
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 3
temp 25
pH 3.07
pe 17
redox pe
units mg/l
density 1
Cl 40.91
S(6) 1264
Al 21.6
As 3.82
Ca 124.8
Cu 40.91
Fe 41.51
K 35.01
Mg 13.42
Mn 24.26
Na 20.89
Zn 9.71
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 3

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

Elements	Molality	Moles
Al	8.019e-004	8.019e-004
As	5.107e-005	5.107e-005
Ca	3.119e-003	3.119e-003
Cl	1.156e-003	1.156e-003
Cu	6.448e-004	6.448e-004
Fe	7.445e-004	7.445e-004
K	8.969e-004	8.969e-004
Mg	5.531e-004	5.531e-004
Mn	4.423e-004	4.423e-004
Na	9.102e-004	9.102e-004
S(6)	1.318e-002	1.318e-002
Zn	1.487e-004	1.487e-004

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

```

              pH = 3.070
              pe = 17.000
      Activity of water = 1.000
      Ionic strength = 3.218e-002
      Mass of water (kg) = 1.000e+000
      Total alkalinity (eq/kg) = -2.266e-003
      Total carbon (mol/kg) = 0.000e+000
      Total CO2 (mol/kg) = 0.000e+000
      Temperature (deg C) = 25.000
      Electrical balance (eq) = -1.053e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -30.80
              Iterations = 8
              Total H = 1.110530e+002
              Total O = 5.557899e+001

```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	9.741e-004	8.511e-004	-3.011	-3.070	-0.059
OH-	1.344e-011	1.132e-011	-10.872	-10.946	-0.075
H2O	5.553e+001	9.996e-001	1.744	-0.000	0.000
Al	8.019e-004				
AlSO4+	4.097e-004	3.464e-004	-3.388	-3.460	-0.073
Al+3	2.262e-004	6.552e-005	-3.646	-4.184	-0.538
Al(SO4)2-	1.643e-004	1.389e-004	-3.784	-3.857	-0.073
AlOH+2	1.676e-006	8.621e-007	-5.776	-6.064	-0.289
Al(OH)2+	2.781e-009	2.351e-009	-8.556	-8.629	-0.073
Al2(OH)2+4	1.546e-009	1.208e-010	-8.811	-9.918	-1.107
HALO2	4.020e-012	4.020e-012	-11.396	-11.396	0.000

Al3(OH)4+5	3.475e-013	7.050e-015	-12.459	-14.152	-1.693
AlO2-	1.914e-015	1.618e-015	-14.718	-14.791	-0.073
NaAlO2	2.296e-019	2.296e-019	-18.639	-18.639	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-51.563	-54.881	-3.319
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-151.256	-151.256	0.000
As(3)	2.419e-026				
HAsO2	1.291e-026	1.291e-026	-25.889	-25.889	0.000
As(OH)3	1.128e-026	1.128e-026	-25.948	-25.948	0.000
H2AsO3-	9.588e-033	8.107e-033	-32.018	-32.091	-0.073
AsO2-	9.170e-033	7.753e-033	-32.038	-32.111	-0.073
AsO2OH-2	1.838e-040	0.000e+000	-39.736	-40.031	-0.296
As(5)	5.107e-005				
H2AsO4-	4.531e-005	3.831e-005	-4.344	-4.417	-0.073
H3AsO4	5.743e-006	5.743e-006	-5.241	-5.241	0.000
HAsO4-2	1.476e-008	7.471e-009	-7.831	-8.127	-0.296
AsO4-3	1.045e-016	2.252e-017	-15.981	-16.647	-0.667
Ca	3.119e-003				
Ca+2	2.219e-003	1.192e-003	-2.654	-2.924	-0.270
CaSO4	8.999e-004	8.999e-004	-3.046	-3.046	0.000
CaCl+	2.891e-007	2.445e-007	-6.539	-6.612	-0.073
CaCl2	2.781e-010	2.781e-010	-9.556	-9.556	0.000
CaOH+	2.340e-013	1.978e-013	-12.631	-12.704	-0.073
Cl(-1)	1.156e-003				
Cl-	1.154e-003	9.673e-004	-2.938	-3.014	-0.077
CuCl+	6.621e-007	5.598e-007	-6.179	-6.252	-0.073
MnCl+	3.434e-007	2.903e-007	-6.464	-6.537	-0.073
CaCl+	2.891e-007	2.445e-007	-6.539	-6.612	-0.073
HCl	1.849e-007	1.849e-007	-6.733	-6.733	0.000
MgCl+	1.568e-007	1.326e-007	-6.805	-6.878	-0.073
NaCl	1.265e-007	1.265e-007	-6.898	-6.898	0.000
ZnCl+	9.697e-008	8.198e-008	-7.013	-7.086	-0.073
KCl	2.345e-008	2.345e-008	-7.630	-7.630	0.000
FeCl+2	9.839e-009	5.061e-009	-8.007	-8.296	-0.289
FeCl2+	4.688e-009	3.963e-009	-8.329	-8.402	-0.073
CuCl2	2.852e-010	2.852e-010	-9.545	-9.545	0.000
CaCl2	2.781e-010	2.781e-010	-9.556	-9.556	0.000
ZnCl2	9.263e-011	9.263e-011	-10.033	-10.033	0.000
FeCl+	2.730e-012	2.308e-012	-11.564	-11.637	-0.073
Zn(OH)Cl	1.646e-012	1.646e-012	-11.783	-11.783	0.000
MnCl3-	7.018e-014	5.934e-014	-13.154	-13.227	-0.073
ZnCl3-	5.853e-014	4.948e-014	-13.233	-13.306	-0.073
ZnCl4-2	7.166e-016	3.628e-016	-15.145	-15.440	-0.296
FeCl2	1.198e-017	1.198e-017	-16.922	-16.922	0.000
FeCl4-	5.273e-018	4.458e-018	-17.278	-17.351	-0.073
CuCl2-	8.492e-020	7.180e-020	-19.071	-19.144	-0.073
CuCl4-2	9.890e-021	5.007e-021	-20.005	-20.300	-0.296
CuCl3-2	8.809e-022	4.460e-022	-21.055	-21.351	-0.296
FeCl4-2	6.397e-023	3.239e-023	-22.194	-22.490	-0.296
Cl(1)	3.282e-017				
HClO	3.282e-017	3.282e-017	-16.484	-16.484	0.000
ClO-	1.230e-021	1.040e-021	-20.910	-20.983	-0.073
Cl(3)	3.477e-032				
HClO2	1.792e-032	1.792e-032	-31.747	-31.747	0.000
ClO2-	1.685e-032	1.424e-032	-31.773	-31.846	-0.073
Cl(5)	1.650e-029				
ClO3-	1.650e-029	1.389e-029	-28.783	-28.857	-0.075
Cl(7)	8.035e-031				
ClO4-	8.027e-031	6.758e-031	-30.095	-30.170	-0.075
ZnClO4+	7.628e-034	6.449e-034	-33.118	-33.191	-0.073
Cu(1)	1.456e-018				
Cu+	1.370e-018	1.158e-018	-17.863	-17.936	-0.073
CuCl2-	8.492e-020	7.180e-020	-19.071	-19.144	-0.073
CuCl3-2	8.809e-022	4.460e-022	-21.055	-21.351	-0.296
Cu(2)	6.448e-004				
Cu+2	3.937e-004	2.116e-004	-3.405	-3.675	-0.270
CuSO4	2.504e-004	2.504e-004	-3.601	-3.601	0.000

CuCl+	6.621e-007	5.598e-007	-6.179	-6.252	-0.073
CuOH+	1.516e-008	1.282e-008	-7.819	-7.892	-0.073
CuCl2	2.852e-010	2.852e-010	-9.545	-9.545	0.000
CuCl4-2	9.890e-021	5.007e-021	-20.005	-20.300	-0.296
CuO2-2	2.825e-031	1.430e-031	-30.549	-30.845	-0.296
Fe(2)	8.779e-009				
Fe+2	6.095e-009	3.275e-009	-8.215	-8.485	-0.270
FeSO4	2.682e-009	2.682e-009	-8.572	-8.572	0.000
FeCl+	2.730e-012	2.308e-012	-11.564	-11.637	-0.073
FeOH+	1.439e-015	1.216e-015	-14.842	-14.915	-0.073
FeCl2	1.198e-017	1.198e-017	-16.922	-16.922	0.000
FeCl4-2	6.397e-023	3.239e-023	-22.194	-22.490	-0.296
Fe(OH)2	1.135e-023	1.135e-023	-22.945	-22.945	0.000
Fe(OH)3-	6.276e-031	5.306e-031	-30.202	-30.275	-0.073
Fe(OH)4-2	0.000e+000	0.000e+000	-41.910	-42.205	-0.296
Fe(3)	7.445e-004				
FeOH+2	4.629e-004	2.381e-004	-3.335	-3.623	-0.289
Fe(OH)2+	1.095e-004	9.261e-005	-3.960	-4.033	-0.073
Fe+3	1.084e-004	3.140e-005	-3.965	-4.503	-0.538
Fe2(OH)2+4	1.953e-005	1.526e-006	-4.709	-5.816	-1.107
FeSO4+	1.857e-005	1.570e-005	-4.731	-4.804	-0.073
Fe(SO4)2-	1.622e-006	1.371e-006	-5.790	-5.863	-0.073
Fe3(OH)4+5	1.455e-006	2.953e-008	-5.837	-7.530	-1.693
Fe(OH)3	5.087e-008	5.087e-008	-7.294	-7.294	0.000
FeCl+2	9.839e-009	5.061e-009	-8.007	-8.296	-0.289
FeCl2+	4.688e-009	3.963e-009	-8.329	-8.402	-0.073
Fe(OH)4-	1.775e-014	1.501e-014	-13.751	-13.824	-0.073
FeCl4-	5.273e-018	4.458e-018	-17.278	-17.351	-0.073
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-43.244	-43.240	0.003
K	8.969e-004				
K+	8.613e-004	7.219e-004	-3.065	-3.141	-0.077
KSO4-	3.561e-005	3.011e-005	-4.448	-4.521	-0.073
KCl	2.345e-008	2.345e-008	-7.630	-7.630	0.000
KHSO4	2.261e-008	2.261e-008	-7.646	-7.646	0.000
KOH	2.940e-015	2.940e-015	-14.532	-14.532	0.000
Mg	5.531e-004				
Mg+2	3.107e-004	1.755e-004	-3.508	-3.756	-0.248
MgSO4	2.422e-004	2.422e-004	-3.616	-3.616	0.000
MgCl+	1.568e-007	1.326e-007	-6.805	-6.878	-0.073
Mg4(OH)4+4	0.000e+000	0.000e+000	-41.386	-42.493	-1.107
Mn(2)	4.423e-004				
Mn+2	2.623e-004	1.410e-004	-3.581	-3.851	-0.270
MnSO4	1.797e-004	1.797e-004	-3.746	-3.746	0.000
MnCl+	3.434e-007	2.903e-007	-6.464	-6.537	-0.073
MnOH+	5.033e-012	4.255e-012	-11.298	-11.371	-0.073
MnCl3-	7.018e-014	5.934e-014	-13.154	-13.227	-0.073
Mn2OH+3	2.782e-015	6.427e-016	-14.556	-15.192	-0.636
Mn(OH)2	1.227e-020	1.227e-020	-19.911	-19.911	0.000
Mn2(OH)3+	4.793e-023	4.052e-023	-22.319	-22.392	-0.073
Mn(OH)3-	1.598e-029	1.351e-029	-28.796	-28.869	-0.073
Mn(OH)4-2	2.655e-040	1.344e-040	-39.576	-39.872	-0.296
Mn(3)	1.627e-012				
Mn+3	1.627e-012	3.760e-013	-11.789	-12.425	-0.636
Mn(6)	3.607e-030				
MnO4-2	3.607e-030	1.826e-030	-29.443	-29.738	-0.296
Mn(7)	9.551e-023				
MnO4-	9.551e-023	8.041e-023	-22.020	-22.095	-0.075
Na	9.102e-004				
Na+	8.800e-004	7.440e-004	-3.056	-3.128	-0.073
NaSO4-	3.004e-005	2.540e-005	-4.522	-4.595	-0.073
NaCl	1.265e-007	1.265e-007	-6.898	-6.898	0.000
NaOH	1.452e-015	1.452e-015	-14.838	-14.838	0.000
NaAlO2	2.296e-019	2.296e-019	-18.639	-18.639	0.000
O(0)	3.822e-006				
O2	1.911e-006	1.926e-006	-5.719	-5.715	0.003
S(6)	1.318e-002				

SO4-2	1.020e-002	5.166e-003	-1.991	-2.287	-0.296
CaSO4	8.999e-004	8.999e-004	-3.046	-3.046	0.000
HSO4-	5.254e-004	4.442e-004	-3.280	-3.352	-0.073
AlSO4+	4.097e-004	3.464e-004	-3.388	-3.460	-0.073
CuSO4	2.504e-004	2.504e-004	-3.601	-3.601	0.000
MgSO4	2.422e-004	2.422e-004	-3.616	-3.616	0.000
MnSO4	1.797e-004	1.797e-004	-3.746	-3.746	0.000
Al(SO4)2-	1.643e-004	1.389e-004	-3.784	-3.857	-0.073
ZnSO4	5.476e-005	5.476e-005	-4.262	-4.262	0.000
KSO4-	3.561e-005	3.011e-005	-4.448	-4.521	-0.073
NaSO4-	3.004e-005	2.540e-005	-4.522	-4.595	-0.073
FeSO4+	1.857e-005	1.570e-005	-4.731	-4.804	-0.073
Fe(SO4)2-	1.622e-006	1.371e-006	-5.790	-5.863	-0.073
KHSO4	2.261e-008	2.261e-008	-7.646	-7.646	0.000
FeSO4	2.682e-009	2.682e-009	-8.572	-8.572	0.000
H2SO4	3.567e-010	3.567e-010	-9.448	-9.448	0.000
Zn	1.487e-004				
Zn+2	9.388e-005	5.045e-005	-4.027	-4.297	-0.270
ZnSO4	5.476e-005	5.476e-005	-4.262	-4.262	0.000
ZnCl+	9.697e-008	8.198e-008	-7.013	-7.086	-0.073
ZnCl2	9.263e-011	9.263e-011	-10.033	-10.033	0.000
ZnOH+	7.685e-011	6.498e-011	-10.114	-10.187	-0.073
Zn(OH)Cl	1.646e-012	1.646e-012	-11.783	-11.783	0.000
ZnCl3-	5.853e-014	4.948e-014	-13.233	-13.306	-0.073
ZnCl4-2	7.166e-016	3.628e-016	-15.145	-15.440	-0.296
Zn(OH)2	3.268e-016	3.268e-016	-15.486	-15.486	0.000
Zn(OH)3-	1.407e-024	1.190e-024	-23.852	-23.925	-0.073
ZnClO4+	7.628e-034	6.449e-034	-33.118	-33.191	-0.073
Zn(OH)4-2	4.705e-034	2.382e-034	-33.327	-33.623	-0.296

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

Phase	SI	log IAP	log KT	
Al	-140.60	9.31	149.91	Al
Al(g)	-191.31	9.31	200.62	Al
Al2(SO4)3	-34.13	-15.23	18.90	Al2(SO4)3
Al2(SO4)3·6H2O	-16.78	-15.23	1.56	Al2(SO4)3·6H2O
Alum-K	-6.93	-11.90	-4.97	KAl(SO4)2·12H2O
Alunite	-1.38	-1.85	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.86	-5.21	-4.35	CaSO4
Antarcticite	-13.05	-8.95	4.09	CaCl2·6H2O
Antlerite	-9.76	-1.03	8.73	Cu3(SO4)(OH)4
Aphthitalite	-13.24	-17.13	-3.89	NaK3(SO4)2
Arcanite	-6.73	-8.57	-1.84	K2SO4
Arsenolite	-50.48	-70.32	-19.84	As2O3
As	-73.56	-30.87	42.68	As
As2O5	-17.11	-14.97	2.14	As2O5
As4O6(cubi)	-100.82	-140.64	-39.82	As4O6
As4O6(mono)	-100.59	-140.64	-40.05	As4O6
Atacamite	-16.57	-2.31	14.26	Cu4Cl2(OH)6
Bassanite	-1.50	-5.21	-3.71	CaSO4·0.5H2O
Birnessite	-10.64	-96.19	-85.55	Mn8O14·5H2O
Bischofite	-14.18	-9.79	4.39	MgCl2·6H2O
Bixbyite	-5.47	-6.43	-0.96	Mn2O3
Bloedite	-12.11	-14.59	-2.48	Na2Mg(SO4)2·4H2O
Boehmite	-2.52	5.03	7.55	AlO2H
Brochantite	-13.99	1.43	15.42	Cu4(SO4)(OH)6
Brucite	-13.90	2.38	16.28	Mg(OH)2
Ca	-133.76	6.07	139.83	Ca
Ca(g)	-159.00	6.07	165.07	Ca
Ca2Al2O5·8H2O	-43.09	16.48	59.57	Ca2Al2O5·8H2O
Ca2Cl2(OH)2·H2O	-32.03	-5.74	26.29	Ca2Cl2(OH)2·H2O
Ca3(AsO4)2	-23.13	-5.32	17.80	Ca3(AsO4)2
Ca3Al2O6	-93.33	19.70	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-108.15	32.33	140.48	Ca4Al2Fe2O10
Ca4Al2O7·13H2O	-84.34	22.92	107.25	Ca4Al2O7·13H2O

Ca4Al2O7:19H2O	-80.77	22.91	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-67.63	0.69	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-33.64	13.27	46.91	CaAl2O4
CaAl2O4:10H2O	-24.73	13.27	37.99	CaAl2O4:10H2O
CaAl4O7	-45.27	23.32	68.59	CaAl4O7
Carnallite	-20.21	-15.94	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.68	-5.21	-3.54	CaSO4:0.5H2O
Chalcanthite	-3.33	-5.96	-2.63	CuSO4:5H2O
Chalcocyanite	-8.87	-5.96	2.91	CuSO4
Chloromagnesite	-31.60	-9.78	21.82	MgCl2
Cl2(g)	-18.02	-15.03	2.99	Cl2
Claudetite	-50.53	-70.32	-19.80	As2O3
Corundum	-8.24	10.05	18.29	Al2O3
Cu	-26.17	5.32	31.50	Cu
Cu(g)	-78.33	5.32	83.66	Cu
CuCl2	-13.42	-9.70	3.72	CuCl2
Cuprite	-27.83	-29.73	-1.91	Cu2O
Delafossite	-3.72	-10.16	-6.44	CuFeO2
Diaspore	-2.12	5.03	7.15	AlHO2
Epsomite	-4.08	-6.04	-1.96	MgSO4:7H2O
Ettringite	-58.40	4.06	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-58.50	0.51	59.02	Fe
Fe(OH)2	-16.24	-2.35	13.89	Fe(OH)2
Fe(OH)3	-0.93	4.71	5.64	Fe(OH)3
Fe2(SO4)3	-18.91	-15.87	3.05	Fe2(SO4)3
FeO	-15.87	-2.34	13.52	FeO
Ferrite-Ca	-8.87	12.63	21.50	CaFe2O4
Ferrite-Cu	1.60	11.88	10.28	CuFe2O4
Ferrite-Dicalcium	-40.95	15.85	56.80	Ca2Fe2O5
Ferrite-Mg	-9.22	11.80	21.02	MgFe2O4
Ferrite-Zn	-0.44	11.26	11.70	ZnFe2O4
FeSO4	-13.38	-10.77	2.61	FeSO4
Gibbsite	-2.71	5.03	7.74	Al(OH)3
Glauberite	-8.29	-13.75	-5.47	Na2Ca(SO4)2
Goethite	4.18	4.71	0.53	FeOOH
Gypsum	-0.68	-5.21	-4.53	CaSO4:2H2O
H2(g)	-40.14	-43.24	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.71	-6.14	1.56	NaCl
Hausmannite	-14.29	-4.14	10.14	Mn3O4
HCl(g)	-12.39	-6.08	6.30	HCl
Hematite	9.34	9.41	0.08	Fe2O3
Hercynite	-21.10	7.71	28.80	FeAl2O4
Hexahydrite	-4.32	-6.04	-1.73	MgSO4:6H2O
Hydrophilite	-20.70	-8.95	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	6.61	-2.81	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	2.66	-2.79	-5.45	NaFe3(SO4)2(OH)6
K	-69.62	1.36	70.98	K
K(g)	-80.22	1.36	81.58	K
K2O	-84.18	-0.14	84.04	K2O
K3H(SO4)2	-13.44	-17.07	-3.62	K3H(SO4)2
Kainite	-11.89	-12.20	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-15.17	-11.90	3.27	KAl(SO4)2
Katoite	-59.24	19.70	78.94	Ca3Al2H12O12
Kieserite	-5.78	-6.04	-0.27	MgSO4:H2O
KMgCl3	-37.19	-15.94	21.25	KMgCl3
KMgCl3:2H2O	-29.90	-15.94	13.96	KMgCl3:2H2O
Lammerite	-9.13	-7.58	1.55	Cu3(AsO4)2
Lawrencite	-23.57	-14.51	9.05	FeCl2
Leonite	-10.50	-14.61	-4.11	K2Mg(SO4)2:4H2O
Lime	-29.35	3.22	32.57	CaO
Magnetite	-3.35	7.07	10.42	Fe3O4
Manganite	-3.05	-3.22	-0.16	MnO(OH)
Manganosite	-15.63	2.29	17.92	MnO
Mayenite	-385.19	108.96	494.15	Ca12Al14O33
Melanterite	-8.37	-10.77	-2.40	FeSO4:7H2O

Mercallite	-7.06	-8.50	-1.44	KHSO4
Mg	-117.28	5.24	122.52	Mg
Mg(g)	-137.00	5.24	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.64	-5.45	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-14.06	-4.85	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.52	-9.78	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.09	-9.79	7.30	MgCl2:4H2O
MgCl2:H2O	-25.86	-9.78	16.07	MgCl2:H2O
MgOHCl	-19.59	-3.70	15.89	MgOHCl
MgSO4	-10.87	-6.04	4.83	MgSO4
Mirabilite	-7.39	-8.55	-1.15	Na2SO4:10H2O
Misenite	-48.48	-59.56	-11.08	K8H6(SO4)7
Mn	-77.79	5.15	82.93	Mn
Mn(OH)2(am)	-13.02	2.29	15.31	Mn(OH)2
Mn(OH)3	-9.56	-3.22	6.34	Mn(OH)3
MnCl2:2H2O	-13.88	-9.88	4.00	MnCl2:2H2O
MnCl2:4H2O	-12.63	-9.88	2.75	MnCl2:4H2O
MnCl2:H2O	-15.42	-9.88	5.54	MnCl2:H2O
MnO2(gamma)	-0.67	-16.79	-16.13	MnO2
MnSO4	-8.75	-6.14	2.61	MnSO4
Molysite	-27.02	-13.55	13.47	FeCl3
Na	-66.00	1.37	67.37	Na
Na(g)	-79.49	1.37	80.86	Na
Na2O	-67.53	-0.12	67.42	Na2O
Na3H(SO4)2	-16.14	-17.03	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.40	-22.30	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-15.24	4.65	19.88	NaFeO2
Nantokite	-14.18	-20.95	-6.77	CuCl
O2(g)	-2.82	-5.72	-2.89	O2
Oxychloride-Mg	-27.15	-1.32	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.66	-6.04	-1.39	MgSO4:5H2O
Periclase	-18.94	2.38	21.33	MgO
Picromerite	-10.17	-14.61	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-10.72	-25.03	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-19.33	3.22	22.55	Ca(OH)2
Pyrolusite	0.87	-16.79	-17.66	MnO2
Scacchite	-18.62	-9.88	8.74	MnCl2
Spinel	-25.17	12.44	37.61	Al2MgO4
Starkeyite	-5.04	-6.04	-1.00	MgSO4:4H2O
Sylvite	-6.98	-6.16	0.83	KCl
Syngenite	-6.18	-13.78	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-45.67	-28.52	17.14	Mg2CaCl6:12H2O
Tenorite	-5.18	2.47	7.65	CuO
Thenardite	-8.19	-8.54	-0.36	Na2SO4
Todorokite	-9.35	-55.17	-45.82	Mn7O12:3H2O
Wustite	-13.88	-1.47	12.40	Fe.947O
Zincite	-9.36	1.84	11.20	ZnO
Zn	-64.09	4.70	68.79	Zn
Zn(ClO4)2:6H2O	-70.27	-64.64	5.63	Zn(ClO4)2:6H2O
Zn(g)	-80.71	4.70	85.41	Zn
Zn(OH)2(beta)	-10.09	1.84	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-9.82	1.84	11.66	Zn(OH)2
Zn(OH)2(gamma)	-10.04	1.84	11.88	Zn(OH)2
Zn2(OH)3Cl	-17.69	-2.40	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-12.32	-4.74	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-18.76	-9.44	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-30.42	-11.33	19.09	Zn3O(SO4)2
ZnCl2	-17.40	-10.33	7.08	ZnCl2
ZnSO4	-10.12	-6.58	3.53	ZnSO4
ZnSO4:6H2O	-4.89	-6.58	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-4.71	-6.59	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.03	-6.58	-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 ₃ (SO ₄)(OH) ₄
Aphthitalite	-17.08	-20.97	-3.89	NaK ₃ (SO ₄) ₂
Arcanite	-9.33	-11.17	-1.84	K ₂ SO ₄
Arsenolite	-123.16	-143.00	-19.84	As ₂ O ₃
As	-102.31	-59.63	42.68	As
As ₂ O ₅	-99.91	-97.77	2.14	As ₂ O ₅
As ₄ O ₆ (cubi)	-246.18	-286.01	-39.82	As ₄ O ₆
As ₄ O ₆ (mono)	-245.96	-286.01	-40.05	As ₄ O ₆
Atacamite	-0.77	13.49	14.26	Cu ₄ Cl ₂ (OH) ₆
Bassanite	-2.05	-5.75	-3.71	CaSO ₄ :0.5H ₂ O
Birnessite	15.35	-70.19	-85.55	Mn ₈ O ₁₄ :5H ₂ O
Bischofite	-14.26	-9.87	4.39	MgCl ₂ :6H ₂ O
Bixbyite	3.56	2.60	-0.96	Mn ₂ O ₃
Bloedite	-12.23	-14.71	-2.48	Na ₂ Mg(SO ₄) ₂ :4H ₂ O
Brochantite	1.64	17.06	15.42	Cu ₄ (SO ₄)(OH) ₆
Brucite	-4.64	11.64	16.28	Mg(OH) ₂
Ca	-119.73	20.10	139.83	Ca
Ca(g)	-144.97	20.10	165.07	Ca
Ca ₂ Cl ₂ (OH) ₂ :H ₂ O	-23.42	2.87	26.29	Ca ₂ Cl ₂ (OH) ₂ :H ₂ O
Ca ₃ (AsO ₄) ₂	-79.02	-61.22	17.80	Ca ₃ (AsO ₄) ₂
Ca ₄ Cl ₂ (OH) ₆ :13H ₂ O	-41.09	27.24	68.33	Ca ₄ Cl ₂ (OH) ₆ :13H ₂ O
Carnallite	-21.51	-17.24	4.27	KMgCl ₃ :6H ₂ O
CaSO ₄ :0.5H ₂ O(beta)	-2.22	-5.75	-3.54	CaSO ₄ :0.5H ₂ O
Chalcanthite	-6.56	-9.19	-2.63	CuSO ₄ :5H ₂ O
Chalcocyanite	-12.10	-9.19	2.91	CuSO ₄
Chloromagnesite	-31.68	-9.87	21.82	MgCl ₂
Cl ₂ (g)	-32.42	-29.42	2.99	Cl ₂
Claudetite	-123.21	-143.00	-19.80	As ₂ O ₃
Cu	-14.83	16.67	31.50	Cu
Cu(g)	-66.99	16.67	83.66	Cu
CuCl ₂	-16.48	-12.76	3.72	CuCl ₂
CuF	-25.65	-18.57	7.08	CuF
CuF ₂	-15.67	-16.29	-0.62	CuF ₂
CuF ₂ :2H ₂ O	-11.74	-16.29	-4.55	CuF ₂ :2H ₂ O
Cuprite	-10.20	-12.10	-1.91	Cu ₂ O
Epsomite	-4.34	-6.30	-1.96	MgSO ₄ :7H ₂ O
F ₂ (g)	-88.67	-32.95	55.71	F ₂
Fluorite	-2.78	-12.85	-10.07	CaF ₂
Glauberite	-8.70	-14.17	-5.47	Na ₂ Ca(SO ₄) ₂
Gypsum	-1.22	-5.75	-4.53	CaSO ₄ :2H ₂ O
H ₂ (g)	-35.08	-38.18	-3.10	H ₂
H ₂ O(g)	-1.59	-0.00	1.59	H ₂ O
Halite	-7.55	-5.99	1.56	NaCl
Hausmannite	1.79	11.93	10.14	Mn ₃ O ₄
HCl(g)	-17.06	-10.75	6.30	HCl
Hexahydrite	-4.57	-6.30	-1.73	MgSO ₄ :6H ₂ O
Hydrophilite	-21.07	-9.32	11.75	CaCl ₂
Ice	-0.14	-0.00	0.14	H ₂ O
K	-63.63	7.34	70.98	K
K(g)	-74.24	7.34	81.58	K
K ₂ O	-77.27	6.77	84.04	K ₂ O
K ₃ H(SO ₄) ₂	-22.10	-25.73	-3.62	K ₃ H(SO ₄) ₂
Kainite	-13.36	-13.67	-0.31	KMgClSO ₄ :3H ₂ O
Kieserite	-6.03	-6.30	-0.27	MgSO ₄ :H ₂ O
KMgCl ₃	-38.48	-17.24	21.25	KMgCl ₃
KMgCl ₃ :2H ₂ O	-31.20	-17.24	13.96	KMgCl ₃ :2H ₂ O
Lammerite	-73.08	-71.52	1.55	Cu ₃ (AsO ₄) ₂
Leonite	-13.36	-17.47	-4.11	K ₂ Mg(SO ₄) ₂ :4H ₂ 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 ₄
Mg	-102.96	19.56	122.52	Mg
Mg(g)	-122.69	19.56	142.25	Mg
Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O	-8.58	-3.39	5.20	Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O
Mg _{1.5} SO ₄ (OH)	-9.69	-0.48	9.21	Mg _{1.5} SO ₄ (OH)
MgCl ₂ :2H ₂ O	-22.60	-9.87	12.73	MgCl ₂ :2H ₂ 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 3
 3.000e+000 Solution 2 AS1

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

Elements	Molality	Moles
Al	2.005e-004	8.019e-004
As	1.374e-005	5.494e-005
Ca	2.405e-003	9.621e-003
Cl	8.011e-004	3.204e-003
Cu	1.625e-004	6.502e-004
F	9.873e-006	3.949e-005
Fe	1.861e-004	7.445e-004
K	2.831e-004	1.133e-003
Mg	6.374e-004	2.550e-003
Mn	1.131e-004	4.522e-004
N	1.553e-004	6.214e-004
Na	1.631e-003	6.525e-003
S	5.194e-003	2.078e-002
Zn	3.942e-005	1.577e-004

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

pH	=	3.507	Charge balance
pe	=	16.454	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	1.608e-002	
Mass of water (kg)	=	4.000e+000	
Total alkalinity (eq/kg)	=	-5.652e-004	
Total carbon (mol/kg)	=	0.000e+000	
Total CO2 (mol/kg)	=	0.000e+000	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	-5.542e-003	
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	-7.83	
Iterations	=	58	
Total H	=	4.442049e+002	
Total O	=	2.221872e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	3.465e-004	3.113e-004	-3.460	-3.507	-0.046
OH-	3.519e-011	3.094e-011	-10.454	-10.509	-0.056
H2O	5.553e+001	9.998e-001	1.744	-0.000	0.000
Al	2.005e-004				
AlSO4+	9.457e-005	8.333e-005	-4.024	-4.079	-0.055
Al+3	8.541e-005	3.220e-005	-4.068	-4.492	-0.424
Al(SO4)2-	1.857e-005	1.636e-005	-4.731	-4.786	-0.055
AlOH+2	1.912e-006	1.158e-006	-5.718	-5.936	-0.218
Al(OH)2+	9.803e-009	8.638e-009	-8.009	-8.064	-0.055
Al2(OH)2+4	1.521e-009	2.182e-010	-8.818	-9.661	-0.843
HALO2	4.038e-011	4.038e-011	-10.394	-10.394	0.000
Al3(OH)4+5	9.247e-013	4.677e-014	-12.034	-13.330	-1.296
AlO2-	5.042e-014	4.443e-014	-13.297	-13.352	-0.055
NaAlO2	1.198e-017	1.198e-017	-16.921	-16.921	0.000
AlF+2	3.485e-040	2.111e-040	-39.458	-39.676	-0.218
Al13O4(OH)24+7	0.000e+000	0.000e+000	-42.372	-44.913	-2.541
AlF2+	0.000e+000	0.000e+000	-76.204	-76.259	-0.055
AlF3	0.000e+000	0.000e+000	-114.342	-114.342	0.000
AlF4-	0.000e+000	0.000e+000	-154.071	-154.125	-0.055
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-151.892	-151.892	0.000

As(3)	1.239e-027					
HAsO2	6.609e-028	6.609e-028	-27.180	-27.180	0.000	
As(OH)3	5.778e-028	5.778e-028	-27.238	-27.238	0.000	
H2AsO3-	1.288e-033	1.135e-033	-32.890	-32.945	-0.055	
AsO2-	1.232e-033	1.085e-033	-32.910	-32.964	-0.055	
AsO2OH-2	0.000e+000	0.000e+000	-40.227	-40.448	-0.222	
HAsS2	0.000e+000	0.000e+000	-277.149	-277.149	0.000	
As(5)	1.374e-005					
HAsO3F-	9.811e-006	8.646e-006	-5.008	-5.063	-0.055	
H2AsO4-	3.681e-006	3.244e-006	-5.434	-5.489	-0.055	
H3AsO4	1.779e-007	1.779e-007	-6.750	-6.750	0.000	
AsO3F-2	6.231e-008	3.740e-008	-7.205	-7.427	-0.222	
HAsO4-2	2.881e-009	1.730e-009	-8.540	-8.762	-0.222	
AsO4-3	4.502e-017	1.425e-017	-16.347	-16.846	-0.499	
Ca	2.405e-003					
Ca+2	1.955e-003	1.215e-003	-2.709	-2.916	-0.207	
CaSO4	4.487e-004	4.487e-004	-3.348	-3.348	0.000	
CaNO3+	9.343e-007	8.233e-007	-6.030	-6.084	-0.055	
CaCl+	2.050e-007	1.807e-007	-6.688	-6.743	-0.055	
CaCl2	1.491e-010	1.491e-010	-9.826	-9.826	0.000	
CaOH+	6.252e-013	5.510e-013	-12.204	-12.259	-0.055	
CaF+	0.000e+000	0.000e+000	-44.338	-44.393	-0.055	
Cl(-1)	8.011e-004					
Cl-	8.002e-004	7.019e-004	-3.097	-3.154	-0.057	
CaCl+	2.050e-007	1.807e-007	-6.688	-6.743	-0.055	
MgCl+	1.771e-007	1.560e-007	-6.752	-6.807	-0.055	
NaCl	1.744e-007	1.744e-007	-6.758	-6.758	0.000	
CuCl+	1.616e-007	1.424e-007	-6.792	-6.847	-0.055	
MnCl+	8.574e-008	7.556e-008	-7.067	-7.122	-0.055	
HCl	4.908e-008	4.908e-008	-7.309	-7.309	0.000	
ZnCl+	2.462e-008	2.169e-008	-7.609	-7.664	-0.055	
KCl	5.736e-009	5.736e-009	-8.241	-8.241	0.000	
FeCl+2	5.728e-010	3.469e-010	-9.242	-9.460	-0.218	
FeCl2+	2.237e-010	1.971e-010	-9.650	-9.705	-0.055	
CaCl2	1.491e-010	1.491e-010	-9.826	-9.826	0.000	
CuCl2	5.262e-011	5.262e-011	-10.279	-10.279	0.000	
ZnCl2	1.779e-011	1.779e-011	-10.750	-10.750	0.000	
Zn(OH)Cl	1.191e-012	1.191e-012	-11.924	-11.924	0.000	
FeCl+	6.312e-013	5.562e-013	-12.200	-12.255	-0.055	
MnCl3-	9.227e-015	8.131e-015	-14.035	-14.090	-0.055	
ZnCl3-	7.823e-015	6.894e-015	-14.107	-14.162	-0.055	
ZnCl4-2	6.110e-017	3.668e-017	-16.214	-16.436	-0.222	
FeCl2	2.095e-018	2.095e-018	-17.679	-17.679	0.000	
FeCl4-	1.325e-019	1.167e-019	-18.878	-18.933	-0.055	
CuCl2-	5.286e-020	4.659e-020	-19.277	-19.332	-0.055	
CuCl4-2	8.104e-022	4.865e-022	-21.091	-21.313	-0.222	
CuCl3-2	3.498e-022	2.100e-022	-21.456	-21.678	-0.222	
FeCl4-2	4.968e-024	2.982e-024	-23.304	-23.525	-0.222	
Cl(1)	5.268e-018					
HClO	5.267e-018	5.267e-018	-17.278	-17.278	0.000	
ClO-	5.177e-022	4.562e-022	-21.286	-21.341	-0.055	
Cl(3)	6.029e-033					
ClO2-	4.289e-033	3.780e-033	-32.368	-32.423	-0.055	
HClO2	1.740e-033	1.740e-033	-32.760	-32.760	0.000	
Cl(5)	2.535e-030					
ClO3-	2.535e-030	2.229e-030	-29.596	-29.652	-0.056	
Cl(7)	7.462e-032					
ClO4-	7.460e-032	6.558e-032	-31.127	-31.183	-0.056	
ZnClO4+	2.590e-035	2.282e-035	-34.587	-34.642	-0.055	
Cu(1)	1.673e-018					
Cu+	1.620e-018	1.427e-018	-17.791	-17.845	-0.055	
CuCl2-	5.286e-020	4.659e-020	-19.277	-19.332	-0.055	
CuCl3-2	3.498e-022	2.100e-022	-21.456	-21.678	-0.222	
Cu(2)	1.625e-004					
Cu+2	1.194e-004	7.416e-005	-3.923	-4.130	-0.207	
CuSO4	4.297e-005	4.297e-005	-4.367	-4.367	0.000	
CuCl+	1.616e-007	1.424e-007	-6.792	-6.847	-0.055	

		CuOH+	1.394e-008	1.229e-008	-7.856	-7.911	-0.055
		CuCl2	5.262e-011	5.262e-011	-10.279	-10.279	0.000
		CuNO2+	8.306e-019	7.319e-019	-18.081	-18.136	-0.055
		CuCl4-2	8.104e-022	4.865e-022	-21.091	-21.313	-0.222
		CuO2-2	4.668e-030	2.802e-030	-29.331	-29.553	-0.222
		Cu(NO2)2	7.059e-034	7.059e-034	-33.151	-33.151	0.000
		CuF+	0.000e+000	0.000e+000	-45.058	-45.113	-0.055
		CuNH3+2	0.000e+000	0.000e+000	-57.011	-57.229	-0.218
		Cu(NH3)2+2	0.000e+000	0.000e+000	-110.717	-110.935	-0.218
		Cu(NH3)3+2	0.000e+000	0.000e+000	-165.036	-165.254	-0.218
F	9.873e-006						
		HAsO3F-	9.811e-006	8.646e-006	-5.008	-5.063	-0.055
		AsO3F-2	6.231e-008	3.740e-008	-7.205	-7.427	-0.222
		AlF+2	3.485e-040	2.111e-040	-39.458	-39.676	-0.218
		F-	0.000e+000	0.000e+000	-42.127	-42.183	-0.056
		HF	0.000e+000	0.000e+000	-42.504	-42.504	0.000
		FeF+2	0.000e+000	0.000e+000	-43.317	-43.535	-0.218
		MgF+	0.000e+000	0.000e+000	-44.291	-44.346	-0.055
		CaF+	0.000e+000	0.000e+000	-44.338	-44.393	-0.055
		MnF+	0.000e+000	0.000e+000	-44.995	-45.050	-0.055
		CuF+	0.000e+000	0.000e+000	-45.058	-45.113	-0.055
		ZnF+	0.000e+000	0.000e+000	-45.714	-45.769	-0.055
		NaF	0.000e+000	0.000e+000	-46.004	-46.004	0.000
		FeF+	0.000e+000	0.000e+000	-49.732	-49.787	-0.055
		AlF2+	0.000e+000	0.000e+000	-76.204	-76.259	-0.055
		FeF2+	0.000e+000	0.000e+000	-81.454	-81.509	-0.055
		H2F2	0.000e+000	0.000e+000	-84.612	-84.612	0.000
		HF2-	0.000e+000	0.000e+000	-85.248	-85.303	-0.055
		AlF3	0.000e+000	0.000e+000	-114.342	-114.342	0.000
		AlF4-	0.000e+000	0.000e+000	-154.071	-154.125	-0.055
Fe(2)	2.188e-009						
		Fe+2	1.751e-009	1.088e-009	-8.757	-8.963	-0.207
		FeSO4	4.361e-010	4.361e-010	-9.360	-9.360	0.000
		FeCl+	6.312e-013	5.562e-013	-12.200	-12.255	-0.055
		FeOH+	1.254e-015	1.105e-015	-14.902	-14.957	-0.055
		FeCl2	2.095e-018	2.095e-018	-17.679	-17.679	0.000
		Fe(OH)2	2.818e-023	2.818e-023	-22.550	-22.550	0.000
		FeCl4-2	4.968e-024	2.982e-024	-23.304	-23.525	-0.222
		Fe(OH)3-	4.089e-030	3.603e-030	-29.388	-29.443	-0.055
		Fe(OH)4-2	0.000e+000	0.000e+000	-40.715	-40.937	-0.222
		FeF+	0.000e+000	0.000e+000	-49.732	-49.787	-0.055
Fe(3)	1.861e-004						
		FeOH+2	1.016e-004	6.151e-005	-3.993	-4.211	-0.218
		Fe(OH)2+	7.423e-005	6.542e-005	-4.129	-4.184	-0.055
		Fe+3	7.869e-006	2.967e-006	-5.104	-5.528	-0.424
		FeSO4+	8.238e-007	7.260e-007	-6.084	-6.139	-0.055
		Fe2(OH)2+4	7.099e-007	1.018e-007	-6.149	-6.992	-0.843
		Fe(OH)3	9.826e-008	9.826e-008	-7.008	-7.008	0.000
		Fe(SO4)2-	3.523e-008	3.104e-008	-7.453	-7.508	-0.055
		Fe3(OH)4+5	2.752e-008	1.392e-009	-7.560	-8.856	-1.296
		FeNO3+2	6.624e-009	4.012e-009	-8.179	-8.397	-0.218
		FeCl+2	5.728e-010	3.469e-010	-9.242	-9.460	-0.218
		FeCl2+	2.237e-010	1.971e-010	-9.650	-9.705	-0.055
		Fe(OH)4-	8.995e-014	7.927e-014	-13.046	-13.101	-0.055
		FeNO2+2	6.520e-019	3.949e-019	-18.186	-18.403	-0.218
		FeCl4-	1.325e-019	1.167e-019	-18.878	-18.933	-0.055
		FeF+2	0.000e+000	0.000e+000	-43.317	-43.535	-0.218
		FeF2+	0.000e+000	0.000e+000	-81.454	-81.509	-0.055
H(0)	0.000e+000						
		H2	0.000e+000	0.000e+000	-43.024	-43.022	0.002
K	2.831e-004						
		K+	2.775e-004	2.434e-004	-3.557	-3.614	-0.057
		KSO4-	5.638e-006	4.969e-006	-5.249	-5.304	-0.055
		KCl	5.736e-009	5.736e-009	-8.241	-8.241	0.000
		KHSO4	1.365e-009	1.365e-009	-8.865	-8.865	0.000
		KOH	2.710e-015	2.710e-015	-14.567	-14.567	0.000
Mg	6.374e-004						

Mg+2	4.449e-004	2.848e-004	-3.352	-3.546	-0.194
MgSO4	1.923e-004	1.923e-004	-3.716	-3.716	0.000
MgCl+	1.771e-007	1.560e-007	-6.752	-6.807	-0.055
Mg4(OH)4+4	8.669e-040	1.244e-040	-39.062	-39.905	-0.843
MgF+	0.000e+000	0.000e+000	-44.291	-44.346	-0.055
Mn(2)	1.131e-004				
Mn+2	8.140e-005	5.056e-005	-4.089	-4.296	-0.207
MnSO4	3.155e-005	3.155e-005	-4.501	-4.501	0.000
MnCl+	8.574e-008	7.556e-008	-7.067	-7.122	-0.055
MnNO3+	1.230e-008	1.084e-008	-7.910	-7.965	-0.055
MnOH+	4.736e-012	4.174e-012	-11.325	-11.379	-0.055
Mn(NO3)2	3.682e-012	3.682e-012	-11.434	-11.434	0.000
MnCl3-	9.227e-015	8.131e-015	-14.035	-14.090	-0.055
Mn2OH+3	6.864e-016	2.261e-016	-15.163	-15.646	-0.482
Mn(OH)2	3.290e-020	3.290e-020	-19.483	-19.483	0.000
Mn2(OH)3+	1.210e-022	1.066e-022	-21.917	-21.972	-0.055
Mn(OH)3-	1.125e-028	9.912e-029	-27.949	-28.004	-0.055
Mn(OH)4-2	4.490e-039	2.696e-039	-38.348	-38.569	-0.222
MnF+	0.000e+000	0.000e+000	-44.995	-45.050	-0.055
Mn(3)	1.164e-013				
Mn+3	1.164e-013	3.836e-014	-12.934	-13.416	-0.482
Mn(6)	2.230e-029				
MnO4-2	2.230e-029	1.339e-029	-28.652	-28.873	-0.222
Mn(7)	1.907e-022				
MnO4-	1.907e-022	1.677e-022	-21.720	-21.776	-0.056
N(-03)	0.000e+000				
HN3	0.000e+000	0.000e+000	-82.073	-82.073	0.000
N3-	0.000e+000	0.000e+000	-83.214	-83.269	-0.055
ZnN3+	0.000e+000	0.000e+000	-87.507	-87.562	-0.055
Zn(N3)2	0.000e+000	0.000e+000	-170.077	-170.077	0.000
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-51.348	-51.406	-0.058
CuNH3+2	0.000e+000	0.000e+000	-57.011	-57.229	-0.218
NH3	0.000e+000	0.000e+000	-57.139	-57.139	0.000
Zn(NH3)+2	0.000e+000	0.000e+000	-59.604	-59.822	-0.218
NH4SO4-	0.000e+000	0.000e+000	-62.248	-62.303	-0.055
Cu(NH3)2+2	0.000e+000	0.000e+000	-110.717	-110.935	-0.218
Zn(NH3)2+2	0.000e+000	0.000e+000	-114.537	-114.755	-0.218
Cu(NH3)3+2	0.000e+000	0.000e+000	-165.036	-165.254	-0.218
Zn(NH3)3+2	0.000e+000	0.000e+000	-169.470	-169.688	-0.218
Zn(NH3)4+2	0.000e+000	0.000e+000	-224.677	-224.894	-0.218
N(0)	1.791e-007				
N2	8.953e-008	8.953e-008	-7.048	-7.048	0.000
N(3)	1.590e-016				
NO2-	1.075e-016	9.425e-017	-15.969	-16.026	-0.057
HNO2	5.008e-017	5.008e-017	-16.300	-16.300	0.000
CuNO2+	8.306e-019	7.319e-019	-18.081	-18.136	-0.055
FeNO2+2	6.520e-019	3.949e-019	-18.186	-18.403	-0.218
Cu(NO2)2	7.059e-034	7.059e-034	-33.151	-33.151	0.000
N(5)	1.552e-004				
NO3-	1.542e-004	1.353e-004	-3.812	-3.869	-0.057
CaNO3+	9.343e-007	8.233e-007	-6.030	-6.084	-0.055
MnNO3+	1.230e-008	1.084e-008	-7.910	-7.965	-0.055
FeNO3+2	6.624e-009	4.012e-009	-8.179	-8.397	-0.218
HNO3	2.202e-009	2.202e-009	-8.657	-8.657	0.000
Mn(NO3)2	3.682e-012	3.682e-012	-11.434	-11.434	0.000
Na	1.631e-003				
Na+	1.604e-003	1.414e-003	-2.795	-2.850	-0.055
NaSO4-	2.681e-005	2.362e-005	-4.572	-4.627	-0.055
NaCl	1.744e-007	1.744e-007	-6.758	-6.758	0.000
NaOH	7.547e-015	7.547e-015	-14.122	-14.122	0.000
NaAlO2	1.198e-017	1.198e-017	-16.921	-16.921	0.000
NaF	0.000e+000	0.000e+000	-46.004	-46.004	0.000
O(0)	1.403e-006				
O2	7.015e-007	7.043e-007	-6.154	-6.152	0.002
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-128.579	-128.579	0.000

HS-	0.000e+000	0.000e+000	-132.026	-132.082	-0.056
S-2	0.000e+000	0.000e+000	-141.287	-141.501	-0.214
S2-2	0.000e+000	0.000e+000	-233.761	-233.982	-0.222
HAsS2	0.000e+000	0.000e+000	-277.149	-277.149	0.000
S3-2	0.000e+000	0.000e+000	-326.283	-326.505	-0.222
S4-2	0.000e+000	0.000e+000	-419.033	-419.254	-0.222
S5-2	0.000e+000	0.000e+000	-511.999	-512.220	-0.222
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-133.155	-133.377	-0.222
HS2O3-	0.000e+000	0.000e+000	-135.815	-135.870	-0.055
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-121.167	-121.381	-0.214
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-42.359	-42.414	-0.055
H2SO3	0.000e+000	0.000e+000	-43.939	-43.939	0.000
SO2	0.000e+000	0.000e+000	-44.039	-44.039	0.000
SO3-2	0.000e+000	0.000e+000	-45.921	-46.139	-0.218
S2O6-2	0.000e+000	0.000e+000	-60.278	-60.500	-0.222
S3O6-2	0.000e+000	0.000e+000	-155.284	-155.505	-0.222
S4O6-2	0.000e+000	0.000e+000	-234.383	-234.605	-0.222
S5O6-2	0.000e+000	0.000e+000	-342.362	-342.584	-0.222
S(5)	0.000e+000				
S2O5-2	0.000e+000	0.000e+000	-89.436	-89.658	-0.222
S(6)	5.194e-003				
SO4-2	4.213e-003	2.529e-003	-2.375	-2.597	-0.222
CaSO4	4.487e-004	4.487e-004	-3.348	-3.348	0.000
MgSO4	1.923e-004	1.923e-004	-3.716	-3.716	0.000
AlSO4+	9.457e-005	8.333e-005	-4.024	-4.079	-0.055
HSO4-	9.026e-005	7.954e-005	-4.045	-4.099	-0.055
CuSO4	4.297e-005	4.297e-005	-4.367	-4.367	0.000
MnSO4	3.155e-005	3.155e-005	-4.501	-4.501	0.000
NaSO4-	2.681e-005	2.362e-005	-4.572	-4.627	-0.055
Al(SO4)2-	1.857e-005	1.636e-005	-4.731	-4.786	-0.055
ZnSO4	9.778e-006	9.778e-006	-5.010	-5.010	0.000
KSO4-	5.638e-006	4.969e-006	-5.249	-5.304	-0.055
FeSO4+	8.238e-007	7.260e-007	-6.084	-6.139	-0.055
Fe(SO4)2-	3.523e-008	3.104e-008	-7.453	-7.508	-0.055
KHSO4	1.365e-009	1.365e-009	-8.865	-8.865	0.000
FeSO4	4.361e-010	4.361e-010	-9.360	-9.360	0.000
H2SO4	2.336e-011	2.336e-011	-10.631	-10.631	0.000
NH4SO4-	0.000e+000	0.000e+000	-62.248	-62.303	-0.055
S(7)	6.081e-038				
S2O8-2	3.040e-038	1.825e-038	-37.517	-37.739	-0.222
S(8)	4.115e-027				
HSO5-	4.115e-027	3.626e-027	-26.386	-26.441	-0.055
Zn	3.942e-005				
Zn+2	2.962e-005	1.840e-005	-4.528	-4.735	-0.207
ZnSO4	9.778e-006	9.778e-006	-5.010	-5.010	0.000
ZnCl+	2.462e-008	2.169e-008	-7.609	-7.664	-0.055
ZnOH+	7.353e-011	6.480e-011	-10.134	-10.188	-0.055
ZnCl2	1.779e-011	1.779e-011	-10.750	-10.750	0.000
Zn(OH)Cl	1.191e-012	1.191e-012	-11.924	-11.924	0.000
ZnCl3-	7.823e-015	6.894e-015	-14.107	-14.162	-0.055
Zn(OH)2	8.912e-016	8.912e-016	-15.050	-15.050	0.000
ZnCl4-2	6.110e-017	3.668e-017	-16.214	-16.436	-0.222
Zn(OH)3-	1.007e-023	8.872e-024	-22.997	-23.052	-0.055
Zn(OH)4-2	8.092e-033	4.857e-033	-32.092	-32.314	-0.222
ZnClO4+	2.590e-035	2.282e-035	-34.587	-34.642	-0.055
ZnF+	0.000e+000	0.000e+000	-45.714	-45.769	-0.055
Zn(NH3)+2	0.000e+000	0.000e+000	-59.604	-59.822	-0.218
ZnN3+	0.000e+000	0.000e+000	-87.507	-87.562	-0.055
Zn(NH3)2+2	0.000e+000	0.000e+000	-114.537	-114.755	-0.218
Zn(NH3)3+2	0.000e+000	0.000e+000	-169.470	-169.688	-0.218
Zn(N3)2	0.000e+000	0.000e+000	-170.077	-170.077	0.000
Zn(NH3)4+2	0.000e+000	0.000e+000	-224.677	-224.894	-0.218

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

Phase	SI	log IAP	log KT	
Al	-139.27	10.64	149.91	Al
Al(g)	-189.98	10.64	200.62	Al
Al2(SO4)3	-35.67	-16.78	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-18.33	-16.78	1.56	Al2(SO4)3:6H2O
Alabandite	-132.45	-132.87	-0.42	MnS
AlF3	-113.78	-131.04	-17.27	AlF3
Alum-K	-8.33	-13.30	-4.97	KAl(SO4)2:12H2O
Alunite	-0.77	-1.24	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.16	-5.51	-4.35	CaSO4
Antarcticite	-13.32	-9.22	4.09	CaCl2:6H2O
Antlerite	-9.69	-0.96	8.73	Cu3(SO4)(OH)4
Aphthitalite	-15.00	-18.88	-3.89	NaK3(SO4)2
Arcanite	-7.98	-9.82	-1.84	K2SO4
Arsenolite	-53.06	-72.90	-19.84	As2O3
Arsenopyrite	-217.26	-231.71	-14.45	FeAsS
As	-74.52	-31.84	42.68	As
As2O5	-20.13	-17.99	2.14	As2O5
As4O6(cubi)	-105.98	-145.81	-39.82	As4O6
As4O6(mono)	-105.76	-145.81	-40.05	As4O6
Atacamite	-16.05	-1.79	14.26	Cu4Cl2(OH)6
Bassanite	-1.81	-5.51	-3.71	CaSO4:0.5H2O
Birnessite	-8.53	-94.07	-85.55	Mn8O14:5H2O
Bischofite	-14.25	-9.85	4.39	MgCl2:6H2O
Bixbyite	-4.83	-5.79	-0.96	Mn2O3
Bloedite	-11.96	-14.44	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-1.52	6.03	7.55	AlO2H
Bornite	-496.24	-598.78	-102.53	Cu5FeS4
Brochantite	-13.50	1.92	15.42	Cu4(SO4)(OH)6
Brucite	-12.82	3.47	16.28	Mg(OH)2
Ca	-132.66	7.17	139.83	Ca
Ca(g)	-157.90	7.17	165.07	Ca
Ca2Al2O5:8H2O	-39.32	20.25	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-31.42	-5.13	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-23.50	-5.70	17.80	Ca3(AsO4)2
Ca3Al2O6	-88.68	24.35	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-102.05	38.43	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-78.81	28.45	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-75.23	28.45	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-65.26	3.07	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-30.75	16.15	46.91	CaAl2O4
CaAl2O4:10H2O	-21.84	16.15	37.99	CaAl2O4:10H2O
CaAl4O7	-40.38	28.21	68.59	CaAl4O7
Carnallite	-20.89	-16.62	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.98	-5.51	-3.54	CaSO4:0.5H2O
Chalcanthite	-4.10	-6.73	-2.63	CuSO4:5H2O
Chalcocite	-129.52	-164.27	-34.74	Cu2S
Chalcocyanite	-9.64	-6.73	2.91	CuSO4
Chalcopyrite	-237.64	-270.24	-32.60	CuFeS2
Chloromagnesite	-31.67	-9.85	21.82	MgCl2
Cl2(g)	-19.39	-16.40	2.99	Cl2
Claudetite	-53.11	-72.90	-19.80	As2O3
Corundum	-6.23	12.06	18.29	Al2O3
Covellite	-109.84	-132.70	-22.86	CuS
Cu	-25.54	5.96	31.50	Cu
Cu(g)	-77.70	5.96	83.66	Cu
CuCl2	-14.16	-10.44	3.72	CuCl2
CuF	-67.11	-60.03	7.08	CuF
CuF2	-87.88	-88.50	-0.62	CuF2
CuF2:2H2O	-83.95	-88.50	-4.55	CuF2:2H2O
Cuprite	-26.77	-28.68	-1.91	Cu2O
Delafoosite	-2.91	-9.35	-6.44	CuFeO2
Diaspore	-1.12	6.03	7.15	AlHO2
Epsomite	-4.18	-6.14	-1.96	MgSO4:7H2O
Ettringite	-54.65	7.81	62.46	Ca6Al2(SO4)3(OH)12:26H2O

F2(g)	-150.17	-94.46	55.71	F2
Fe	-57.89	1.13	59.02	Fe
Fe(OH)2	-15.84	-1.95	13.89	Fe(OH)2
Fe(OH)3	-0.65	4.99	5.64	Fe(OH)3
Fe2(SO4)3	-21.89	-18.85	3.05	Fe2(SO4)3
FeF2	-90.91	-93.33	-2.42	FeF2
FeF3	-112.82	-132.08	-19.26	FeF3
FeO	-15.47	-1.95	13.52	FeO
Ferrite-Ca	-7.41	14.08	21.50	CaFe2O4
Ferrite-Cu	2.59	12.87	10.28	CuFe2O4
Ferrite-Dicalcium	-38.62	18.18	56.80	Ca2Fe2O5
Ferrite-Mg	-7.57	13.45	21.02	MgFe2O4
Ferrite-Zn	0.56	12.26	11.70	ZnFe2O4
FeSO4	-14.17	-11.56	2.61	FeSO4
Fluorite	-77.21	-87.28	-10.07	CaF2
Gibbsite	-1.71	6.03	7.74	Al(OH)3
Glauberite	-8.34	-13.81	-5.47	Na2Ca(SO4)2
Goethite	4.46	4.99	0.53	FeOOH
Gypsum	-0.98	-5.51	-4.53	CaSO4·2H2O
H2(g)	-39.92	-43.02	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-127.60	-135.59	-7.99	H2S
Halite	-7.57	-6.00	1.56	NaCl
Hausmannite	-13.22	-3.07	10.14	Mn3O4
HCl(g)	-12.96	-6.66	6.30	HCl
Hematite	9.91	9.99	0.08	Fe2O3
Hercynite	-18.70	10.11	28.80	FeAl2O4
Hexahydrite	-4.42	-6.14	-1.73	MgSO4·6H2O
Hydrophilite	-20.97	-9.22	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	5.06	-4.35	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	1.86	-3.59	-5.45	NaFe3(SO4)2(OH)6
K	-69.55	1.43	70.98	K
K(g)	-80.15	1.43	81.58	K
K2O	-84.25	-0.21	84.04	K2O
K3H(SO4)2	-15.92	-19.54	-3.62	K3H(SO4)2
Kainite	-12.60	-12.91	-0.31	KMgClSO4·3H2O
KAl(SO4)2	-16.57	-13.30	3.27	KAl(SO4)2
Katoite	-54.59	24.35	78.94	Ca3Al2H12O12
Kieserite	-5.88	-6.14	-0.27	MgSO4·H2O
KMgCl3	-37.87	-16.62	21.25	KMgCl3
KMgCl3·2H2O	-30.58	-16.62	13.96	KMgCl3·2H2O
Lammerite	-10.89	-9.34	1.55	Cu3(AsO4)2
Lawrencite	-24.33	-15.27	9.05	FeCl2
Leonite	-11.85	-15.97	-4.11	K2Mg(SO4)2·4H2O
Lime	-28.47	4.10	32.57	CaO
Magnetite	-2.38	8.04	10.42	Fe3O4
Manganite	-2.73	-2.90	-0.16	MnO(OH)
Manganosite	-15.20	2.72	17.92	MnO
Mayenite	-360.58	133.57	494.15	Ca12Al14O33
Melanterite	-9.16	-11.56	-2.40	FeSO4·7H2O
Mercallite	-8.28	-9.72	-1.44	KHSO4
Mg	-115.98	6.54	122.52	Mg
Mg(g)	-135.70	6.54	142.25	Mg
Mg1.25SO4(OH)0.5·0.5H2O	-10.47	-5.28	5.20	Mg1.25SO4(OH)0.5·0.5H2O
Mg1.5SO4(OH)	-13.62	-4.41	9.21	Mg1.5SO4(OH)
MgCl2·2H2O	-22.58	-9.85	12.73	MgCl2·2H2O
MgCl2·4H2O	-17.15	-9.85	7.30	MgCl2·4H2O
MgCl2·H2O	-25.93	-9.85	16.07	MgCl2·H2O
MgOHCl	-19.08	-3.19	15.89	MgOHCl
MgSO4	-10.97	-6.14	4.83	MgSO4
Mirabilite	-7.14	-8.30	-1.15	Na2SO4·10H2O
Misenite	-57.05	-68.13	-11.08	K8H6(SO4)7
Mn	-77.14	5.79	82.93	Mn
Mn(OH)2(am)	-12.59	2.72	15.31	Mn(OH)2
Mn(OH)3	-9.24	-2.90	6.34	Mn(OH)3
MnCl2·2H2O	-14.60	-10.60	4.00	MnCl2·2H2O

MnCl2:4H2O	-13.36	-10.60	2.75	MnCl2:4H2O
MnCl2:H2O	-16.15	-10.60	5.54	MnCl2:H2O
MnO2 (gamma)	-0.46	-16.58	-16.13	MnO2
MnSO4	-9.50	-6.89	2.61	MnSO4
Molysite	-28.46	-14.99	13.47	FeCl3
N2(g)	-3.87	-7.05	-3.18	N2
Na	-65.18	2.20	67.37	Na
Na(g)	-78.66	2.20	80.86	Na
Na2O	-66.10	1.31	67.42	Na2O
Na3H(SO4)2	-16.36	-17.25	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.21	-22.11	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-14.23	5.65	19.88	NaFeO2
Nantokite	-14.23	-21.00	-6.77	CuCl
NH3(g)	-58.94	-57.14	1.80	NH3
Niter	-7.26	-7.48	-0.22	KNO3
NO(g)	-18.73	-17.99	0.74	NO
NO2(g)	-14.19	-5.84	8.35	NO2
O2(g)	-3.26	-6.15	-2.89	O2
Orpiment	-400.18	-479.67	-79.49	As2S3
Oxychloride-Mg	-25.56	0.27	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.76	-6.14	-1.39	MgSO4:5H2O
Periclase	-17.86	3.47	21.33	MgO
Picromerite	-11.53	-15.97	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-12.68	-26.99	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-18.45	4.10	22.55	Ca(OH)2
Pyrite	-216.93	-241.63	-24.70	FeS2
Pyrolusite	1.08	-16.58	-17.66	MnO2
Pyrrhotite	-133.80	-137.54	-3.74	FeS
Realgar	-155.81	-216.09	-60.28	AsS
S	-93.55	-138.66	-45.11	S
S2(g)	-201.00	-208.19	-7.19	S2
Scacchite	-19.34	-10.60	8.74	MnCl2
Sellaite	-78.47	-87.91	-9.44	MgF2
SO2(g)	-44.21	-44.04	0.18	SO2
Sphalerite	-121.84	-133.31	-11.47	ZnS
Spinel	-22.08	15.52	37.61	Al2MgO4
Starkeyite	-5.14	-6.14	-1.00	MgSO4:4H2O
Sylvite	-7.59	-6.77	0.83	KCl
Syngenite	-7.74	-15.34	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-46.07	-28.93	17.14	Mg2CaCl6:12H2O
Tenorite	-4.76	2.88	7.65	CuO
Thenardite	-7.94	-8.30	-0.36	Na2SO4
Todorokite	-7.44	-53.26	-45.82	Mn7O12:3H2O
Troilite	-133.70	-137.54	-3.84	FeS
Wurtzite	-124.14	-133.31	-9.17	ZnS
Wustite	-13.51	-1.11	12.40	Fe.947O
Zincite	-8.92	2.28	11.20	ZnO
Zn	-63.43	5.35	68.79	Zn
Zn(ClO4)2:6H2O	-72.74	-67.10	5.63	Zn(ClO4)2:6H2O
Zn(g)	-80.05	5.35	85.41	Zn
Zn(NO3)2:6H2O	-15.87	-12.47	3.40	Zn(NO3)2:6H2O
Zn(OH)2(beta)	-9.65	2.28	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-9.38	2.28	11.66	Zn(OH)2
Zn(OH)2(gamma)	-9.61	2.28	11.88	Zn(OH)2
Zn2(OH)3Cl	-17.40	-2.10	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-12.64	-5.05	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-20.47	-11.16	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-31.48	-12.39	19.09	Zn3O(SO4)2
Zn5(NO3)2(OH)8	-46.03	-3.36	42.67	Zn5(NO3)2(OH)8
ZnCl2	-18.12	-11.04	7.08	ZnCl2
ZnCl2(NH3)2	-118.31	-125.32	-7.01	ZnCl2(NH3)2
ZnCl2(NH3)4	-232.89	-239.60	-6.71	ZnCl2(NH3)4
ZnCl2(NH3)6	-349.14	-353.88	-4.74	ZnCl2(NH3)6
ZnF2	-88.61	-89.10	-0.49	ZnF2
ZnSO4	-10.87	-7.33	3.53	ZnSO4
ZnSO4:6H2O	-5.63	-7.33	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.46	-7.33	-1.88	ZnSO4:7H2O

ZnSO4:H2O -6.78 -7.33 -0.55 ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
