+	5.386e-025	4.647e-025	-24.269	-24.333	-0.064
Mn(OH)3-	6.602e-031	5.696e-031	-30.180	-30.244	-0.064
Mn(OH)4-2	0.000e+000	0.000e+000	-41.257	-41.517	-0.259
Mn(3)	3.722e-013				
Mn+3	3.722e-013	1.023e-013	-12.429	-12.990	-0.561
Mn(6)	6.246e-033				
MnO4-2	6.246e-033	3.439e-033	-32.204	-32.464	-0.259
Mn(7)	1.761e-025				
MnO4-	1.761e-025	1.514e-025	-24.754	-24.820	-0.065
Na	6.184e-004				
Na+	6.004e-004	5.180e-004	-3.222	-3.286	-0.064
NaSO4-	1.791e-005	1.545e-005	-4.747	-4.811	-0.064
NaCl	9.975e-008	9.975e-008	-7.001	-7.001	0.000
NaOH	5.431e-016	5.431e-016	-15.265	-15.265	0.000
NaAlO2	6.150e-021	6.150e-021	-20.211	-20.211	0.000
O(0)	3.186e-007				
O2	1.593e-007	1.602e-007	-6.798	-6.795	0.002
S(6)	9.875e-003				

SO4-2	8.202e-003	4.515e-003	-2.086	-2.345	-0.259
HSO4-	8.378e-004	7.229e-004	-3.077	-3.141	-0.064
CaSO4	2.402e-004	2.402e-004	-3.619	-3.619	0.000
MgSO4	1.987e-004	1.987e-004	-3.702	-3.702	0.000
AlSO4+	1.622e-004	1.400e-004	-3.790	-3.854	-0.064
Al(SO4)2-	5.687e-005	4.907e-005	-4.245	-4.309	-0.064
MnSO4	4.272e-005	4.272e-005	-4.369	-4.369	0.000
FeSO4+	3.166e-005	2.732e-005	-4.499	-4.564	-0.064
NaSO4-	1.791e-005	1.545e-005	-4.747	-4.811	-0.064
KSO4-	1.414e-005	1.220e-005	-4.850	-4.914	-0.064
ZnSO4	8.114e-006	8.114e-006	-5.091	-5.091	0.000
Fe(SO4)2-	2.417e-006	2.085e-006	-5.617	-5.681	-0.064
CuSO4	5.878e-007	5.878e-007	-6.231	-6.231	0.000
KHSO4	1.705e-008	1.705e-008	-7.768	-7.768	0.000
FeSO4	4.667e-009	4.667e-009	-8.331	-8.331	0.000
H2SO4	1.081e-009	1.081e-009	-8.966	-8.966	0.000
Zn	2.297e-005				
Zn+2	1.483e-005	8.552e-006	-4.829	-5.068	-0.239
ZnSO4	8.114e-006	8.114e-006	-5.091	-5.091	0.000
ZnCl+	1.825e-008	1.574e-008	-7.739	-7.803	-0.064
ZnCl2	2.015e-011	2.015e-011	-10.696	-10.696	0.000
ZnOH+	6.857e-012	5.916e-012	-11.164	-11.228	-0.064
Zn(OH)Cl	1.698e-013	1.698e-013	-12.770	-12.770	0.000
ZnCl3-	1.413e-014	1.219e-014	-13.850	-13.914	-0.064
ZnCl4-2	1.840e-016	1.013e-016	-15.735	-15.994	-0.259
Zn(OH)2	1.598e-017	1.598e-017	-16.796	-16.796	0.000
Zn(OH)3-	3.622e-026	3.125e-026	-25.441	-25.505	-0.064
Zn(OH)4-2	6.104e-036	3.361e-036	-35.214	-35.474	-0.259
ZnClO4+	9.934e-037	8.571e-037	-36.003	-36.067	-0.064

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

Phase	SI	log IAP	log KT	
Al	-140.94	8.98	149.91	Al
Al(g)	-191.64	8.98	200.62	Al
Al2(SO4)3	-34.97	-16.07	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-17.63	-16.07	1.56	Al2(SO4)3:6H2O
Alum-K	-7.72	-12.69	-4.97	KAl(SO4)2:12H2O
Alunite	-4.45	-4.92	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.43	-5.78	-4.35	CaSO4
Antarcticite	-13.45	-9.36	4.09	CaCl2:6H2O
Antlerite	-18.61	-9.88	8.73	Cu3(SO4)(OH)4
Aphthitalite	-14.51	-18.40	-3.89	NaK3(SO4)2
Arcanite	-7.45	-9.30	-1.84	K2SO4
Arsenolite	-51.14	-70.98	-19.84	As2O3
As	-73.08	-30.39	42.68	As
As2O5	-18.84	-16.71	2.14	As2O5
As4O6(cubi)	-102.13	-141.96	-39.82	As4O6
As4O6(mono)	-101.91	-141.96	-40.05	As4O6
Atacamite	-28.37	-14.10	14.26	Cu4Cl2(OH)6
Bassanite	-2.08	-5.78	-3.71	CaSO4:0.5H2O
Birnessite	-22.73	-108.27	-85.55	Mn8O14:5H2O
Bischofite	-14.10	-9.70	4.39	MgCl2:6H2O
Bixbyite	-8.22	-9.18	-0.96	Mn2O3
Bloedite	-12.57	-15.05	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-3.67	3.88	7.55	AlO2H
Brochantite	-25.95	-10.53	15.42	Cu4(SO4)(OH)6
Brucite	-14.47	1.82	16.28	Mg(OH)2
Ca	-134.27	5.56	139.83	Ca
Ca(g)	-159.51	5.56	165.07	Ca
Ca2Al2O5:8H2O	-47.48	12.08	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-33.49	-7.20	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-28.03	-10.23	17.80	Ca3(AsO4)2
Ca3Al2O6	-98.79	14.25	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-115.68	24.80	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-90.85	16.41	107.25	Ca4Al2O7:13H2O

Ca4Al2O7:19H2O	-87.28	16.40	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-71.21	-2.88	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-36.98	9.92	46.91	CaAl2O4
CaAl2O4:10H2O	-28.07	9.92	37.99	CaAl2O4:10H2O
CaAl4O7	-50.90	17.69	68.59	CaAl4O7
Carnallite	-20.41	-16.14	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-2.25	-5.78	-3.54	CaSO4:0.5H2O
Chalcanthite	-5.96	-8.59	-2.63	CuSO4:5H2O
Chalcocyanite	-11.50	-8.59	2.91	CuSO4
Chloromagnesite	-31.52	-9.70	21.82	MgCl2
Cl2(g)	-17.91	-14.92	2.99	Cl2
Claudetite	-51.18	-70.98	-19.80	As2O3
Corundum	-10.53	7.76	18.29	Al2O3
Cu	-28.74	2.75	31.50	Cu
Cu(g)	-80.90	2.75	83.66	Cu
CuCl2	-15.89	-12.17	3.72	CuCl2
Cuprite	-33.51	-35.41	-1.91	Cu2O
Delafossite	-7.08	-13.51	-6.44	CuFeO2
Diaspore	-3.27	3.88	7.15	AlHO2
Epsomite	-4.17	-6.13	-1.96	MgSO4:7H2O
Ettringite	-65.57	-3.11	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-58.21	0.81	59.02	Fe
Fe(OH)2	-16.48	-2.59	13.89	Fe(OH)2
Fe(OH)3	-1.44	4.20	5.64	Fe(OH)3
Fe2(SO4)3	-18.49	-15.44	3.05	Fe2(SO4)3
FeO	-16.11	-2.59	13.52	FeO
Ferrite-Ca	-10.94	10.55	21.50	CaFe2O4
Ferrite-Cu	-2.54	7.75	10.28	CuFe2O4
Ferrite-Dicalcium	-44.08	12.71	56.80	Ca2Fe2O5
Ferrite-Mg	-10.81	10.21	21.02	MgFe2O4
Ferrite-Zn	-2.78	8.92	11.70	ZnFe2O4
FeSO4	-13.14	-10.53	2.61	FeSO4
Gibbsite	-3.86	3.88	7.74	Al(OH)3
Glauberite	-9.23	-14.70	-5.47	Na2Ca(SO4)2
Goethite	3.67	4.20	0.53	FeOOH
Gypsum	-1.25	-5.78	-4.53	CaSO4:2H2O
H2(g)	-39.60	-42.70	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.81	-6.25	1.56	NaCl
Hausmannite	-18.14	-8.00	10.14	Mn3O4
HCl(g)	-12.06	-5.76	6.30	HCl
Hematite	8.32	8.39	0.08	Fe2O3
Hercynite	-23.63	5.18	28.80	FeAl2O4
Hexahydrate	-4.40	-6.13	-1.73	MgSO4:6H2O
Hydrophilite	-21.11	-9.36	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	5.43	-3.98	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	1.66	-3.79	-5.45	NaFe3(SO4)2(OH)6
K	-69.95	1.02	70.98	K
K(g)	-80.56	1.02	81.58	K
K2O	-85.39	-1.35	84.04	K2O
K3H(SO4)2	-14.29	-17.92	-3.62	K3H(SO4)2
Kainite	-12.25	-12.56	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-15.96	-12.68	3.27	KAl(SO4)2
Katoite	-64.70	14.25	78.94	Ca3Al2H12O12
Kieserite	-5.86	-6.13	-0.27	MgSO4:H2O
KMgCl3	-37.39	-16.14	21.25	KMgCl3
KMgCl3:2H2O	-30.10	-16.14	13.96	KMgCl3:2H2O
Lammerite	-20.20	-18.65	1.55	Cu3(AsO4)2
Lawrencite	-23.16	-14.11	9.05	FeCl2
Leonite	-11.31	-15.42	-4.11	K2Mg(SO4)2:4H2O
Lime	-30.41	2.16	32.57	CaO
Magnetite	-4.61	5.81	10.42	Fe3O4
Manganite	-4.43	-4.59	-0.16	MnO(OH)
Manganosite	-16.73	1.18	17.92	MnO
Mayenite	-413.88	80.27	494.15	Ca12Al14O33
Melanterite	-8.13	-10.53	-2.40	FeSO4:7H2O

Mercallite	-7.18	-8.62	-1.44	KHSO4
Mg	-117.31	5.21	122.52	Mg
Mg(g)	-137.03	5.21	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.87	-5.67	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-14.43	-5.22	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.44	-9.70	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.01	-9.70	7.30	MgCl2:4H2O
MgCl2:H2O	-25.78	-9.70	16.07	MgCl2:H2O
MgOHCl	-19.83	-3.94	15.89	MgOHCl
MgSO4	-10.96	-6.13	4.83	MgSO4
Mirabilite	-7.76	-8.92	-1.15	Na2SO4:10H2O
Misenite	-49.94	-61.02	-11.08	K8H6(SO4)7
Mn	-78.35	4.58	82.93	Mn
Mn(OH)2(am)	-14.12	1.18	15.31	Mn(OH)2
Mn(OH)3	-10.93	-4.59	6.34	Mn(OH)3
MnCl2:2H2O	-14.33	-10.34	4.00	MnCl2:2H2O
MnCl2:4H2O	-13.09	-10.34	2.75	MnCl2:4H2O
MnCl2:H2O	-15.88	-10.34	5.54	MnCl2:H2O
MnO2(gamma)	-2.31	-18.44	-16.13	MnO2
MnSO4	-9.37	-6.76	2.61	MnSO4
Molysite	-26.56	-13.08	13.47	FeCl3
Na	-66.16	1.21	67.37	Na
Na(g)	-79.65	1.21	80.86	Na
Na2O	-68.39	-0.97	67.42	Na2O
Na3H(SO4)2	-16.46	-17.35	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-17.72	-23.62	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-16.17	3.71	19.88	NaFeO2
Nantokite	-16.70	-23.47	-6.77	CuCl
O2(g)	-3.90	-6.80	-2.89	O2
Oxychloride-Mg	-27.96	-2.13	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.74	-6.13	-1.39	MgSO4:5H2O
Periclase	-19.51	1.82	21.33	MgO
Picromerite	-10.99	-15.43	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-12.68	-26.99	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-20.39	2.16	22.55	Ca(OH)2
Pyrolusite	-0.78	-18.44	-17.66	MnO2
Scacchite	-19.08	-10.34	8.74	MnCl2
Spinel	-28.03	9.58	37.61	Al2MgO4
Starkeyite	-5.13	-6.13	-1.00	MgSO4:4H2O
Sylvite	-7.26	-6.44	0.83	KCl
Syngenite	-7.48	-15.08	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-45.91	-28.77	17.14	Mg2CaCl6:12H2O
Tenorite	-8.29	-0.65	7.65	CuO
Thenardite	-8.56	-8.92	-0.36	Na2SO4
Todorokite	-19.78	-65.61	-45.82	Mn7O12:3H2O
Wustite	-14.13	-1.73	12.40	Fe.947O
Zincite	-10.67	0.53	11.20	ZnO
Zn	-64.86	3.93	68.79	Zn
Zn(ClO4)2:6H2O	-75.25	-69.62	5.63	Zn(ClO4)2:6H2O
Zn(g)	-81.48	3.93	85.41	Zn
Zn(OH)2(beta)	-11.40	0.53	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-11.13	0.53	11.66	Zn(OH)2
Zn(OH)2(gamma)	-11.35	0.53	11.88	Zn(OH)2
Zn2(OH)3Cl	-19.99	-4.70	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-14.46	-6.88	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-24.43	-15.11	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-33.38	-14.29	19.09	Zn3O(SO4)2
ZnCl2	-18.07	-10.99	7.08	ZnCl2
ZnSO4	-10.95	-7.41	3.53	ZnSO4
ZnSO4:6H2O	-5.71	-7.41	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.54	-7.41	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.86	-7.41	-0.55	ZnSO4:H2O

Initial solution 2. AS1

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

Elements	Molality	Moles
As	1.290e-006	1.290e-006
Ca	2.167e-003	2.167e-003
Cl	6.829e-004	6.829e-004
Cu	1.779e-006	1.779e-006
F	1.316e-005	1.316e-005
K	7.855e-005	7.855e-005
Mg	6.656e-004	6.656e-004
Mn	3.296e-006	3.296e-006
N(5)	2.071e-004	2.071e-004
Na	1.872e-003	1.872e-003
S(6)	2.531e-003	2.531e-003
Zn	2.983e-006	2.983e-006

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

pH = 7.540  
 pe = 10.000  
 Activity of water = 1.000  
 Ionic strength = 1.056e-002  
 Mass of water (kg) = 1.000e+000  
 Total alkalinity (eq/kg) = 1.343e-006  
 Total carbon (mol/kg) = 0.000e+000  
 Total CO2 (mol/kg) = 0.000e+000  
 Temperature (deg C) = 25.000  
 Electrical balance (eq) = 1.664e-003  
 Percent error,  $100 \cdot (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$  = 13.88  
 Iterations = 24  
 Total H = 1.110507e+002  
 Total O = 5.553608e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	3.718e-007	3.340e-007	-6.430	-6.476	-0.047
H+	3.161e-008	2.884e-008	-7.500	-7.540	-0.040
H2O	5.553e+001	9.999e-001	1.744	-0.000	0.000
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-172.417	-172.417	0.000
As(3)	0.000e+000				
HAsO2	0.000e+000	0.000e+000	-62.230	-62.230	0.000
As(OH)3	0.000e+000	0.000e+000	-62.288	-62.288	0.000
H2AsO3-	0.000e+000	0.000e+000	-63.916	-63.962	-0.046
AsO2-	0.000e+000	0.000e+000	-63.936	-63.981	-0.046
AsO2OH-2	0.000e+000	0.000e+000	-67.247	-67.432	-0.185
As(5)	1.290e-006				
AsO3F-2	1.270e-006	8.301e-007	-5.896	-6.081	-0.185
HAsO3F-	1.976e-008	1.778e-008	-7.704	-7.750	-0.046
HAsO4-2	0.000e+000	0.000e+000	-40.403	-40.587	-0.185
H2AsO4-	0.000e+000	0.000e+000	-41.302	-41.347	-0.046
AsO4-3	0.000e+000	0.000e+000	-44.222	-44.638	-0.416
H3AsO4	0.000e+000	0.000e+000	-46.642	-46.642	0.000
Ca	2.167e-003				
Ca+2	1.907e-003	1.277e-003	-2.720	-2.894	-0.174
CaSO4	2.583e-004	2.583e-004	-3.588	-3.588	0.000
CaNO3+	1.313e-006	1.181e-006	-5.882	-5.928	-0.046
CaCl+	1.840e-007	1.656e-007	-6.735	-6.781	-0.046
CaF+	7.576e-008	6.817e-008	-7.121	-7.166	-0.046
CaOH+	6.949e-009	6.252e-009	-8.158	-8.204	-0.046
CaCl2	1.192e-010	1.192e-010	-9.924	-9.924	0.000
Cl(-1)	6.829e-004				
Cl-	6.823e-004	6.119e-004	-3.166	-3.213	-0.047
MgCl+	1.928e-007	1.735e-007	-6.715	-6.761	-0.046
CaCl+	1.840e-007	1.656e-007	-6.735	-6.781	-0.046

NaCl	1.795e-007	1.795e-007	-6.746	-6.746	0.000
MnCl+	2.596e-009	2.336e-009	-8.586	-8.632	-0.046
ZnCl+	1.858e-009	1.672e-009	-8.731	-8.777	-0.046
KCl	1.432e-009	1.432e-009	-8.844	-8.844	0.000
Zn(OH)Cl	9.910e-010	9.910e-010	-9.004	-9.004	0.000
CuCl+	8.707e-010	7.835e-010	-9.060	-9.106	-0.046
CaCl2	1.192e-010	1.192e-010	-9.924	-9.924	0.000
HCl	3.964e-012	3.964e-012	-11.402	-11.402	0.000
ZnCl2	1.195e-012	1.195e-012	-11.923	-11.923	0.000
CuCl2	2.525e-013	2.525e-013	-12.598	-12.598	0.000
CuCl2-	7.065e-016	6.357e-016	-15.151	-15.197	-0.046
ZnCl3-	4.488e-016	4.039e-016	-15.348	-15.394	-0.046
MnCl3-	2.124e-016	1.911e-016	-15.673	-15.719	-0.046
CuCl3-2	3.823e-018	2.498e-018	-17.418	-17.602	-0.185
ZnCl4-2	2.866e-018	1.873e-018	-17.543	-17.727	-0.185
CuCl4-2	2.715e-024	1.774e-024	-23.566	-23.751	-0.185
Cl(1)	1.250e-026				
ClO-	6.368e-027	5.730e-027	-26.196	-26.242	-0.046
HClO	6.129e-027	6.129e-027	-26.213	-26.213	0.000
Cl(3)	0.000e+000				
ClO2-	0.000e+000	0.000e+000	-42.119	-42.165	-0.046
HClO2	0.000e+000	0.000e+000	-46.535	-46.535	0.000
Cl(5)	0.000e+000				
ClO3-	0.000e+000	0.000e+000	-44.189	-44.236	-0.047
Cl(7)	0.000e+000				
ClO4-	0.000e+000	0.000e+000	-50.562	-50.609	-0.047
ZnClO4+	0.000e+000	0.000e+000	-55.075	-55.121	-0.046
Cu(1)	2.919e-014				
Cu+	2.848e-014	2.562e-014	-13.546	-13.591	-0.046
CuCl2-	7.065e-016	6.357e-016	-15.151	-15.197	-0.046
CuCl3-2	3.823e-018	2.498e-018	-17.418	-17.602	-0.185
Cu(2)	1.779e-006				
CuOH+	9.303e-007	8.370e-007	-6.031	-6.077	-0.046
Cu+2	6.992e-007	4.681e-007	-6.155	-6.330	-0.174
CuSO4	1.485e-007	1.485e-007	-6.828	-6.828	0.000
CuCl+	8.707e-010	7.835e-010	-9.060	-9.106	-0.046
CuF+	8.661e-011	7.793e-011	-10.062	-10.108	-0.046
CuCl2	2.525e-013	2.525e-013	-12.598	-12.598	0.000
CuO2-2	3.675e-016	2.402e-016	-15.435	-15.620	-0.185
CuCl4-2	2.715e-024	1.774e-024	-23.566	-23.751	-0.185
F	1.316e-005				
F-	1.169e-005	1.050e-005	-4.932	-4.979	-0.047
AsO3F-2	1.270e-006	8.301e-007	-5.896	-6.081	-0.185
MgF+	1.023e-007	9.206e-008	-6.990	-7.036	-0.046
CaF+	7.576e-008	6.817e-008	-7.121	-7.166	-0.046
HAsO3F-	1.976e-008	1.778e-008	-7.704	-7.750	-0.046
NaF	1.875e-009	1.875e-009	-8.727	-8.727	0.000
MnF+	5.633e-010	5.068e-010	-9.249	-9.295	-0.046
HF	4.651e-010	4.651e-010	-9.332	-9.332	0.000
ZnF+	2.681e-010	2.413e-010	-9.572	-9.617	-0.046
CuF+	8.661e-011	7.793e-011	-10.062	-10.108	-0.046
HF2-	1.315e-015	1.183e-015	-14.881	-14.927	-0.046
H2F2	5.380e-019	5.380e-019	-18.269	-18.269	0.000
H(0)	1.317e-038				
H2	6.583e-039	6.600e-039	-38.182	-38.180	0.001
K	7.855e-005				
K+	7.769e-005	6.967e-005	-4.110	-4.157	-0.047
KSO4-	8.657e-007	7.790e-007	-6.063	-6.108	-0.046
KCl	1.432e-009	1.432e-009	-8.844	-8.844	0.000
KOH	8.375e-012	8.375e-012	-11.077	-11.077	0.000
KHSO4	1.982e-014	1.982e-014	-13.703	-13.703	0.000
Mg	6.656e-004				
Mg+2	5.310e-004	3.631e-004	-3.275	-3.440	-0.165
MgSO4	1.343e-004	1.343e-004	-3.872	-3.872	0.000
MgCl+	1.928e-007	1.735e-007	-6.715	-6.761	-0.046
MgF+	1.023e-007	9.206e-008	-6.990	-7.036	-0.046
Mg4(OH)4+4	2.283e-023	4.466e-024	-22.642	-23.350	-0.709

Mn(2)	3.296e-006					
Mn+2	2.678e-006	1.793e-006	-5.572	-5.747	-0.174	
MnSO4	6.126e-007	6.126e-007	-6.213	-6.213	0.000	
MnCl+	2.596e-009	2.336e-009	-8.586	-8.632	-0.046	
MnOH+	1.775e-009	1.597e-009	-8.751	-8.797	-0.046	
MnNO3+	5.828e-010	5.244e-010	-9.234	-9.280	-0.046	
MnF+	5.633e-010	5.068e-010	-9.249	-9.295	-0.046	
Mn(NO3)2	2.432e-013	2.432e-013	-12.614	-12.614	0.000	
Mn2(OH)3+	1.873e-013	1.686e-013	-12.727	-12.773	-0.046	
Mn(OH)2	1.359e-013	1.359e-013	-12.867	-12.867	0.000	
Mn2OH+3	7.780e-015	3.068e-015	-14.109	-14.513	-0.404	
MnCl3-	2.124e-016	1.911e-016	-15.673	-15.719	-0.046	
Mn(OH)3-	4.913e-018	4.421e-018	-17.309	-17.355	-0.046	
Mn(OH)4-2	1.986e-024	1.298e-024	-23.702	-23.887	-0.185	
Mn(3)	1.212e-021					
Mn+3	1.212e-021	4.781e-022	-20.916	-21.320	-0.404	
Mn(6)	2.047e-024					
MnO4-2	2.047e-024	1.338e-024	-23.689	-23.874	-0.185	
Mn(7)	6.557e-024					
MnO4-	6.557e-024	5.890e-024	-23.183	-23.230	-0.047	
N(5)	2.071e-004					
NO3-	2.058e-004	1.846e-004	-3.687	-3.734	-0.047	
CaNO3+	1.313e-006	1.181e-006	-5.882	-5.928	-0.046	
MnNO3+	5.828e-010	5.244e-010	-9.234	-9.280	-0.046	
HNO3	2.784e-013	2.784e-013	-12.555	-12.555	0.000	
Mn(NO3)2	2.432e-013	2.432e-013	-12.614	-12.614	0.000	
Na	1.872e-003					
Na+	1.854e-003	1.669e-003	-2.732	-2.778	-0.046	
NaSO4-	1.697e-005	1.527e-005	-4.770	-4.816	-0.046	
NaCl	1.795e-007	1.795e-007	-6.746	-6.746	0.000	
NaF	1.875e-009	1.875e-009	-8.727	-8.727	0.000	
NaOH	9.616e-011	9.616e-011	-10.017	-10.017	0.000	
O(0)	2.916e-016					
O2	1.458e-016	1.462e-016	-15.836	-15.835	0.001	
S(6)	2.531e-003					
SO4-2	2.119e-003	1.385e-003	-2.674	-2.858	-0.185	
CaSO4	2.583e-004	2.583e-004	-3.588	-3.588	0.000	
MgSO4	1.343e-004	1.343e-004	-3.872	-3.872	0.000	
NaSO4-	1.697e-005	1.527e-005	-4.770	-4.816	-0.046	
KSO4-	8.657e-007	7.790e-007	-6.063	-6.108	-0.046	
MnSO4	6.126e-007	6.126e-007	-6.213	-6.213	0.000	
ZnSO4	4.733e-007	4.733e-007	-6.325	-6.325	0.000	
CuSO4	1.485e-007	1.485e-007	-6.828	-6.828	0.000	
HSO4-	4.485e-009	4.035e-009	-8.348	-8.394	-0.046	
KHSO4	1.982e-014	1.982e-014	-13.703	-13.703	0.000	
H2SO4	1.098e-019	1.098e-019	-18.959	-18.959	0.000	
Zn	2.983e-006					
Zn+2	2.429e-006	1.626e-006	-5.615	-5.789	-0.174	
ZnSO4	4.733e-007	4.733e-007	-6.325	-6.325	0.000	
ZnOH+	6.871e-008	6.182e-008	-7.163	-7.209	-0.046	
Zn(OH)2	9.179e-009	9.179e-009	-8.037	-8.037	0.000	
ZnCl+	1.858e-009	1.672e-009	-8.731	-8.777	-0.046	
Zn(OH)Cl	9.910e-010	9.910e-010	-9.004	-9.004	0.000	
ZnF+	2.681e-010	2.413e-010	-9.572	-9.617	-0.046	
ZnCl2	1.195e-012	1.195e-012	-11.923	-11.923	0.000	
Zn(OH)3-	1.096e-012	9.864e-013	-11.960	-12.006	-0.046	
ZnCl3-	4.488e-016	4.039e-016	-15.348	-15.394	-0.046	
Zn(OH)4-2	8.921e-018	5.830e-018	-17.050	-17.234	-0.185	
ZnCl4-2	2.866e-018	1.873e-018	-17.543	-17.727	-0.185	
ZnClO4+	0.000e+000	0.000e+000	-55.075	-55.121	-0.046	

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

Phase	SI	log IAP	log KT	
Anhydrite	-1.40	-5.75	-4.35	CaSO4
Antarcticite	-13.41	-9.32	4.09	CaCl2:6H2O

Antlerite	-0.42	8.31	8.73	Cu <sub>3</sub> (SO <sub>4</sub> )(OH) <sub>4</sub>
Aphthitalite	-17.08	-20.97	-3.89	NaK <sub>3</sub> (SO <sub>4</sub> ) <sub>2</sub>
Arcanite	-9.33	-11.17	-1.84	K <sub>2</sub> SO <sub>4</sub>
Arsenolite	-123.16	-143.00	-19.84	As <sub>2</sub> O <sub>3</sub>
As	-102.31	-59.63	42.68	As
As <sub>2</sub> O <sub>5</sub>	-99.91	-97.77	2.14	As <sub>2</sub> O <sub>5</sub>
As <sub>4</sub> O <sub>6</sub> (cubi)	-246.18	-286.01	-39.82	As <sub>4</sub> O <sub>6</sub>
As <sub>4</sub> O <sub>6</sub> (mono)	-245.96	-286.01	-40.05	As <sub>4</sub> O <sub>6</sub>
Atacamite	-0.77	13.49	14.26	Cu <sub>4</sub> Cl <sub>2</sub> (OH) <sub>6</sub>
Bassanite	-2.05	-5.75	-3.71	CaSO <sub>4</sub> :0.5H <sub>2</sub> O
Birnessite	15.35	-70.19	-85.55	Mn <sub>8</sub> O <sub>14</sub> :5H <sub>2</sub> O
Bischofite	-14.26	-9.87	4.39	MgCl <sub>2</sub> :6H <sub>2</sub> O
Bixbyite	3.56	2.60	-0.96	Mn <sub>2</sub> O <sub>3</sub>
Bloedite	-12.23	-14.71	-2.48	Na <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub> :4H <sub>2</sub> O
Brochantite	1.64	17.06	15.42	Cu <sub>4</sub> (SO <sub>4</sub> )(OH) <sub>6</sub>
Brucite	-4.64	11.64	16.28	Mg(OH) <sub>2</sub>
Ca	-119.73	20.10	139.83	Ca
Ca(g)	-144.97	20.10	165.07	Ca
Ca <sub>2</sub> Cl <sub>2</sub> (OH) <sub>2</sub> :H <sub>2</sub> O	-23.42	2.87	26.29	Ca <sub>2</sub> Cl <sub>2</sub> (OH) <sub>2</sub> :H <sub>2</sub> O
Ca <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub>	-79.02	-61.22	17.80	Ca <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub>
Ca <sub>4</sub> Cl <sub>2</sub> (OH) <sub>6</sub> :13H <sub>2</sub> O	-41.09	27.24	68.33	Ca <sub>4</sub> Cl <sub>2</sub> (OH) <sub>6</sub> :13H <sub>2</sub> O
Carnallite	-21.51	-17.24	4.27	KMgCl <sub>3</sub> :6H <sub>2</sub> O
CaSO <sub>4</sub> :0.5H <sub>2</sub> O(beta)	-2.22	-5.75	-3.54	CaSO <sub>4</sub> :0.5H <sub>2</sub> O
Chalcanthite	-6.56	-9.19	-2.63	CuSO <sub>4</sub> :5H <sub>2</sub> O
Chalcocyanite	-12.10	-9.19	2.91	CuSO <sub>4</sub>
Chloromagnesite	-31.68	-9.87	21.82	MgCl <sub>2</sub>
Cl <sub>2</sub> (g)	-32.42	-29.42	2.99	Cl <sub>2</sub>
Claudetite	-123.21	-143.00	-19.80	As <sub>2</sub> O <sub>3</sub>
Cu	-14.83	16.67	31.50	Cu
Cu(g)	-66.99	16.67	83.66	Cu
CuCl <sub>2</sub>	-16.48	-12.76	3.72	CuCl <sub>2</sub>
CuF	-25.65	-18.57	7.08	CuF
CuF <sub>2</sub>	-15.67	-16.29	-0.62	CuF <sub>2</sub>
CuF <sub>2</sub> :2H <sub>2</sub> O	-11.74	-16.29	-4.55	CuF <sub>2</sub> :2H <sub>2</sub> O
Cuprite	-10.20	-12.10	-1.91	Cu <sub>2</sub> O
Epsomite	-4.34	-6.30	-1.96	MgSO <sub>4</sub> :7H <sub>2</sub> O
F <sub>2</sub> (g)	-88.67	-32.95	55.71	F <sub>2</sub>
Fluorite	-2.78	-12.85	-10.07	CaF <sub>2</sub>
Glauberite	-8.70	-14.17	-5.47	Na <sub>2</sub> Ca(SO <sub>4</sub> ) <sub>2</sub>
Gypsum	-1.22	-5.75	-4.53	CaSO <sub>4</sub> :2H <sub>2</sub> O
H <sub>2</sub> (g)	-35.08	-38.18	-3.10	H <sub>2</sub>
H <sub>2</sub> O(g)	-1.59	-0.00	1.59	H <sub>2</sub> O
Halite	-7.55	-5.99	1.56	NaCl
Hausmannite	1.79	11.93	10.14	Mn <sub>3</sub> O <sub>4</sub>
HCl(g)	-17.06	-10.75	6.30	HCl
Hexahydrate	-4.57	-6.30	-1.73	MgSO <sub>4</sub> :6H <sub>2</sub> O
Hydrophilite	-21.07	-9.32	11.75	CaCl <sub>2</sub>
Ice	-0.14	-0.00	0.14	H <sub>2</sub> O
K	-63.63	7.34	70.98	K
K(g)	-74.24	7.34	81.58	K
K <sub>2</sub> O	-77.27	6.77	84.04	K <sub>2</sub> O
K <sub>3</sub> H(SO <sub>4</sub> ) <sub>2</sub>	-22.10	-25.73	-3.62	K <sub>3</sub> H(SO <sub>4</sub> ) <sub>2</sub>
Kainite	-13.36	-13.67	-0.31	KMgClSO <sub>4</sub> :3H <sub>2</sub> O
Kieserite	-6.03	-6.30	-0.27	MgSO <sub>4</sub> :H <sub>2</sub> O
KMgCl <sub>3</sub>	-38.48	-17.24	21.25	KMgCl <sub>3</sub>
KMgCl <sub>3</sub> :2H <sub>2</sub> O	-31.20	-17.24	13.96	KMgCl <sub>3</sub> :2H <sub>2</sub> O
Lammerite	-73.08	-71.52	1.55	Cu <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub>
Leonite	-13.36	-17.47	-4.11	K <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub> :4H <sub>2</sub> O
Lime	-20.38	12.19	32.57	CaO
Manganite	1.46	1.30	-0.16	MnO(OH)
Manganosite	-8.58	9.33	17.92	MnO
Mercallite	-13.12	-14.56	-1.44	KHSO <sub>4</sub>
Mg	-102.96	19.56	122.52	Mg
Mg(g)	-122.69	19.56	142.25	Mg
Mg <sub>1.25</sub> SO <sub>4</sub> (OH)0.5:0.5H <sub>2</sub> O	-8.58	-3.39	5.20	Mg <sub>1.25</sub> SO <sub>4</sub> (OH)0.5:0.5H <sub>2</sub> O
Mg <sub>1.5</sub> SO <sub>4</sub> (OH)	-9.69	-0.48	9.21	Mg <sub>1.5</sub> SO <sub>4</sub> (OH)
MgCl <sub>2</sub> :2H <sub>2</sub> O	-22.60	-9.87	12.73	MgCl <sub>2</sub> :2H <sub>2</sub> O

MgCl2:4H2O	-17.17	-9.87	7.30	MgCl2:4H2O
MgCl2:H2O	-25.94	-9.87	16.07	MgCl2:H2O
MgOHCl	-15.00	0.89	15.89	MgOHCl
MgSO4	-11.13	-6.30	4.83	MgSO4
Mirabilite	-7.26	-8.41	-1.15	Na2SO4:10H2O
Misenite	-87.43	-98.50	-11.08	K8H6(SO4)7
Mn	-65.68	17.25	82.93	Mn
Mn(OH)2(am)	-5.97	9.33	15.31	Mn(OH)2
Mn(OH)3	-5.04	1.30	6.34	Mn(OH)3
MnCl2:2H2O	-16.17	-12.17	4.00	MnCl2:2H2O
MnCl2:4H2O	-14.92	-12.17	2.75	MnCl2:4H2O
MnCl2:H2O	-17.71	-12.17	5.54	MnCl2:H2O
MnO2(gamma)	1.32	-14.81	-16.13	MnO2
MnSO4	-11.21	-8.61	2.61	MnSO4
Na	-58.65	8.72	67.37	Na
Na(g)	-72.14	8.72	80.86	Na
Na2O	-57.89	9.52	67.42	Na2O
Na3H(SO4)2	-20.70	-21.59	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.69	-22.58	-5.89	Na4Ca(SO4)3:2H2O
Nantokite	-10.04	-16.80	-6.77	CuCl
Niter	-7.67	-7.89	-0.22	KNO3
NO2(g)	-15.66	-7.31	8.35	NO2
O2(g)	-12.94	-15.84	-2.89	O2
Oxychloride-Mg	-13.31	12.53	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.91	-6.30	-1.39	MgSO4:5H2O
Periclase	-9.69	11.64	21.33	MgO
Picromerite	-13.03	-17.47	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-14.66	-28.98	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-10.36	12.19	22.55	Ca(OH)2
Pyrolusite	2.85	-14.81	-17.66	MnO2
Scacchite	-20.91	-12.17	8.74	MnCl2
Sellaite	-3.95	-13.40	-9.44	MgF2
Starkeyite	-5.30	-6.30	-1.00	MgSO4:4H2O
Sylvite	-8.20	-7.37	0.83	KCl
Syngenite	-9.32	-16.92	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-46.20	-29.05	17.14	Mg2CaCl6:12H2O
Tenorite	1.10	8.75	7.65	CuO
Thenardite	-8.06	-8.41	-0.36	Na2SO4
Todorokite	14.67	-31.16	-45.82	Mn7O12:3H2O
Zincite	-1.91	9.29	11.20	ZnO
Zn	-51.58	17.21	68.79	Zn
Zn(ClO4)2:6H2O	-112.64	-107.01	5.63	Zn(ClO4)2:6H2O
Zn(g)	-68.20	17.21	85.41	Zn
Zn(NO3)2:6H2O	-16.66	-13.26	3.40	Zn(NO3)2:6H2O
Zn(OH)2(beta)	-2.64	9.29	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-2.37	9.29	11.66	Zn(OH)2
Zn(OH)2(gamma)	-2.59	9.29	11.88	Zn(OH)2
Zn2(OH)3Cl	-7.46	7.83	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-6.94	0.64	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-79.21	-69.90	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-27.09	-8.00	19.09	Zn3O(SO4)2
Zn5(NO3)2(OH)8	-18.76	23.91	42.67	Zn5(NO3)2(OH)8
ZnCl2	-19.29	-12.22	7.08	ZnCl2
ZnF2	-15.25	-15.75	-0.49	ZnF2
ZnSO4	-12.18	-8.65	3.53	ZnSO4
ZnSO4:6H2O	-6.95	-8.65	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-6.77	-8.65	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-8.10	-8.65	-0.55	ZnSO4:H2O

-----  
Beginning of batch-reaction calculations.  
-----

Reaction step 1.

Using mix 4.

## Mixture 4.

1.000e+000 Solution 1 Flujo 2  
3.000e+000 Solution 2 AS1

## -----Solution composition-----

Elements	Molality	Moles
Al	7.792e-005	3.117e-004
As	1.970e-006	7.878e-006
Ca	1.843e-003	7.373e-003
Cl	8.320e-004	3.328e-003
Cu	1.728e-006	6.912e-006
F	9.873e-006	3.949e-005
Fe	1.945e-004	7.780e-004
K	1.601e-004	6.402e-004
Mg	6.176e-004	2.470e-003
Mn	2.981e-005	1.192e-004
N	1.553e-004	6.214e-004
Na	1.558e-003	6.233e-003
S	4.367e-003	1.747e-002
Zn	7.979e-006	3.192e-005

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

pH	=	3.271	Charge balance
pe	=	16.690	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	1.352e-002	
Mass of water (kg)	=	4.000e+000	
Total alkalinity (eq/kg)	=	-8.906e-004	
Total carbon (mol/kg)	=	0.000e+000	
Total CO2 (mol/kg)	=	0.000e+000	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	-6.778e-003	
Percent error, 100*(Cat- An )/(Cat+ An )	=	-11.14	
Iterations	=	12	
Total H	=	4.442059e+002	
Total O	=	2.221737e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	5.921e-004	5.354e-004	-3.228	-3.271	-0.044
OH-	2.028e-011	1.799e-011	-10.693	-10.745	-0.052
H2O	5.553e+001	9.998e-001	1.744	-0.000	0.000
Al	7.792e-005				
AlSO4+	3.272e-005	2.909e-005	-4.485	-4.536	-0.051
Al+3	3.127e-005	1.252e-005	-4.505	-4.902	-0.398
AlF+2	7.657e-006	4.805e-006	-5.116	-5.318	-0.202
Al(SO4)2-	5.768e-006	5.129e-006	-5.239	-5.290	-0.051
AlOH+2	4.173e-007	2.619e-007	-6.380	-6.582	-0.202
AlF2+	8.258e-008	7.343e-008	-7.083	-7.134	-0.051
Al(OH)2+	1.277e-009	1.136e-009	-8.894	-8.945	-0.051
Al2(OH)2+4	6.806e-011	1.115e-011	-10.167	-10.953	-0.786
AlF3	3.548e-011	3.548e-011	-10.450	-10.450	0.000
HAlo2	3.087e-012	3.087e-012	-11.511	-11.511	0.000
Al3(OH)4+5	5.080e-015	3.142e-016	-14.294	-15.503	-1.209
AlO2-	2.221e-015	1.975e-015	-14.653	-14.704	-0.051
AlF4-	3.847e-016	3.421e-016	-15.415	-15.466	-0.051
NaAlO2	5.142e-019	5.142e-019	-18.289	-18.289	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-55.413	-57.782	-2.369
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-187.358	-187.358	0.000

As(3)	0.000e+000					
HAsO2	0.000e+000	0.000e+000	0.000e+000	-62.643	-62.643	0.000
As(OH)3	0.000e+000	0.000e+000	0.000e+000	-62.702	-62.702	0.000
H2AsO3-	0.000e+000	0.000e+000	0.000e+000	-68.593	-68.644	-0.051
AsO2-	0.000e+000	0.000e+000	0.000e+000	-68.612	-68.663	-0.051
AsO2OH-2	0.000e+000	0.000e+000	0.000e+000	-76.177	-76.383	-0.206
HAsS2	0.000e+000	0.000e+000	0.000e+000	-311.772	-311.772	0.000
As(5)	1.970e-006					
HAsO3F-	1.963e-006	1.745e-006		-5.707	-5.758	-0.051
AsO3F-2	7.049e-009	4.389e-009		-8.152	-8.358	-0.206
H2AsO4-	0.000e+000	0.000e+000		-41.136	-41.187	-0.051
H3AsO4	0.000e+000	0.000e+000		-42.212	-42.212	0.000
HAsO4-2	0.000e+000	0.000e+000		-44.490	-44.696	-0.206
AsO4-3	0.000e+000	0.000e+000		-52.551	-53.015	-0.464
Ca	1.843e-003					
Ca+2	1.519e-003	9.743e-004		-2.818	-3.011	-0.193
CaSO4	3.232e-004	3.232e-004		-3.490	-3.490	0.000
CaNO3+	7.492e-007	6.661e-007		-6.125	-6.176	-0.051
CaCl+	1.710e-007	1.520e-007		-6.767	-6.818	-0.051
CaF+	2.138e-010	1.901e-010		-9.670	-9.721	-0.051
CaCl2	1.316e-010	1.316e-010		-9.881	-9.881	0.000
CaOH+	2.890e-013	2.570e-013		-12.539	-12.590	-0.051
Cl(-1)	8.320e-004					
Cl-	8.313e-004	7.362e-004		-3.080	-3.133	-0.053
MgCl+	1.877e-007	1.669e-007		-6.726	-6.777	-0.051
NaCl	1.766e-007	1.766e-007		-6.753	-6.753	0.000
CaCl+	1.710e-007	1.520e-007		-6.767	-6.818	-0.051
HCl	8.853e-008	8.853e-008		-7.053	-7.053	0.000
MnCl+	2.477e-008	2.202e-008		-7.606	-7.657	-0.051
ZnCl+	5.446e-009	4.842e-009		-8.264	-8.315	-0.051
KCl	3.441e-009	3.441e-009		-8.463	-8.463	0.000
CuCl+	1.880e-009	1.671e-009		-8.726	-8.777	-0.051
FeCl+2	1.239e-009	7.777e-010		-8.907	-9.109	-0.202
FeCl2+	5.213e-010	4.635e-010		-9.283	-9.334	-0.051
CaCl2	1.316e-010	1.316e-010		-9.881	-9.881	0.000
ZnCl2	4.164e-012	4.164e-012		-11.380	-11.380	0.000
FeCl+	8.145e-013	7.242e-013		-12.089	-12.140	-0.051
CuCl2	6.480e-013	6.480e-013		-12.188	-12.188	0.000
Zn(OH)Cl	1.546e-013	1.546e-013		-12.811	-12.811	0.000
MnCl3-	2.932e-015	2.607e-015		-14.533	-14.584	-0.051
ZnCl3-	1.904e-015	1.693e-015		-14.720	-14.771	-0.051
ZnCl4-2	1.517e-017	9.447e-018		-16.819	-17.025	-0.206
FeCl2	2.861e-018	2.861e-018		-17.544	-17.544	0.000
FeCl4-	3.396e-019	3.020e-019		-18.469	-18.520	-0.051
CuCl2-	3.747e-022	3.331e-022		-21.426	-21.477	-0.051
CuCl4-2	1.058e-023	6.590e-024		-22.975	-23.181	-0.206
FeCl4-2	7.195e-024	4.480e-024		-23.143	-23.349	-0.206
CuCl3-2	2.530e-024	1.575e-024		-23.597	-23.803	-0.206
Cl(1)	9.524e-018					
HClO	9.523e-018	9.523e-018		-17.021	-17.021	0.000
ClO-	5.394e-022	4.796e-022		-21.268	-21.319	-0.051
Cl(3)	7.632e-033					
ClO2-	4.479e-033	3.983e-033		-32.349	-32.400	-0.051
HClO2	3.153e-033	3.153e-033		-32.501	-32.501	0.000
Cl(5)	2.652e-030					
ClO3-	2.652e-030	2.354e-030		-29.576	-29.628	-0.052
Cl(7)	7.824e-032					
ClO4-	7.824e-032	6.943e-032		-31.107	-31.158	-0.052
ZnClO4+	5.782e-036	5.141e-036		-35.238	-35.289	-0.051
Cu(1)	1.081e-020					
Cu+	1.044e-020	9.279e-021		-19.981	-20.033	-0.051
CuCl2-	3.747e-022	3.331e-022		-21.426	-21.477	-0.051
CuCl3-2	2.530e-024	1.575e-024		-23.597	-23.803	-0.206
Cu(2)	1.728e-006					
Cu+2	1.294e-006	8.301e-007		-5.888	-6.081	-0.193
CuSO4	4.319e-007	4.319e-007		-6.365	-6.365	0.000
CuCl+	1.880e-009	1.671e-009		-8.726	-8.777	-0.051

	CuOH+	8.992e-011	7.995e-011	-10.046	-10.097	-0.051
	CuCl2	6.480e-013	6.480e-013	-12.188	-12.188	0.000
	CuF+	5.679e-013	5.050e-013	-12.246	-12.297	-0.051
	CuNO2+	9.271e-021	8.243e-021	-20.033	-20.084	-0.051
	CuCl4-2	1.058e-023	6.590e-024	-22.975	-23.181	-0.206
	CuO2-2	5.757e-033	3.585e-033	-32.240	-32.446	-0.206
	Cu(NO2)2	8.000e-036	8.000e-036	-35.097	-35.097	0.000
	CuNH3+2	0.000e+000	0.000e+000	-58.743	-58.945	-0.202
	Cu(NH3)2+2	0.000e+000	0.000e+000	-112.213	-112.415	-0.202
	Cu(NH3)3+2	0.000e+000	0.000e+000	-166.297	-166.499	-0.202
F		9.873e-006				
	AlF+2	7.657e-006	4.805e-006	-5.116	-5.318	-0.202
	HAsO3F-	1.963e-006	1.745e-006	-5.707	-5.758	-0.051
	AlF2+	8.258e-008	7.343e-008	-7.083	-7.134	-0.051
	F-	4.326e-008	3.838e-008	-7.364	-7.416	-0.052
	HF	3.155e-008	3.155e-008	-7.501	-7.501	0.000
	AsO3F-2	7.049e-009	4.389e-009	-8.152	-8.358	-0.206
	FeF+2	5.816e-009	3.650e-009	-8.235	-8.438	-0.202
	MgF+	3.026e-010	2.691e-010	-9.519	-9.570	-0.051
	CaF+	2.138e-010	1.901e-010	-9.670	-9.721	-0.051
	AlF3	3.548e-011	3.548e-011	-10.450	-10.450	0.000
	MnF+	1.632e-011	1.451e-011	-10.787	-10.838	-0.051
	NaF	5.604e-012	5.604e-012	-11.252	-11.252	0.000
	FeF2+	2.549e-012	2.267e-012	-11.594	-11.645	-0.051
	ZnF+	2.387e-012	2.123e-012	-11.622	-11.673	-0.051
	CuF+	5.679e-013	5.050e-013	-12.246	-12.297	-0.051
	H2F2	2.476e-015	2.476e-015	-14.606	-14.606	0.000
	FeF+	1.335e-015	1.187e-015	-14.874	-14.925	-0.051
	AlF4-	3.847e-016	3.421e-016	-15.415	-15.466	-0.051
	HF2-	3.299e-016	2.934e-016	-15.482	-15.533	-0.051
Fe(2)		2.592e-009				
	Fe+2	2.105e-009	1.350e-009	-8.677	-8.870	-0.193
	FeSO4	4.860e-010	4.860e-010	-9.313	-9.313	0.000
	FeCl+	8.145e-013	7.242e-013	-12.089	-12.140	-0.051
	FeF+	1.335e-015	1.187e-015	-14.874	-14.925	-0.051
	FeOH+	8.968e-016	7.974e-016	-15.047	-15.098	-0.051
	FeCl2	2.861e-018	2.861e-018	-17.544	-17.544	0.000
	Fe(OH)2	1.183e-023	1.183e-023	-22.927	-22.927	0.000
	FeCl4-2	7.195e-024	4.480e-024	-23.143	-23.349	-0.206
	Fe(OH)3-	9.889e-031	8.793e-031	-30.005	-30.056	-0.051
	Fe(OH)4-2	0.000e+000	0.000e+000	-41.579	-41.785	-0.206
Fe(3)		1.945e-004				
	FeOH+2	1.218e-004	7.644e-005	-3.914	-4.117	-0.202
	Fe(OH)2+	5.316e-005	4.727e-005	-4.274	-4.325	-0.051
	Fe+3	1.584e-005	6.340e-006	-4.800	-5.198	-0.398
	FeSO4+	1.567e-006	1.393e-006	-5.805	-5.856	-0.051
	Fe2(OH)2+4	9.598e-007	1.573e-007	-6.018	-6.803	-0.786
	Fe(SO4)2-	6.016e-008	5.349e-008	-7.221	-7.272	-0.051
	Fe(OH)3	4.128e-008	4.128e-008	-7.384	-7.384	0.000
	Fe3(OH)4+5	2.511e-008	1.553e-009	-7.600	-8.809	-1.209
	FeNO3+2	1.378e-008	8.649e-009	-7.861	-8.063	-0.202
	FeF+2	5.816e-009	3.650e-009	-8.235	-8.438	-0.202
	FeCl+2	1.239e-009	7.777e-010	-8.907	-9.109	-0.202
	FeCl2+	5.213e-010	4.635e-010	-9.283	-9.334	-0.051
	FeF2+	2.549e-012	2.267e-012	-11.594	-11.645	-0.051
	Fe(OH)4-	2.178e-014	1.937e-014	-13.662	-13.713	-0.051
	FeNO2+2	1.353e-018	8.493e-019	-17.869	-18.071	-0.202
	FeCl4-	3.396e-019	3.020e-019	-18.469	-18.520	-0.051
H(0)		0.000e+000				
	H2	0.000e+000	0.000e+000	-43.024	-43.023	0.001
K		1.601e-004				
	K+	1.572e-004	1.392e-004	-3.804	-3.856	-0.053
	KSO4-	2.870e-006	2.552e-006	-5.542	-5.593	-0.051
	KCl	3.441e-009	3.441e-009	-8.463	-8.463	0.000
	KHSO4	1.205e-009	1.205e-009	-8.919	-8.919	0.000
	KOH	9.013e-016	9.013e-016	-15.045	-15.045	0.000
Mg		6.176e-004				

Mg+2	4.412e-004	2.905e-004	-3.355	-3.537	-0.182
MgSO4	1.762e-004	1.762e-004	-3.754	-3.754	0.000
MgCl+	1.877e-007	1.669e-007	-6.726	-6.777	-0.051
MgF+	3.026e-010	2.691e-010	-9.519	-9.570	-0.051
Mg4(OH)4+4	0.000e+000	0.000e+000	-40.027	-40.813	-0.786
Mn(2)	2.981e-005				
Mn+2	2.191e-005	1.405e-005	-4.659	-4.852	-0.193
MnSO4	7.873e-006	7.873e-006	-5.104	-5.104	0.000
MnCl+	2.477e-008	2.202e-008	-7.606	-7.657	-0.051
MnNO3+	3.416e-009	3.037e-009	-8.466	-8.517	-0.051
MnF+	1.632e-011	1.451e-011	-10.787	-10.838	-0.051
Mn(NO3)2	1.041e-012	1.041e-012	-11.983	-11.983	0.000
MnOH+	7.584e-013	6.743e-013	-12.120	-12.171	-0.051
MnCl3-	2.932e-015	2.607e-015	-14.533	-14.584	-0.051
Mn2OH+3	2.853e-017	1.015e-017	-16.545	-16.993	-0.449
Mn(OH)2	3.091e-021	3.091e-021	-20.510	-20.510	0.000
Mn2(OH)3+	1.820e-024	1.618e-024	-23.740	-23.791	-0.051
Mn(OH)3-	6.089e-030	5.414e-030	-29.215	-29.266	-0.051
Mn(OH)4-2	1.375e-040	0.000e+000	-39.862	-40.067	-0.206
Mn(3)	5.157e-014				
Mn+3	5.157e-014	1.835e-014	-13.288	-13.736	-0.449
Mn(6)	6.861e-031				
MnO4-2	6.861e-031	4.272e-031	-30.164	-30.369	-0.206
Mn(7)	1.038e-023				
MnO4-	1.038e-023	9.212e-024	-22.984	-23.036	-0.052
N(-03)	0.000e+000				
HN3	0.000e+000	0.000e+000	-81.364	-81.364	0.000
N3-	0.000e+000	0.000e+000	-82.744	-82.795	-0.051
ZnN3+	0.000e+000	0.000e+000	-87.709	-87.760	-0.051
Zn(N3)2	0.000e+000	0.000e+000	-169.801	-169.801	0.000
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-50.882	-50.935	-0.054
NH3	0.000e+000	0.000e+000	-56.904	-56.904	0.000
CuNH3+2	0.000e+000	0.000e+000	-58.743	-58.945	-0.202
Zn(NH3)+2	0.000e+000	0.000e+000	-60.056	-60.259	-0.202
NH4SO4-	0.000e+000	0.000e+000	-61.828	-61.879	-0.051
Cu(NH3)2+2	0.000e+000	0.000e+000	-112.213	-112.415	-0.202
Zn(NH3)2+2	0.000e+000	0.000e+000	-114.754	-114.956	-0.202
Cu(NH3)3+2	0.000e+000	0.000e+000	-166.297	-166.499	-0.202
Zn(NH3)3+2	0.000e+000	0.000e+000	-169.452	-169.654	-0.202
Zn(NH3)4+2	0.000e+000	0.000e+000	-224.423	-224.626	-0.202
N(0)	5.326e-007				
N2	2.663e-007	2.663e-007	-6.575	-6.575	0.000
N(3)	1.951e-016				
NO2-	1.071e-016	9.484e-017	-15.970	-16.023	-0.053
HNO2	8.666e-017	8.666e-017	-16.062	-16.062	0.000
FeNO2+2	1.353e-018	8.493e-019	-17.869	-18.071	-0.202
CuNO2+	9.271e-021	8.243e-021	-20.033	-20.084	-0.051
Cu(NO2)2	8.000e-036	8.000e-036	-35.097	-35.097	0.000
N(5)	1.548e-004				
NO3-	1.540e-004	1.364e-004	-3.812	-3.865	-0.053
CaNO3+	7.492e-007	6.661e-007	-6.125	-6.176	-0.051
FeNO3+2	1.378e-008	8.649e-009	-7.861	-8.063	-0.202
HNO3	3.820e-009	3.820e-009	-8.418	-8.418	0.000
MnNO3+	3.416e-009	3.037e-009	-8.466	-8.517	-0.051
Mn(NO3)2	1.041e-012	1.041e-012	-11.983	-11.983	0.000
Na	1.558e-003				
Na+	1.535e-003	1.365e-003	-2.814	-2.865	-0.051
NaSO4-	2.303e-005	2.048e-005	-4.638	-4.689	-0.051
NaCl	1.766e-007	1.766e-007	-6.753	-6.753	0.000
NaF	5.604e-012	5.604e-012	-11.252	-11.252	0.000
NaOH	4.237e-015	4.237e-015	-14.373	-14.373	0.000
NaAlO2	5.142e-019	5.142e-019	-18.289	-18.289	0.000
O(0)	1.410e-006				
O2	7.052e-007	7.075e-007	-6.152	-6.150	0.001
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-128.159	-128.159	0.000

HS-	0.000e+000	0.000e+000	-131.845	-131.897	-0.052
S-2	0.000e+000	0.000e+000	-141.353	-141.552	-0.199
S2-2	0.000e+000	0.000e+000	-233.406	-233.612	-0.206
HAsS2	0.000e+000	0.000e+000	-311.772	-311.772	0.000
S3-2	0.000e+000	0.000e+000	-325.507	-325.713	-0.206
S4-2	0.000e+000	0.000e+000	-417.836	-418.041	-0.206
S5-2	0.000e+000	0.000e+000	-510.381	-510.586	-0.206
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-132.797	-133.003	-0.206
HS2O3-	0.000e+000	0.000e+000	-135.210	-135.261	-0.051
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-120.808	-121.007	-0.199
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-42.175	-42.226	-0.051
H2SO3	0.000e+000	0.000e+000	-43.516	-43.516	0.000
SO2	0.000e+000	0.000e+000	-43.616	-43.616	0.000
SO3-2	0.000e+000	0.000e+000	-45.984	-46.186	-0.202
S2O6-2	0.000e+000	0.000e+000	-59.918	-60.124	-0.206
S3O6-2	0.000e+000	0.000e+000	-154.502	-154.708	-0.206
S4O6-2	0.000e+000	0.000e+000	-233.180	-233.386	-0.206
S5O6-2	0.000e+000	0.000e+000	-340.738	-340.944	-0.206
S(5)	0.000e+000				
S2O5-2	0.000e+000	0.000e+000	-89.077	-89.282	-0.206
S(6)	4.367e-003				
SO4-2	3.647e-003	2.271e-003	-2.438	-2.644	-0.206
CaSO4	3.232e-004	3.232e-004	-3.490	-3.490	0.000
MgSO4	1.762e-004	1.762e-004	-3.754	-3.754	0.000
HSO4-	1.381e-004	1.228e-004	-3.860	-3.911	-0.051
AlSO4+	3.272e-005	2.909e-005	-4.485	-4.536	-0.051
NaSO4-	2.303e-005	2.048e-005	-4.638	-4.689	-0.051
MnSO4	7.873e-006	7.873e-006	-5.104	-5.104	0.000
Al(SO4)2-	5.768e-006	5.129e-006	-5.239	-5.290	-0.051
KSO4-	2.870e-006	2.552e-006	-5.542	-5.593	-0.051
ZnSO4	1.868e-006	1.868e-006	-5.729	-5.729	0.000
FeSO4+	1.567e-006	1.393e-006	-5.805	-5.856	-0.051
CuSO4	4.319e-007	4.319e-007	-6.365	-6.365	0.000
Fe(SO4)2-	6.016e-008	5.349e-008	-7.221	-7.272	-0.051
KHSO4	1.205e-009	1.205e-009	-8.919	-8.919	0.000
FeSO4	4.860e-010	4.860e-010	-9.313	-9.313	0.000
H2SO4	6.205e-011	6.205e-011	-10.207	-10.207	0.000
NH4SO4-	0.000e+000	0.000e+000	-61.828	-61.879	-0.051
S(7)	1.401e-037				
S2O8-2	7.006e-038	4.363e-038	-37.154	-37.360	-0.206
S(8)	6.312e-027				
HSO5-	6.312e-027	5.613e-027	-26.200	-26.251	-0.051
Zn	7.979e-006				
Zn+2	6.105e-006	3.915e-006	-5.214	-5.407	-0.193
ZnSO4	1.868e-006	1.868e-006	-5.729	-5.729	0.000
ZnCl+	5.446e-009	4.842e-009	-8.264	-8.315	-0.051
ZnOH+	9.018e-012	8.018e-012	-11.045	-11.096	-0.051
ZnCl2	4.164e-012	4.164e-012	-11.380	-11.380	0.000
ZnF+	2.387e-012	2.123e-012	-11.622	-11.673	-0.051
Zn(OH)Cl	1.546e-013	1.546e-013	-12.811	-12.811	0.000
ZnCl3-	1.904e-015	1.693e-015	-14.720	-14.771	-0.051
Zn(OH)2	6.412e-017	6.412e-017	-16.193	-16.193	0.000
ZnCl4-2	1.517e-017	9.447e-018	-16.819	-17.025	-0.206
Zn(OH)3-	4.174e-025	3.712e-025	-24.379	-24.430	-0.051
Zn(OH)4-2	1.898e-034	1.182e-034	-33.722	-33.928	-0.206
ZnClO4+	5.782e-036	5.141e-036	-35.238	-35.289	-0.051
Zn(NH3)+2	0.000e+000	0.000e+000	-60.056	-60.259	-0.202
ZnN3+	0.000e+000	0.000e+000	-87.709	-87.760	-0.051
Zn(NH3)2+2	0.000e+000	0.000e+000	-114.754	-114.956	-0.202
Zn(NH3)3+2	0.000e+000	0.000e+000	-169.452	-169.654	-0.202
Zn(N3)2	0.000e+000	0.000e+000	-169.801	-169.801	0.000
Zn(NH3)4+2	0.000e+000	0.000e+000	-224.423	-224.626	-0.202

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

Phase	SI	log IAP	log KT	
Al	-140.39	9.52	149.91	Al
Al(g)	-191.09	9.52	200.62	Al
Al2(SO4)3	-36.63	-17.74	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-19.29	-17.74	1.56	Al2(SO4)3:6H2O
Alabandite	-133.06	-133.48	-0.42	MnS
AlF3	-9.88	-27.15	-17.27	AlF3
Alum-K	-9.08	-14.05	-4.97	KAl(SO4)2:12H2O
Alunite	-3.75	-4.22	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.31	-5.66	-4.35	CaSO4
Antarcticite	-13.37	-9.28	4.09	CaCl2:6H2O
Antlerite	-16.53	-7.80	8.73	Cu3(SO4)(OH)4
Aphthitalite	-15.83	-19.72	-3.89	NaK3(SO4)2
Arcanite	-8.51	-10.36	-1.84	K2SO4
Arsenolite	-123.99	-143.83	-19.84	As2O3
Arsenopyrite	-252.69	-267.13	-14.45	FeAsS
As	-109.99	-67.30	42.68	As
As2O5	-91.05	-88.92	2.14	As2O5
As4O6(cubi)	-247.84	-287.66	-39.82	As4O6
As4O6(mono)	-247.61	-287.66	-40.05	As4O6
Atacamite	-25.23	-10.96	14.26	Cu4Cl2(OH)6
Bassanite	-1.95	-5.66	-3.71	CaSO4:0.5H2O
Birnessite	-16.74	-102.29	-85.55	Mn8O14:5H2O
Bischofite	-14.20	-9.80	4.39	MgCl2:6H2O
Bixbyite	-6.88	-7.85	-0.96	Mn2O3
Bloedite	-12.08	-14.55	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-2.64	4.91	7.55	AlO2H
Bornite	-507.05	-609.58	-102.53	Cu5FeS4
Brochantite	-22.76	-7.34	15.42	Cu4(SO4)(OH)6
Brucite	-13.28	3.01	16.28	Mg(OH)2
Ca	-133.23	6.61	139.83	Ca
Ca(g)	-158.47	6.61	165.07	Ca
Ca2Al2O5:8H2O	-42.68	16.88	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-32.04	-5.75	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-96.13	-78.32	17.80	Ca3(AsO4)2
Ca3Al2O6	-92.62	20.42	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-107.30	33.18	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-83.31	23.95	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-79.73	23.95	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-67.01	1.32	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-33.55	13.35	46.91	CaAl2O4
CaAl2O4:10H2O	-24.64	13.35	37.99	CaAl2O4:10H2O
CaAl4O7	-45.41	23.18	68.59	CaAl4O7
Carnallite	-21.06	-16.79	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-2.12	-5.66	-3.54	CaSO4:0.5H2O
Chalcanthite	-6.10	-8.73	-2.63	CuSO4:5H2O
Chalcocite	-133.95	-168.69	-34.74	Cu2S
Chalcocyanite	-11.64	-8.72	2.91	CuSO4
Chalcopyrite	-239.60	-272.20	-32.60	CuFeS2
Chloromagnesite	-31.62	-9.80	21.82	MgCl2
Cl2(g)	-18.88	-15.88	2.99	Cl2
Claudetite	-124.04	-143.83	-19.80	As2O3
Corundum	-8.47	9.82	18.29	Al2O3
Covellite	-111.85	-134.71	-22.86	CuS
Cu	-27.96	3.54	31.50	Cu
Cu(g)	-80.12	3.54	83.66	Cu
CuCl2	-16.07	-12.35	3.72	CuCl2
CuF	-34.53	-27.45	7.08	CuF
CuF2	-20.29	-20.91	-0.62	CuF2
CuF2:2H2O	-16.36	-20.91	-4.55	CuF2:2H2O
Cuprite	-31.62	-33.52	-1.91	Cu2O
Delafossite	-5.71	-12.15	-6.44	CuFeO2
Diaspore	-2.24	4.91	7.15	AlHO2
Epsomite	-4.22	-6.18	-1.96	MgSO4:7H2O
Ettringite	-59.01	3.45	62.46	Ca6Al2(SO4)3(OH)12:26H2O

F2(g)	-80.16	-24.45	55.71	F2
Fe	-58.27	0.75	59.02	Fe
Fe(OH)2	-16.22	-2.33	13.89	Fe(OH)2
Fe(OH)3	-1.02	4.62	5.64	Fe(OH)3
Fe2(SO4)3	-21.37	-18.33	3.05	Fe2(SO4)3
FeF2	-21.28	-23.70	-2.42	FeF2
FeF3	-8.19	-27.45	-19.26	FeF3
FeO	-15.85	-2.33	13.52	FeO
Ferrite-Ca	-8.73	12.76	21.50	CaFe2O4
Ferrite-Cu	-0.59	9.69	10.28	CuFe2O4
Ferrite-Dicalcium	-40.50	16.29	56.80	Ca2Fe2O5
Ferrite-Mg	-8.78	12.24	21.02	MgFe2O4
Ferrite-Zn	-1.33	10.37	11.70	ZnFe2O4
FeSO4	-14.12	-11.51	2.61	FeSO4
Fluorite	-7.78	-17.84	-10.07	CaF2
Gibbsite	-2.83	4.91	7.74	Al(OH)3
Glauberite	-8.56	-14.03	-5.47	Na2Ca(SO4)2
Goethite	4.09	4.62	0.53	FeOOH
Gypsum	-1.12	-5.66	-4.53	CaSO4:2H2O
H2(g)	-39.92	-43.02	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-127.18	-135.17	-7.99	H2S
Halite	-7.56	-6.00	1.56	NaCl
Hausmannite	-16.30	-6.15	10.14	Mn3O4
HCl(g)	-12.71	-6.40	6.30	HCl
Hematite	9.16	9.23	0.08	Fe2O3
Hercynite	-21.31	7.50	28.80	FeAl2O4
Hexahydrate	-4.45	-6.18	-1.73	MgSO4:6H2O
Hydrophilite	-21.02	-9.28	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	4.30	-5.11	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	1.33	-4.12	-5.45	NaFe3(SO4)2(OH)6
K	-70.02	0.95	70.98	K
K(g)	-80.63	0.95	81.58	K
K2O	-85.21	-1.17	84.04	K2O
K3H(SO4)2	-16.50	-20.13	-3.62	K3H(SO4)2
Kainite	-12.86	-13.17	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-17.32	-14.05	3.27	KAl(SO4)2
Katoite	-58.53	20.42	78.94	Ca3Al2H12O12
Kieserite	-5.91	-6.18	-0.27	MgSO4:H2O
KMgCl3	-38.04	-16.79	21.25	KMgCl3
KMgCl3:2H2O	-30.75	-16.79	13.96	KMgCl3:2H2O
Lammerite	-89.09	-87.53	1.55	Cu3(AsO4)2
Lawrencite	-24.19	-15.14	9.05	FeCl2
Leonite	-12.43	-16.54	-4.11	K2Mg(SO4)2:4H2O
Lime	-29.04	3.53	32.57	CaO
Magnetite	-3.51	6.90	10.42	Fe3O4
Manganite	-3.76	-3.92	-0.16	MnO(OH)
Manganosite	-16.23	1.69	17.92	MnO
Mayenite	-383.02	111.13	494.15	Ca12Al14O33
Melanterite	-9.12	-11.51	-2.40	FeSO4:7H2O
Mercallite	-8.33	-9.77	-1.44	KHSO4
Mg	-116.44	6.08	122.52	Mg
Mg(g)	-136.16	6.08	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.62	-5.43	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-13.89	-4.68	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.53	-9.80	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.10	-9.80	7.30	MgCl2:4H2O
MgCl2:H2O	-25.88	-9.80	16.07	MgCl2:H2O
MgOHCl	-19.29	-3.40	15.89	MgOHCl
MgSO4	-11.01	-6.18	4.83	MgSO4
Mirabilite	-7.22	-8.37	-1.15	Na2SO4:10H2O
Misenite	-57.91	-68.99	-11.08	K8H6(SO4)7
Mn	-78.17	4.77	82.93	Mn
Mn(OH)2(am)	-13.62	1.69	15.31	Mn(OH)2
Mn(OH)3	-10.26	-3.92	6.34	Mn(OH)3
MnCl2:2H2O	-15.12	-11.12	4.00	MnCl2:2H2O

MnCl2:4H2O	-13.87	-11.12	2.75	MnCl2:4H2O
MnCl2:H2O	-16.66	-11.12	5.54	MnCl2:H2O
MnO2 (gamma)	-1.48	-17.61	-16.13	MnO2
MnSO4	-10.10	-7.50	2.61	MnSO4
Molysite	-28.07	-14.60	13.47	FeCl3
N2(g)	-3.40	-6.57	-3.18	N2
Na	-65.43	1.94	67.37	Na
Na(g)	-78.92	1.94	80.86	Na
Na2O	-66.60	0.81	67.42	Na2O
Na3H(SO4)2	-16.26	-17.15	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.51	-22.40	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-14.86	5.02	19.88	NaFeO2
Nantokite	-16.40	-23.17	-6.77	CuCl
NH3(g)	-58.70	-56.90	1.80	NH3
Niter	-7.50	-7.72	-0.22	KNO3
NO(g)	-18.49	-17.76	0.74	NO
NO2(g)	-13.95	-5.60	8.35	NO2
O2(g)	-3.26	-6.15	-2.89	O2
Orpiment	-469.85	-549.34	-79.49	As2S3
Oxychloride-Mg	-26.23	-0.39	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.79	-6.18	-1.39	MgSO4:5H2O
Periclase	-18.32	3.01	21.33	MgO
Picromerite	-12.10	-16.54	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-13.54	-27.85	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-19.02	3.53	22.55	Ca(OH)2
Pyrite	-216.47	-241.17	-24.70	FeS2
Pyrolusite	0.05	-17.61	-17.66	MnO2
Pyrrhotite	-133.76	-137.50	-3.74	FeS
Realgar	-190.86	-251.13	-60.28	AsS
S	-93.13	-138.24	-45.11	S
S2(g)	-200.16	-207.35	-7.19	S2
Scacchite	-19.86	-11.12	8.74	MnCl2
Sellaite	-8.93	-18.37	-9.44	MgF2
SO2(g)	-43.79	-43.62	0.18	SO2
Sphalerite	-122.56	-134.03	-11.47	ZnS
Spinel	-24.78	12.83	37.61	Al2MgO4
Starkeyite	-5.18	-6.18	-1.00	MgSO4:4H2O
Sylvite	-7.82	-6.99	0.83	KCl
Syngenite	-8.41	-16.01	-7.60	K2Ca(SO4)2:H2O
Tachyhydrate	-46.03	-28.88	17.14	Mg2CaCl6:12H2O
Tenorite	-7.19	0.46	7.65	CuO
Thenardite	-8.02	-8.37	-0.36	Na2SO4
Todorokite	-14.62	-60.45	-45.82	Mn7O12:3H2O
Troilite	-133.65	-137.50	-3.84	FeS
Wurtzite	-124.86	-134.03	-9.17	ZnS
Wustite	-13.87	-1.47	12.40	Fe.947O
Zincite	-10.06	1.14	11.20	ZnO
Zn	-64.58	4.21	68.79	Zn
Zn(ClO4)2:6H2O	-73.36	-67.72	5.63	Zn(ClO4)2:6H2O
Zn(g)	-81.20	4.21	85.41	Zn
Zn(NO3)2:6H2O	-16.54	-13.14	3.40	Zn(NO3)2:6H2O
Zn(OH)2(beta)	-10.80	1.14	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-10.52	1.14	11.66	Zn(OH)2
Zn(OH)2(gamma)	-10.75	1.14	11.88	Zn(OH)2
Zn2(OH)3Cl	-19.43	-4.13	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-14.50	-6.92	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-94.82	-85.51	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-34.06	-14.97	19.09	Zn3O(SO4)2
Zn5(NO3)2(OH)8	-51.26	-8.60	42.67	Zn5(NO3)2(OH)8
ZnCl2	-18.75	-11.67	7.08	ZnCl2
ZnCl2(NH3)2	-118.47	-125.48	-7.01	ZnCl2(NH3)2
ZnCl2(NH3)4	-232.58	-239.29	-6.71	ZnCl2(NH3)4
ZnCl2(NH3)6	-348.35	-353.10	-4.74	ZnCl2(NH3)6
ZnF2	-19.75	-20.24	-0.49	ZnF2
ZnSO4	-11.58	-8.05	3.53	ZnSO4
ZnSO4:6H2O	-6.35	-8.05	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-6.17	-8.05	-1.88	ZnSO4:7H2O

ZnSO4:H2O            -7.50    -8.05    -0.55    ZnSO4:H2O

-----  
End of simulation.  
-----

-----  
Reading input data for simulation 2.  
-----

-----  
End of run.  
-----