
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 4
temp 25
pH 3.17
pe 12
redox pe
units mg/l
density 1
Cl 46.9
S(6) 1089.6
Al 25.6
As 5.0
Ca 201.4
Cu 35.1
Fe 170.2
K 69.2
Mg 19.8
Mn 20.6
Na 33.2
Zn 17.4
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 4

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

Elements	Molality	Moles
Al	9.504e-004	9.504e-004
As	6.685e-005	6.685e-005
Ca	5.034e-003	5.034e-003
Cl	1.325e-003	1.325e-003
Cu	5.533e-004	5.533e-004
Fe	3.053e-003	3.053e-003
K	1.773e-003	1.773e-003
Mg	8.161e-004	8.161e-004
Mn	3.756e-004	3.756e-004
Na	1.447e-003	1.447e-003
S(6)	1.136e-002	1.136e-002
Zn	2.666e-004	2.666e-004

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

```

pH      = 3.170
pe      = 12.000
Activity of water      = 1.000
Ionic strength      = 3.718e-002
Mass of water (kg)      = 1.000e+000
Total alkalinity (eq/kg)      = -2.718e-003
Total carbon (mol/kg)      = 0.000e+000
Total CO2 (mol/kg)      = 0.000e+000
Temperature (deg C)      = 25.000
Electrical balance (eq)      = 3.154e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|)      = 8.05
Iterations      = 8
Total H      = 1.110537e+002
Total O      = 5.557286e+001

```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	7.785e-004	6.761e-004	-3.109	-3.170	-0.061
OH-	1.709e-011	1.424e-011	-10.767	-10.846	-0.079
H2O	5.553e+001	9.996e-001	1.744	-0.000	0.000
Al	9.504e-004				
AlSO4+	4.577e-004	3.832e-004	-3.339	-3.417	-0.077
Al+3	3.507e-004	9.580e-005	-3.455	-4.019	-0.564
Al(SO4)2-	1.389e-004	1.163e-004	-3.857	-3.935	-0.077
AlOH+2	3.206e-006	1.587e-006	-5.494	-5.799	-0.305
Al(OH)2+	6.507e-009	5.448e-009	-8.187	-8.264	-0.077
Al2(OH)2+4	6.033e-009	4.095e-010	-8.219	-9.388	-1.168
HALO2	1.173e-011	1.173e-011	-10.931	-10.931	0.000

Al3(OH)4+5	3.369e-012	5.535e-014	-11.472	-13.257	-1.784
AlO2-	7.097e-015	5.942e-015	-14.149	-14.226	-0.077
NaAlO2	1.338e-018	1.338e-018	-17.874	-17.874	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-46.038	-49.537	-3.499
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-112.033	-112.033	0.000
As(3)	1.610e-016				
HAsO2	8.593e-017	8.593e-017	-16.066	-16.066	0.000
As(OH)3	7.510e-017	7.510e-017	-16.124	-16.124	0.000
H2AsO3-	8.114e-023	6.793e-023	-22.091	-22.168	-0.077
AsO2-	7.760e-023	6.497e-023	-22.110	-22.187	-0.077
AsO2OH-2	2.019e-030	9.817e-031	-29.695	-30.008	-0.313
As(5)	6.685e-005				
H2AsO4-	6.077e-005	5.088e-005	-4.216	-4.293	-0.077
H3AsO4	6.059e-006	6.059e-006	-5.218	-5.218	0.000
HAsO4-2	2.569e-008	1.249e-008	-7.590	-7.903	-0.313
AsO4-3	2.411e-016	4.740e-017	-15.618	-16.324	-0.706
Ca	5.034e-003				
Ca+2	3.882e-003	2.017e-003	-2.411	-2.695	-0.284
CaSO4	1.152e-003	1.152e-003	-2.939	-2.939	0.000
CaCl+	5.599e-007	4.688e-007	-6.252	-6.329	-0.077
CaCl2	6.044e-010	6.044e-010	-9.219	-9.219	0.000
CaOH+	5.032e-013	4.213e-013	-12.298	-12.375	-0.077
Cl(-1)	1.325e-003				
Cl-	1.322e-003	1.096e-003	-2.879	-2.960	-0.081
CuCl+	7.019e-007	5.877e-007	-6.154	-6.231	-0.077
CaCl+	5.599e-007	4.688e-007	-6.252	-6.329	-0.077
FeCl+	5.035e-007	4.215e-007	-6.298	-6.375	-0.077
MnCl+	3.622e-007	3.033e-007	-6.441	-6.518	-0.077
MgCl+	2.911e-007	2.438e-007	-6.536	-6.613	-0.077
NaCl	2.275e-007	2.275e-007	-6.643	-6.643	0.000
ZnCl+	2.134e-007	1.787e-007	-6.671	-6.748	-0.077
HCl	1.665e-007	1.665e-007	-6.779	-6.779	0.000
KCl	5.248e-008	5.248e-008	-7.280	-7.280	0.000
FeCl+2	1.867e-008	9.244e-009	-7.729	-8.034	-0.305
FeCl2+	9.799e-009	8.204e-009	-8.009	-8.086	-0.077
CaCl2	6.044e-010	6.044e-010	-9.219	-9.219	0.000
CuCl2	3.393e-010	3.393e-010	-9.469	-9.469	0.000
ZnCl2	2.288e-010	2.288e-010	-9.640	-9.640	0.000
Zn(OH)Cl	4.517e-012	4.517e-012	-11.345	-11.345	0.000
FeCl2	2.480e-012	2.480e-012	-11.606	-11.606	0.000
ZnCl3-	1.655e-013	1.385e-013	-12.781	-12.858	-0.077
MnCl3-	9.510e-014	7.962e-014	-13.022	-13.099	-0.077
CuCl2-	1.020e-014	8.543e-015	-13.991	-14.068	-0.077
ZnCl4-2	2.368e-015	1.151e-015	-14.626	-14.939	-0.313
CuCl3-2	1.237e-016	6.015e-017	-15.908	-16.221	-0.313
FeCl4-2	1.771e-017	8.612e-018	-16.752	-17.065	-0.313
FeCl4-	1.416e-017	1.185e-017	-16.849	-16.926	-0.077
CuCl4-2	1.574e-020	7.653e-021	-19.803	-20.116	-0.313
Cl(1)	4.682e-027				
HClO	4.682e-027	4.682e-027	-26.330	-26.330	0.000
ClO-	2.230e-031	1.867e-031	-30.652	-30.729	-0.077
Cl(3)	0.000e+000				
ClO2-	0.000e+000	0.000e+000	-51.315	-51.392	-0.077
HClO2	0.000e+000	0.000e+000	-51.392	-51.392	0.000
Cl(5)	0.000e+000				
ClO3-	0.000e+000	0.000e+000	-58.124	-58.203	-0.079
Cl(7)	0.000e+000				
ClO4-	0.000e+000	0.000e+000	-69.237	-69.316	-0.079
ZnClO4+	0.000e+000	0.000e+000	-71.975	-72.052	-0.077
Cu(1)	1.385e-013				
Cu+	1.281e-013	1.073e-013	-12.892	-12.969	-0.077
CuCl2-	1.020e-014	8.543e-015	-13.991	-14.068	-0.077
CuCl3-2	1.237e-016	6.015e-017	-15.908	-16.221	-0.313
Cu(2)	5.533e-004				
Cu+2	3.771e-004	1.960e-004	-3.424	-3.708	-0.284
CuSO4	1.755e-004	1.755e-004	-3.756	-3.756	0.000

CuCl+	7.019e-007	5.877e-007	-6.154	-6.231	-0.077
CuOH+	1.785e-008	1.495e-008	-7.748	-7.825	-0.077
CuCl2	3.393e-010	3.393e-010	-9.469	-9.469	0.000
CuCl4-2	1.574e-020	7.653e-021	-19.803	-20.116	-0.313
CuO2-2	6.844e-031	3.328e-031	-30.165	-30.478	-0.313
Fe(2)	1.343e-003				
Fe+2	1.016e-003	5.278e-004	-2.993	-3.278	-0.284
FeSO4	3.270e-004	3.270e-004	-3.486	-3.486	0.000
FeCl+	5.035e-007	4.215e-007	-6.298	-6.375	-0.077
FeOH+	2.947e-010	2.468e-010	-9.531	-9.608	-0.077
FeCl2	2.480e-012	2.480e-012	-11.606	-11.606	0.000
FeCl4-2	1.771e-017	8.612e-018	-16.752	-17.065	-0.313
Fe(OH)2	2.898e-018	2.898e-018	-17.538	-17.538	0.000
Fe(OH)3-	2.037e-025	1.706e-025	-24.691	-24.768	-0.077
Fe(OH)4-2	5.187e-037	2.522e-037	-36.285	-36.598	-0.313
Fe(3)	1.710e-003				
FeOH+2	9.759e-004	4.831e-004	-3.011	-3.316	-0.305
Fe(OH)2+	2.825e-004	2.365e-004	-3.549	-3.626	-0.077
Fe+3	1.852e-004	5.061e-005	-3.732	-4.296	-0.564
Fe2(OH)2+4	9.255e-005	6.281e-006	-4.034	-5.202	-1.168
FeSO4+	2.286e-005	1.914e-005	-4.641	-4.718	-0.077
Fe3(OH)4+5	1.889e-005	3.104e-007	-4.724	-6.508	-1.784
Fe(SO4)2-	1.510e-006	1.265e-006	-5.821	-5.898	-0.077
Fe(OH)3	1.635e-007	1.635e-007	-6.786	-6.786	0.000
FeCl+2	1.867e-008	9.244e-009	-7.729	-8.034	-0.305
FeCl2+	9.799e-009	8.204e-009	-8.009	-8.086	-0.077
Fe(OH)4-	7.254e-014	6.074e-014	-13.139	-13.217	-0.077
FeCl4-	1.416e-017	1.185e-017	-16.849	-16.926	-0.077
H(0)	7.189e-034				
H2	3.595e-034	3.627e-034	-33.444	-33.440	0.004
K	1.773e-003				
K+	1.719e-003	1.426e-003	-2.765	-2.846	-0.081
KSO4-	5.372e-005	4.497e-005	-4.270	-4.347	-0.077
KCl	5.248e-008	5.248e-008	-7.280	-7.280	0.000
KHSO4	2.683e-008	2.683e-008	-7.571	-7.571	0.000
KOH	7.308e-015	7.308e-015	-14.136	-14.136	0.000
Mg	8.161e-004				
Mg+2	5.185e-004	2.848e-004	-3.285	-3.545	-0.260
MgSO4	2.973e-004	2.973e-004	-3.527	-3.527	0.000
MgCl+	2.911e-007	2.438e-007	-6.536	-6.613	-0.077
Mg4(OH)4+4	0.000e+000	0.000e+000	-40.084	-41.252	-1.168
Mn(2)	3.756e-004				
Mn+2	2.500e-004	1.299e-004	-3.602	-3.886	-0.284
MnSO4	1.253e-004	1.253e-004	-3.902	-3.902	0.000
MnCl+	3.622e-007	3.033e-007	-6.441	-6.518	-0.077
MnOH+	5.897e-012	4.937e-012	-11.229	-11.307	-0.077
MnCl3-	9.510e-014	7.962e-014	-13.022	-13.099	-0.077
Mn2OH+3	3.232e-015	6.873e-016	-14.490	-15.163	-0.672
Mn(OH)2	1.792e-020	1.792e-020	-19.747	-19.747	0.000
Mn2(OH)3+	8.202e-023	6.867e-023	-22.086	-22.163	-0.077
Mn(OH)3-	2.968e-029	2.485e-029	-28.528	-28.605	-0.077
Mn(OH)4-2	6.398e-040	3.111e-040	-39.194	-39.507	-0.313
Mn(3)	1.630e-017				
Mn+3	1.630e-017	3.465e-018	-16.788	-17.460	-0.672
Mn(6)	0.000e+000				
MnO4-2	0.000e+000	0.000e+000	-48.661	-48.974	-0.313
Mn(7)	0.000e+000				
MnO4-	0.000e+000	0.000e+000	-46.251	-46.330	-0.079
Na	1.447e-003				
Na+	1.410e-003	1.181e-003	-2.851	-2.928	-0.077
NaSO4-	3.641e-005	3.049e-005	-4.439	-4.516	-0.077
NaCl	2.275e-007	2.275e-007	-6.643	-6.643	0.000
NaOH	2.901e-015	2.901e-015	-14.537	-14.537	0.000
NaAlO2	1.338e-018	1.338e-018	-17.874	-17.874	0.000
O(0)	9.587e-026				
O2	4.793e-026	4.837e-026	-25.319	-25.315	0.004
S(6)	1.136e-002				

SO4-2	8.038e-003	3.909e-003	-2.095	-2.408	-0.313
CaSO4	1.152e-003	1.152e-003	-2.939	-2.939	0.000
AlSO4+	4.577e-004	3.832e-004	-3.339	-3.417	-0.077
FeSO4	3.270e-004	3.270e-004	-3.486	-3.486	0.000
HSO4-	3.188e-004	2.669e-004	-3.496	-3.574	-0.077
MgSO4	2.973e-004	2.973e-004	-3.527	-3.527	0.000
CuSO4	1.755e-004	1.755e-004	-3.756	-3.756	0.000
Al(SO4)2-	1.389e-004	1.163e-004	-3.857	-3.935	-0.077
MnSO4	1.253e-004	1.253e-004	-3.902	-3.902	0.000
ZnSO4	7.968e-005	7.968e-005	-4.099	-4.099	0.000
KSO4-	5.372e-005	4.497e-005	-4.270	-4.347	-0.077
NaSO4-	3.641e-005	3.049e-005	-4.439	-4.516	-0.077
FeSO4+	2.286e-005	1.914e-005	-4.641	-4.718	-0.077
Fe(SO4)2-	1.510e-006	1.265e-006	-5.821	-5.898	-0.077
KHSO4	2.683e-008	2.683e-008	-7.571	-7.571	0.000
H2SO4	1.703e-010	1.703e-010	-9.769	-9.769	0.000
Zn	2.666e-004				
Zn+2	1.867e-004	9.702e-005	-3.729	-4.013	-0.284
ZnSO4	7.968e-005	7.968e-005	-4.099	-4.099	0.000
ZnCl+	2.134e-007	1.787e-007	-6.671	-6.748	-0.077
ZnCl2	2.288e-010	2.288e-010	-9.640	-9.640	0.000
ZnOH+	1.879e-010	1.573e-010	-9.726	-9.803	-0.077
Zn(OH)Cl	4.517e-012	4.517e-012	-11.345	-11.345	0.000
ZnCl3-	1.655e-013	1.385e-013	-12.781	-12.858	-0.077
ZnCl4-2	2.368e-015	1.151e-015	-14.626	-14.939	-0.313
Zn(OH)2	9.960e-016	9.960e-016	-15.002	-15.002	0.000
Zn(OH)3-	5.452e-024	4.565e-024	-23.263	-23.341	-0.077
Zn(OH)4-2	2.366e-033	1.151e-033	-32.626	-32.939	-0.313
ZnClO4+	0.000e+000	0.000e+000	-71.975	-72.052	-0.077

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

Phase	SI	log IAP	log KT	
Al	-125.44	24.48	149.91	Al
Al(g)	-176.14	24.48	200.62	Al
Al2(SO4)3	-34.16	-15.26	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-16.82	-15.26	1.56	Al2(SO4)3:6H2O
Alum-K	-6.71	-11.68	-4.97	KAl(SO4)2:12H2O
Alunite	-0.23	-0.70	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.75	-5.10	-4.35	CaSO4
Antarcticite	-12.71	-8.62	4.09	CaCl2:6H2O
Antlerite	-9.58	-0.85	8.73	Cu3(SO4)(OH)4
Aphthitalite	-12.39	-16.28	-3.89	NaK3(SO4)2
Arcanite	-6.26	-8.10	-1.84	K2SO4
Arsenolite	-30.83	-50.68	-19.84	As2O3
As	-49.03	-6.35	42.68	As
As2O5	-17.06	-14.93	2.14	As2O5
As4O6(cubi)	-61.53	-101.35	-39.82	As4O6
As4O6(mono)	-61.30	-101.35	-40.05	As4O6
Atacamite	-16.00	-1.73	14.26	Cu4Cl2(OH)6
Bassanite	-1.40	-5.10	-3.71	CaSO4:0.5H2O
Birnessite	-68.13	-153.67	-85.55	Mn8O14:5H2O
Bischofite	-13.86	-9.47	4.39	MgCl2:6H2O
Bixbyite	-14.94	-15.90	-0.96	Mn2O3
Bloedite	-11.74	-14.22	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-2.06	5.49	7.55	AlO2H
Brochantite	-13.64	1.78	15.42	Cu4(SO4)(OH)6
Brucite	-13.49	2.79	16.28	Mg(OH)2
Ca	-123.53	16.30	139.83	Ca
Ca(g)	-148.77	16.30	165.07	Ca
Ca2Al2O5:8H2O	-41.30	18.27	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-31.26	-4.97	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-21.80	-3.99	17.80	Ca3(AsO4)2
Ca3Al2O6	-91.12	21.92	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-104.49	35.99	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-81.70	25.56	107.25	Ca4Al2O7:13H2O

Ca4Al2O7:19H2O	-78.12	25.56	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-66.01	2.32	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-32.28	14.63	46.91	CaAl2O4
CaAl2O4:10H2O	-23.37	14.63	37.99	CaAl2O4:10H2O
CaAl4O7	-42.98	25.61	68.59	CaAl4O7
Carnallite	-19.54	-15.27	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.57	-5.10	-3.54	CaSO4:0.5H2O
Chalcanthite	-3.49	-6.12	-2.63	CuSO4:5H2O
Chalcocyanite	-9.03	-6.12	2.91	CuSO4
Chloromagnesite	-31.28	-9.47	21.82	MgCl2
Cl2(g)	-27.91	-24.92	2.99	Cl2
Claudetite	-30.88	-50.68	-19.80	As2O3
Corundum	-7.31	10.98	18.29	Al2O3
Cu	-16.21	15.29	31.50	Cu
Cu(g)	-68.37	15.29	83.66	Cu
CuCl2	-13.35	-9.63	3.72	CuCl2
Cuprite	-17.69	-19.60	-1.91	Cu2O
Delafossite	1.85	-4.59	-6.44	CuFeO2
Diaspore	-1.66	5.49	7.15	AlHO2
Epsomite	-3.99	-5.95	-1.96	MgSO4:7H2O
Ettringite	-55.86	6.60	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-43.30	15.72	59.02	Fe
Fe(OH)2	-10.83	3.06	13.89	Fe(OH)2
Fe(OH)3	-0.43	5.21	5.64	Fe(OH)3
Fe2(SO4)3	-18.86	-15.82	3.05	Fe2(SO4)3
FeO	-10.46	3.06	13.52	FeO
Ferrite-Ca	-7.42	14.07	21.50	CaFe2O4
Ferrite-Cu	2.78	13.06	10.28	CuFe2O4
Ferrite-Dicalcium	-39.08	17.72	56.80	Ca2Fe2O5
Ferrite-Mg	-7.80	13.22	21.02	MgFe2O4
Ferrite-Zn	1.05	12.75	11.70	ZnFe2O4
FeSO4	-8.29	-5.69	2.61	FeSO4
Gibbsite	-2.25	5.49	7.74	Al(OH)3
Glauberite	-7.90	-13.37	-5.47	Na2Ca(SO4)2
Goethite	4.68	5.21	0.53	FeOOH
Gypsum	-0.57	-5.10	-4.53	CaSO4:2H2O
H2(g)	-30.34	-33.44	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.45	-5.89	1.56	NaCl
Hausmannite	-23.59	-13.45	10.14	Mn3O4
HCl(g)	-12.43	-6.13	6.30	HCl
Hematite	10.35	10.43	0.08	Fe2O3
Hercynite	-14.76	14.04	28.80	FeAl2O4
Hexahydrite	-4.23	-5.95	-1.73	MgSO4:6H2O
Hydrophilite	-20.36	-8.62	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	7.88	-1.53	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	3.84	-1.61	-5.45	NaFe3(SO4)2(OH)6
K	-64.32	6.65	70.98	K
K(g)	-74.93	6.65	81.58	K
K2O	-83.39	0.65	84.04	K2O
K3H(SO4)2	-12.90	-16.52	-3.62	K3H(SO4)2
Kainite	-11.45	-11.76	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-14.95	-11.68	3.27	KAl(SO4)2
Katoite	-57.03	21.91	78.94	Ca3Al2H12O12
Kieserite	-5.69	-5.95	-0.27	MgSO4:H2O
KMgCl3	-36.52	-15.27	21.25	KMgCl3
KMgCl3:2H2O	-29.23	-15.27	13.96	KMgCl3:2H2O
Lammerite	-8.58	-7.03	1.55	Cu3(AsO4)2
Lawrencite	-18.25	-9.20	9.05	FeCl2
Leonite	-9.94	-14.05	-4.11	K2Mg(SO4)2:4H2O
Lime	-28.92	3.64	32.57	CaO
Magnetite	3.07	13.49	10.42	Fe3O4
Manganite	-7.79	-7.95	-0.16	MnO(OH)
Manganosite	-15.46	2.45	17.92	MnO
Mayenite	-373.54	120.61	494.15	Ca12Al14O33
Melanterite	-3.29	-5.69	-2.40	FeSO4:7H2O

Mercallite	-6.99	-8.42	-1.44	KHSO4
Mg	-107.07	15.45	122.52	Mg
Mg(g)	-126.79	15.45	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.45	-5.25	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-13.77	-4.56	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.20	-9.47	12.73	MgCl2:2H2O
MgCl2:4H2O	-16.77	-9.47	7.30	MgCl2:4H2O
MgCl2:H2O	-25.54	-9.47	16.07	MgCl2:H2O
MgOHCl	-19.23	-3.34	15.89	MgOHCl
MgSO4	-10.78	-5.95	4.83	MgSO4
Mirabilite	-7.11	-8.27	-1.15	Na2SO4:10H2O
Misenite	-47.57	-58.64	-11.08	K8H6(SO4)7
Mn	-67.82	15.11	82.93	Mn
Mn(OH)2(am)	-12.85	2.45	15.31	Mn(OH)2
Mn(OH)3	-14.29	-7.95	6.34	Mn(OH)3
MnCl2:2H2O	-13.80	-9.81	4.00	MnCl2:2H2O
MnCl2:4H2O	-12.56	-9.81	2.75	MnCl2:4H2O
MnCl2:H2O	-15.35	-9.81	5.54	MnCl2:H2O
MnO2(gamma)	-10.30	-26.43	-16.13	MnO2
MnSO4	-8.90	-6.29	2.61	MnSO4
Molysite	-26.65	-13.18	13.47	FeCl3
Na	-60.80	6.57	67.37	Na
Na(g)	-74.29	6.57	80.86	Na
Na2O	-66.93	0.48	67.42	Na2O
Na3H(SO4)2	-15.88	-16.77	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-15.74	-21.63	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-14.43	5.46	19.88	NaFeO2
Nantokite	-9.16	-15.93	-6.77	CuCl
O2(g)	-22.42	-25.32	-2.89	O2
Oxychloride-Mg	-26.37	-0.54	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.57	-5.95	-1.39	MgSO4:5H2O
Periclase	-18.53	2.79	21.33	MgO
Picromerite	-9.61	-14.05	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-9.95	-24.26	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-18.90	3.64	22.55	Ca(OH)2
Pyrolusite	-8.77	-26.43	-17.66	MnO2
Scacchite	-18.55	-9.81	8.74	MnCl2
Spinel	-23.83	13.78	37.61	Al2MgO4
Starkeyite	-4.95	-5.95	-1.00	MgSO4:4H2O
Sylvite	-6.63	-5.81	0.83	KCl
Syngenite	-5.60	-13.20	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-44.69	-27.55	17.14	Mg2CaCl6:12H2O
Tenorite	-5.01	2.63	7.65	CuO
Thenardite	-7.91	-8.26	-0.36	Na2SO4
Todorokite	-57.19	-103.02	-45.82	Mn7O12:3H2O
Wustite	-9.27	3.13	12.40	Fe.947O
Zincite	-8.87	2.33	11.20	ZnO
Zn	-53.80	14.98	68.79	Zn
Zn(ClO4)2:6H2O	-148.28	-142.65	5.63	Zn(ClO4)2:6H2O
Zn(g)	-70.42	14.98	85.41	Zn
Zn(OH)2(beta)	-9.61	2.33	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-9.33	2.33	11.66	Zn(OH)2
Zn(OH)2(gamma)	-9.56	2.33	11.88	Zn(OH)2
Zn2(OH)3Cl	-16.77	-1.48	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-11.68	-4.09	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-17.26	-7.95	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-29.61	-10.52	19.09	Zn3O(SO4)2
ZnCl2	-17.01	-9.93	7.08	ZnCl2
ZnSO4	-9.95	-6.42	3.53	ZnSO4
ZnSO4:6H2O	-4.72	-6.42	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-4.54	-6.42	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-5.87	-6.42	-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
Hexahydrate	-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 4
 3.000e+000 Solution 2 AS1

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

Elements	Molality	Moles
Al	2.376e-004	9.504e-004
As	1.768e-005	7.072e-005
Ca	2.884e-003	1.154e-002
Cl	8.435e-004	3.374e-003
Cu	1.397e-004	5.587e-004
F	9.873e-006	3.949e-005
Fe	7.632e-004	3.053e-003
K	5.022e-004	2.009e-003
Mg	7.032e-004	2.813e-003
Mn	9.638e-005	3.855e-004
N	1.553e-004	6.214e-004
Na	1.765e-003	7.061e-003
S	4.740e-003	1.896e-002
Zn	6.888e-005	2.755e-004

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

pH	=	3.500	Charge balance
pe	=	16.155	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	1.741e-002	
Mass of water (kg)	=	4.000e+000	
Total alkalinity (eq/kg)	=	-9.471e-004	
Total carbon (mol/kg)	=	0.000e+000	
Total CO2 (mol/kg)	=	0.000e+000	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	8.145e-003	
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	10.62	
Iterations	=	53	
Total H	=	4.442056e+002	
Total O	=	2.221811e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	3.529e-004	3.161e-004	-3.452	-3.500	-0.048
OH-	3.481e-011	3.047e-011	-10.458	-10.516	-0.058
H2O	5.553e+001	9.998e-001	1.744	-0.000	0.000
Al	2.376e-004				
Al+3	1.117e-004	4.093e-005	-3.952	-4.388	-0.436
AlSO4+	1.054e-004	9.246e-005	-3.977	-4.034	-0.057
Al(SO4)2-	1.806e-005	1.584e-005	-4.743	-4.800	-0.057
AlOH+2	2.435e-006	1.450e-006	-5.613	-5.839	-0.225
Al(OH)2+	1.214e-008	1.065e-008	-7.916	-7.973	-0.057
Al2(OH)2+4	2.541e-009	3.420e-010	-8.595	-9.466	-0.871
HALO2	4.903e-011	4.903e-011	-10.310	-10.310	0.000
Al3(OH)4+5	1.968e-012	9.038e-014	-11.706	-13.044	-1.338
AlO2-	6.054e-014	5.312e-014	-13.218	-13.275	-0.057
NaAlO2	1.547e-017	1.547e-017	-16.811	-16.811	0.000
AlF+2	2.196e-040	1.308e-040	-39.658	-39.883	-0.225
Al13O4(OH)24+7	0.000e+000	0.000e+000	-41.149	-43.772	-2.623
AlF2+	0.000e+000	0.000e+000	-76.722	-76.779	-0.057
AlF3	0.000e+000	0.000e+000	-115.174	-115.174	0.000
AlF4-	0.000e+000	0.000e+000	-155.213	-155.270	-0.057
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-149.136	-149.136	0.000

As (3)	1.034e-026					
HAsO2	5.519e-027	5.519e-027	-26.258	-26.258	0.000	
As (OH) 3	4.825e-027	4.825e-027	-26.316	-26.316	0.000	
H2AsO3-	1.064e-032	9.334e-033	-31.973	-32.030	-0.057	
AsO2-	1.017e-032	8.925e-033	-31.993	-32.049	-0.057	
AsO2OH-2	4.891e-040	2.885e-040	-39.311	-39.540	-0.229	
HAsS2	0.000e+000	0.000e+000	-271.427	-271.427	0.000	
As (5)	1.768e-005					
HAsO3F-	9.811e-006	8.609e-006	-5.008	-5.065	-0.057	
H2AsO4-	7.438e-006	6.526e-006	-5.129	-5.185	-0.057	
H3AsO4	3.634e-007	3.634e-007	-6.440	-6.440	0.000	
AsO3F-2	6.218e-008	3.667e-008	-7.206	-7.436	-0.229	
HAsO4-2	5.810e-009	3.427e-009	-8.236	-8.465	-0.229	
AsO4-3	9.140e-017	2.781e-017	-16.039	-16.556	-0.517	
Ca	2.884e-003					
Ca+2	2.408e-003	1.473e-003	-2.618	-2.832	-0.213	
CaSO4	4.750e-004	4.750e-004	-3.323	-3.323	0.000	
CaNO3+	6.427e-007	5.639e-007	-6.192	-6.249	-0.057	
CaCl+	2.617e-007	2.296e-007	-6.582	-6.639	-0.057	
CaCl2	1.986e-010	1.986e-010	-9.702	-9.702	0.000	
CaOH+	7.499e-013	6.580e-013	-12.125	-12.182	-0.057	
CaF+	0.000e+000	0.000e+000	-44.564	-44.621	-0.057	
Cl (-1)	8.435e-004					
Cl-	8.425e-004	7.354e-004	-3.074	-3.133	-0.059	
CaCl+	2.617e-007	2.296e-007	-6.582	-6.639	-0.057	
MgCl+	2.117e-007	1.857e-007	-6.674	-6.731	-0.057	
NaCl	1.973e-007	1.973e-007	-6.705	-6.705	0.000	
CuCl+	1.494e-007	1.311e-007	-6.826	-6.882	-0.057	
MnCl+	7.885e-008	6.919e-008	-7.103	-7.160	-0.057	
HCl	5.222e-008	5.222e-008	-7.282	-7.282	0.000	
ZnCl+	4.619e-008	4.053e-008	-7.335	-7.392	-0.057	
KCl	1.064e-008	1.064e-008	-7.973	-7.973	0.000	
FeCl+2	2.449e-009	1.459e-009	-8.611	-8.836	-0.225	
FeCl2+	9.898e-010	8.684e-010	-9.004	-9.061	-0.057	
CaCl2	1.986e-010	1.986e-010	-9.702	-9.702	0.000	
CuCl2	5.078e-011	5.078e-011	-10.294	-10.294	0.000	
ZnCl2	3.482e-011	3.482e-011	-10.458	-10.458	0.000	
FeCl+	5.306e-012	4.656e-012	-11.275	-11.332	-0.057	
Zn(OH)Cl	2.191e-012	2.191e-012	-11.659	-11.659	0.000	
ZnCl3-	1.612e-014	1.414e-014	-13.793	-13.850	-0.057	
MnCl3-	9.317e-015	8.175e-015	-14.031	-14.087	-0.057	
ZnCl4-2	1.337e-016	7.883e-017	-15.874	-16.103	-0.229	
FeCl2	1.837e-017	1.837e-017	-16.736	-16.736	0.000	
FeCl4-	6.436e-019	5.647e-019	-18.191	-18.248	-0.057	
CuCl2-	1.020e-019	8.949e-020	-18.991	-19.048	-0.057	
CuCl4-2	8.739e-022	5.154e-022	-21.059	-21.288	-0.229	
CuCl3-2	7.167e-022	4.227e-022	-21.145	-21.374	-0.229	
FeCl4-2	4.869e-023	2.872e-023	-22.313	-22.542	-0.229	
Cl (1)	1.371e-018					
HClO	1.371e-018	1.371e-018	-17.863	-17.863	0.000	
ClO-	1.333e-022	1.170e-022	-21.875	-21.932	-0.057	
Cl (3)	3.810e-034					
ClO2-	2.702e-034	2.371e-034	-33.568	-33.625	-0.057	
HClO2	1.108e-034	1.108e-034	-33.955	-33.955	0.000	
Cl (5)	3.908e-032					
ClO3-	3.908e-032	3.420e-032	-31.408	-31.466	-0.058	
Cl (7)	2.815e-034					
ClO4-	2.814e-034	2.463e-034	-33.551	-33.609	-0.058	
ZnClO4+	1.741e-037	1.528e-037	-36.759	-36.816	-0.057	
Cu (1)	2.949e-018					
Cu+	2.846e-018	2.497e-018	-17.546	-17.603	-0.057	
CuCl2-	1.020e-019	8.949e-020	-18.991	-19.048	-0.057	
CuCl3-2	7.167e-022	4.227e-022	-21.145	-21.374	-0.229	
Cu (2)	1.397e-004					
Cu+2	1.065e-004	6.517e-005	-3.972	-4.186	-0.213	
CuSO4	3.296e-005	3.296e-005	-4.482	-4.482	0.000	
CuCl+	1.494e-007	1.311e-007	-6.826	-6.882	-0.057	

	CuOH+	1.212e-008	1.063e-008	-7.917	-7.973	-0.057
	CuCl2	5.078e-011	5.078e-011	-10.294	-10.294	0.000
	CuNO2+	1.692e-018	1.485e-018	-17.772	-17.828	-0.057
	CuCl4-2	8.739e-022	5.154e-022	-21.059	-21.288	-0.229
	CuO2-2	3.926e-030	2.316e-030	-29.406	-29.635	-0.229
	Cu(NO2)2	3.305e-033	3.305e-033	-32.481	-32.481	0.000
	CuF+	0.000e+000	0.000e+000	-45.425	-45.481	-0.057
	CuNH3+2	0.000e+000	0.000e+000	-54.856	-55.081	-0.225
	Cu(NH3)2+2	0.000e+000	0.000e+000	-106.357	-106.582	-0.225
	Cu(NH3)3+2	0.000e+000	0.000e+000	-158.472	-158.697	-0.225
F		9.873e-006				
	HAsO3F-	9.811e-006	8.609e-006	-5.008	-5.065	-0.057
	AsO3F-2	6.218e-008	3.667e-008	-7.206	-7.436	-0.229
	AlF+2	2.196e-040	1.308e-040	-39.658	-39.883	-0.225
	F-	0.000e+000	0.000e+000	-42.438	-42.495	-0.058
	HF	0.000e+000	0.000e+000	-42.809	-42.809	0.000
	FeF+2	0.000e+000	0.000e+000	-43.019	-43.244	-0.225
	MgF+	0.000e+000	0.000e+000	-44.546	-44.603	-0.057
	CaF+	0.000e+000	0.000e+000	-44.564	-44.621	-0.057
	MnF+	0.000e+000	0.000e+000	-45.363	-45.420	-0.057
	CuF+	0.000e+000	0.000e+000	-45.425	-45.481	-0.057
	ZnF+	0.000e+000	0.000e+000	-45.773	-45.830	-0.057
	NaF	0.000e+000	0.000e+000	-46.283	-46.283	0.000
	FeF+	0.000e+000	0.000e+000	-49.140	-49.196	-0.057
	AlF2+	0.000e+000	0.000e+000	-76.722	-76.779	-0.057
	FeF2+	0.000e+000	0.000e+000	-81.474	-81.530	-0.057
	H2F2	0.000e+000	0.000e+000	-85.223	-85.223	0.000
	HF2-	0.000e+000	0.000e+000	-85.864	-85.921	-0.057
	AlF3	0.000e+000	0.000e+000	-115.174	-115.174	0.000
	AlF4-	0.000e+000	0.000e+000	-155.213	-155.270	-0.057
Fe(2)		1.725e-008				
	Fe+2	1.421e-008	8.690e-009	-7.848	-8.061	-0.213
	FeSO4	3.040e-009	3.040e-009	-8.517	-8.517	0.000
	FeCl+	5.306e-012	4.656e-012	-11.275	-11.332	-0.057
	FeOH+	9.904e-015	8.690e-015	-14.004	-14.061	-0.057
	FeCl2	1.837e-017	1.837e-017	-16.736	-16.736	0.000
	Fe(OH)2	2.183e-022	2.183e-022	-21.661	-21.661	0.000
	FeCl4-2	4.869e-023	2.872e-023	-22.313	-22.542	-0.229
	Fe(OH)3-	3.132e-029	2.749e-029	-28.504	-28.561	-0.057
	Fe(OH)4-2	1.474e-040	0.000e+000	-39.832	-40.061	-0.229
	FeF+	0.000e+000	0.000e+000	-49.140	-49.196	-0.057
Fe(3)		7.632e-004				
	FeOH+2	4.081e-004	2.430e-004	-3.389	-3.614	-0.225
	Fe(OH)2+	2.901e-004	2.545e-004	-3.538	-3.594	-0.057
	Fe+3	3.249e-005	1.190e-005	-4.488	-4.924	-0.436
	Fe2(OH)2+4	1.181e-005	1.590e-006	-4.928	-5.799	-0.871
	FeSO4+	2.897e-006	2.542e-006	-5.538	-5.595	-0.057
	Fe3(OH)4+5	1.840e-006	8.454e-008	-5.735	-7.073	-1.338
	Fe(OH)3	3.765e-007	3.765e-007	-6.424	-6.424	0.000
	Fe(SO4)2-	1.081e-007	9.487e-008	-6.966	-7.023	-0.057
	FeNO3+2	1.527e-008	9.092e-009	-7.816	-8.041	-0.225
	FeCl+2	2.449e-009	1.459e-009	-8.611	-8.836	-0.225
	FeCl2+	9.898e-010	8.684e-010	-9.004	-9.061	-0.057
	Fe(OH)4-	3.408e-013	2.991e-013	-12.467	-12.524	-0.057
	FeNO2+2	6.142e-018	3.658e-018	-17.212	-17.437	-0.225
	FeCl4-	6.436e-019	5.647e-019	-18.191	-18.248	-0.057
	FeF+2	0.000e+000	0.000e+000	-43.019	-43.244	-0.225
	FeF2+	0.000e+000	0.000e+000	-81.474	-81.530	-0.057
H(0)		0.000e+000				
	H2	0.000e+000	0.000e+000	-42.412	-42.411	0.002
K		5.022e-004				
	K+	4.934e-004	4.307e-004	-3.307	-3.366	-0.059
	KSO4-	8.747e-006	7.675e-006	-5.058	-5.115	-0.057
	KCl	1.064e-008	1.064e-008	-7.973	-7.973	0.000
	KHSO4	2.141e-009	2.141e-009	-8.669	-8.669	0.000
	KOH	4.723e-015	4.723e-015	-14.326	-14.326	0.000
Mg		7.032e-004				

Mg+2	5.123e-004	3.235e-004	-3.290	-3.490	-0.200
MgSO4	1.907e-004	1.907e-004	-3.720	-3.720	0.000
MgCl+	2.117e-007	1.857e-007	-6.674	-6.731	-0.057
Mg4(OH)4+4	1.447e-039	1.948e-040	-38.839	-39.710	-0.871
MgF+	0.000e+000	0.000e+000	-44.546	-44.603	-0.057
Mn(2)	9.638e-005				
Mn+2	7.223e-005	4.418e-005	-4.141	-4.355	-0.213
MnSO4	2.406e-005	2.406e-005	-4.619	-4.619	0.000
MnCl+	7.885e-008	6.919e-008	-7.103	-7.160	-0.057
MnNO3+	6.096e-009	5.349e-009	-8.215	-8.272	-0.057
MnOH+	4.093e-012	3.592e-012	-11.388	-11.445	-0.057
Mn(NO3)2	1.026e-012	1.026e-012	-11.989	-11.989	0.000
MnCl3-	9.317e-015	8.175e-015	-14.031	-14.087	-0.057
Mn2OH+3	5.357e-016	1.700e-016	-15.271	-15.769	-0.498
Mn(OH)2	2.788e-020	2.788e-020	-19.555	-19.555	0.000
Mn2(OH)3+	8.859e-023	7.773e-023	-22.053	-22.109	-0.057
Mn(OH)3-	9.426e-029	8.271e-029	-28.026	-28.082	-0.057
Mn(OH)4-2	3.756e-039	2.215e-039	-38.425	-38.655	-0.229
MnF+	0.000e+000	0.000e+000	-45.363	-45.420	-0.057
Mn(3)	5.304e-014				
Mn+3	5.304e-014	1.684e-014	-13.275	-13.774	-0.498
Mn(6)	1.117e-030				
MnO4-2	1.117e-030	6.586e-031	-29.952	-30.181	-0.229
Mn(7)	4.734e-024				
MnO4-	4.734e-024	4.143e-024	-23.325	-23.383	-0.058
N(-03)	0.000e+000				
HN3	0.000e+000	0.000e+000	-77.906	-77.906	0.000
N3-	0.000e+000	0.000e+000	-79.051	-79.108	-0.057
ZnN3+	0.000e+000	0.000e+000	-83.094	-83.150	-0.057
Zn(N3)2	0.000e+000	0.000e+000	-161.505	-161.505	0.000
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-49.135	-49.195	-0.060
CuNH3+2	0.000e+000	0.000e+000	-54.856	-55.081	-0.225
NH3	0.000e+000	0.000e+000	-54.935	-54.935	0.000
Zn(NH3)+2	0.000e+000	0.000e+000	-57.141	-57.366	-0.225
NH4SO4-	0.000e+000	0.000e+000	-60.094	-60.151	-0.057
Cu(NH3)2+2	0.000e+000	0.000e+000	-106.357	-106.582	-0.225
Zn(NH3)2+2	0.000e+000	0.000e+000	-109.870	-110.095	-0.225
Cu(NH3)3+2	0.000e+000	0.000e+000	-158.472	-158.697	-0.225
Zn(NH3)3+2	0.000e+000	0.000e+000	-162.599	-162.824	-0.225
Zn(NH3)4+2	0.000e+000	0.000e+000	-215.601	-215.826	-0.225
N(0)	6.718e-005				
N2	3.359e-005	3.359e-005	-4.474	-4.474	0.000
N(3)	3.744e-016				
NO2-	2.492e-016	2.176e-016	-15.603	-15.662	-0.059
HNO2	1.174e-016	1.174e-016	-15.930	-15.930	0.000
FeNO2+2	6.142e-018	3.658e-018	-17.212	-17.437	-0.225
CuNO2+	1.692e-018	1.485e-018	-17.772	-17.828	-0.057
Cu(NO2)2	3.305e-033	3.305e-033	-32.481	-32.481	0.000
N(5)	8.817e-005				
NO3-	8.750e-005	7.639e-005	-4.058	-4.117	-0.059
CaNO3+	6.427e-007	5.639e-007	-6.192	-6.249	-0.057
FeNO3+2	1.527e-008	9.092e-009	-7.816	-8.041	-0.225
MnNO3+	6.096e-009	5.349e-009	-8.215	-8.272	-0.057
HNO3	1.263e-009	1.263e-009	-8.899	-8.899	0.000
Mn(NO3)2	1.026e-012	1.026e-012	-11.989	-11.989	0.000
Na	1.765e-003				
Na+	1.740e-003	1.527e-003	-2.759	-2.816	-0.057
NaSO4-	2.537e-005	2.226e-005	-4.596	-4.652	-0.057
NaCl	1.973e-007	1.973e-007	-6.705	-6.705	0.000
NaOH	8.025e-015	8.025e-015	-14.096	-14.096	0.000
NaAlO2	1.547e-017	1.547e-017	-16.811	-16.811	0.000
NaF	0.000e+000	0.000e+000	-46.283	-46.283	0.000
O(0)	8.396e-008				
O2	4.198e-008	4.216e-008	-7.377	-7.375	0.002
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-126.179	-126.179	0.000

HS-	0.000e+000	0.000e+000	-129.631	-129.689	-0.058
S-2	0.000e+000	0.000e+000	-138.893	-139.114	-0.221
S2-2	0.000e+000	0.000e+000	-229.578	-229.807	-0.229
HAsS2	0.000e+000	0.000e+000	-271.427	-271.427	0.000
S3-2	0.000e+000	0.000e+000	-320.312	-320.541	-0.229
S4-2	0.000e+000	0.000e+000	-411.273	-411.502	-0.229
S5-2	0.000e+000	0.000e+000	-502.450	-502.680	-0.229
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-130.807	-131.036	-0.229
HS2O3-	0.000e+000	0.000e+000	-133.465	-133.522	-0.057
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-119.431	-119.652	-0.221
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-41.798	-41.855	-0.057
H2SO3	0.000e+000	0.000e+000	-43.373	-43.373	0.000
SO2	0.000e+000	0.000e+000	-43.474	-43.474	0.000
SO3-2	0.000e+000	0.000e+000	-45.361	-45.586	-0.225
S2O6-2	0.000e+000	0.000e+000	-59.764	-59.994	-0.229
S3O6-2	0.000e+000	0.000e+000	-152.981	-153.210	-0.229
S4O6-2	0.000e+000	0.000e+000	-230.292	-230.521	-0.229
S5O6-2	0.000e+000	0.000e+000	-336.482	-336.712	-0.229
S(5)	0.000e+000				
S2O5-2	0.000e+000	0.000e+000	-88.311	-88.540	-0.229
S(6)	4.740e-003				
SO4-2	3.743e-003	2.207e-003	-2.427	-2.656	-0.229
CaSO4	4.750e-004	4.750e-004	-3.323	-3.323	0.000
MgSO4	1.907e-004	1.907e-004	-3.720	-3.720	0.000
AlSO4+	1.054e-004	9.246e-005	-3.977	-4.034	-0.057
HSO4-	8.034e-005	7.049e-005	-4.095	-4.152	-0.057
CuSO4	3.296e-005	3.296e-005	-4.482	-4.482	0.000
NaSO4-	2.537e-005	2.226e-005	-4.596	-4.652	-0.057
MnSO4	2.406e-005	2.406e-005	-4.619	-4.619	0.000
Al(SO4)2-	1.806e-005	1.584e-005	-4.743	-4.800	-0.057
ZnSO4	1.521e-005	1.521e-005	-4.818	-4.818	0.000
KSO4-	8.747e-006	7.675e-006	-5.058	-5.115	-0.057
FeSO4+	2.897e-006	2.542e-006	-5.538	-5.595	-0.057
Fe(SO4)2-	1.081e-007	9.487e-008	-6.966	-7.023	-0.057
FeSO4	3.040e-009	3.040e-009	-8.517	-8.517	0.000
KHSO4	2.141e-009	2.141e-009	-8.669	-8.669	0.000
H2SO4	2.103e-011	2.103e-011	-10.677	-10.677	0.000
NH4SO4-	0.000e+000	0.000e+000	-60.094	-60.151	-0.057
S(7)	1.189e-038				
S2O8-2	5.947e-039	3.507e-039	-38.226	-38.455	-0.229
S(8)	8.961e-028				
HSO5-	8.961e-028	7.862e-028	-27.048	-27.104	-0.057
Zn	6.888e-005				
Zn+2	5.362e-005	3.280e-005	-4.271	-4.484	-0.213
ZnSO4	1.521e-005	1.521e-005	-4.818	-4.818	0.000
ZnCl+	4.619e-008	4.053e-008	-7.335	-7.392	-0.057
ZnOH+	1.296e-010	1.138e-010	-9.887	-9.944	-0.057
ZnCl2	3.482e-011	3.482e-011	-10.458	-10.458	0.000
Zn(OH)Cl	2.191e-012	2.191e-012	-11.659	-11.659	0.000
ZnCl3-	1.612e-014	1.414e-014	-13.793	-13.850	-0.057
Zn(OH)2	1.541e-015	1.541e-015	-14.812	-14.812	0.000
ZnCl4-2	1.337e-016	7.883e-017	-15.874	-16.103	-0.229
Zn(OH)3-	1.721e-023	1.510e-023	-22.764	-22.821	-0.057
Zn(OH)4-2	1.381e-032	8.143e-033	-31.860	-32.089	-0.229
ZnClO4+	1.741e-037	1.528e-037	-36.759	-36.816	-0.057
ZnF+	0.000e+000	0.000e+000	-45.773	-45.830	-0.057
Zn(NH3)+2	0.000e+000	0.000e+000	-57.141	-57.366	-0.225
ZnN3+	0.000e+000	0.000e+000	-83.094	-83.150	-0.057
Zn(NH3)2+2	0.000e+000	0.000e+000	-109.870	-110.095	-0.225
Zn(N3)2	0.000e+000	0.000e+000	-161.505	-161.505	0.000
Zn(NH3)3+2	0.000e+000	0.000e+000	-162.599	-162.824	-0.225
Zn(NH3)4+2	0.000e+000	0.000e+000	-215.601	-215.826	-0.225

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

Phase	SI	log IAP	log KT	
Al	-138.27	11.64	149.91	Al
Al(g)	-188.97	11.64	200.62	Al
Al2(SO4)3	-35.64	-16.74	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-18.30	-16.74	1.56	Al2(SO4)3:6H2O
Alabandite	-130.12	-130.54	-0.42	MnS
AlF3	-114.61	-131.87	-17.27	AlF3
Alum-K	-8.10	-13.07	-4.97	KAl(SO4)2:12H2O
Alunite	-0.37	-0.84	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.14	-5.49	-4.35	CaSO4
Antarcticite	-13.19	-9.10	4.09	CaCl2:6H2O
Antlerite	-9.94	-1.21	8.73	Cu3(SO4)(OH)4
Aphthitalite	-14.34	-18.23	-3.89	NaK3(SO4)2
Arcanite	-7.54	-9.39	-1.84	K2SO4
Arsenolite	-51.22	-71.06	-19.84	As2O3
Arsenopyrite	-212.14	-226.58	-14.45	FeAsS
As	-72.68	-30.00	42.68	As
As2O5	-19.51	-17.37	2.14	As2O5
As4O6(cubi)	-102.30	-142.12	-39.82	As4O6
As4O6(mono)	-102.07	-142.12	-40.05	As4O6
Atacamite	-16.27	-2.01	14.26	Cu4Cl2(OH)6
Bassanite	-1.78	-5.49	-3.71	CaSO4:0.5H2O
Birnessite	-12.77	-98.32	-85.55	Mn8O14:5H2O
Bischofite	-14.15	-9.76	4.39	MgCl2:6H2O
Bixbyite	-5.58	-6.55	-0.96	Mn2O3
Bloedite	-11.96	-14.44	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-1.44	6.11	7.55	AlO2H
Bornite	-484.88	-587.41	-102.53	Cu5FeS4
Brochantite	-13.82	1.60	15.42	Cu4(SO4)(OH)6
Brucite	-12.77	3.51	16.28	Mg(OH)2
Ca	-131.98	7.86	139.83	Ca
Ca(g)	-157.22	7.86	165.07	Ca
Ca2Al2O5:8H2O	-39.01	20.56	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-31.22	-4.93	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-22.67	-4.87	17.80	Ca3(AsO4)2
Ca3Al2O6	-88.30	24.73	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-100.43	40.05	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-78.36	28.90	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-74.78	28.90	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-64.92	3.40	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-30.52	16.39	46.91	CaAl2O4
CaAl2O4:10H2O	-21.60	16.39	37.99	CaAl2O4:10H2O
CaAl4O7	-39.97	28.62	68.59	CaAl4O7
Carnallite	-20.53	-16.26	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.95	-5.49	-3.54	CaSO4:0.5H2O
Chalcanthite	-4.21	-6.84	-2.63	CuSO4:5H2O
Chalcocite	-126.65	-161.39	-34.74	Cu2S
Chalcocyanite	-9.75	-6.84	2.91	CuSO4
Chalcopyrite	-232.02	-264.62	-32.60	CuFeS2
Chloromagnesite	-31.57	-9.76	21.82	MgCl2
Cl2(g)	-19.95	-16.95	2.99	Cl2
Claudetite	-51.26	-71.06	-19.80	As2O3
Corundum	-6.07	12.22	18.29	Al2O3
Covellite	-107.51	-130.37	-22.86	CuS
Cu	-24.99	6.50	31.50	Cu
Cu(g)	-77.15	6.50	83.66	Cu
CuCl2	-14.17	-10.45	3.72	CuCl2
CuF	-67.18	-60.10	7.08	CuF
CuF2	-88.56	-89.18	-0.62	CuF2
CuF2:2H2O	-84.63	-89.18	-4.55	CuF2:2H2O
Cuprite	-26.30	-28.20	-1.91	Cu2O
Delafoosite	-2.09	-8.53	-6.44	CuFeO2
Diaspore	-1.03	6.11	7.15	AlHO2
Epsomite	-4.18	-6.15	-1.96	MgSO4:7H2O
Ettringite	-54.20	8.26	62.46	Ca6Al2(SO4)3(OH)12:26H2O

F2(g)	-151.39	-95.68	55.71	F2
Fe	-56.39	2.63	59.02	Fe
Fe(OH)2	-14.96	-1.06	13.89	Fe(OH)2
Fe(OH)3	-0.06	5.58	5.64	Fe(OH)3
Fe2(SO4)3	-20.86	-17.82	3.05	Fe2(SO4)3
FeF2	-90.63	-93.05	-2.42	FeF2
FeF3	-113.15	-132.41	-19.26	FeF3
FeO	-14.58	-1.06	13.52	FeO
Ferrite-Ca	-6.18	15.32	21.50	CaFe2O4
Ferrite-Cu	3.68	13.97	10.28	CuFe2O4
Ferrite-Dicalcium	-37.31	19.49	56.80	Ca2Fe2O5
Ferrite-Mg	-6.36	14.66	21.02	MgFe2O4
Ferrite-Zn	1.97	13.67	11.70	ZnFe2O4
FeSO4	-13.32	-10.72	2.61	FeSO4
Fluorite	-77.75	-87.82	-10.07	CaF2
Gibbsite	-1.63	6.11	7.74	Al(OH)3
Glauberite	-8.31	-13.78	-5.47	Na2Ca(SO4)2
Goethite	5.05	5.58	0.53	FeOOH
Gypsum	-0.96	-5.49	-4.53	CaSO4:2H2O
H2(g)	-39.31	-42.41	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-125.20	-133.19	-7.99	H2S
Halite	-7.51	-5.95	1.56	NaCl
Hausmannite	-14.05	-3.90	10.14	Mn3O4
HCl(g)	-12.94	-6.63	6.30	HCl
Hematite	11.08	11.15	0.08	Fe2O3
Hercynite	-17.64	11.16	28.80	FeAl2O4
Hexahydrate	-4.42	-6.15	-1.73	MgSO4:6H2O
Hydrophilite	-20.84	-9.10	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	6.96	-2.45	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	3.55	-1.90	-5.45	NaFe3(SO4)2(OH)6
K	-69.00	1.98	70.98	K
K(g)	-79.60	1.98	81.58	K
K2O	-83.77	0.27	84.04	K2O
K3H(SO4)2	-15.29	-18.91	-3.62	K3H(SO4)2
Kainite	-12.33	-12.65	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-16.34	-13.07	3.27	KAl(SO4)2
Katoite	-54.21	24.73	78.94	Ca3Al2H12O12
Kieserite	-5.88	-6.15	-0.27	MgSO4:H2O
KMgCl3	-37.50	-16.26	21.25	KMgCl3
KMgCl3:2H2O	-30.22	-16.26	13.96	KMgCl3:2H2O
Lammerite	-10.48	-8.93	1.55	Cu3(AsO4)2
Lawrencite	-23.38	-14.33	9.05	FeCl2
Leonite	-11.42	-15.53	-4.11	K2Mg(SO4)2:4H2O
Lime	-28.40	4.17	32.57	CaO
Magnetite	-0.33	10.09	10.42	Fe3O4
Manganite	-3.11	-3.27	-0.16	MnO(OH)
Manganosite	-15.27	2.65	17.92	MnO
Mayenite	-358.56	135.59	494.15	Ca12Al14O33
Melanterite	-8.32	-10.72	-2.40	FeSO4:7H2O
Mercallite	-8.08	-9.52	-1.44	KHSO4
Mg	-115.32	7.20	122.52	Mg
Mg(g)	-135.05	7.20	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.46	-5.27	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-13.60	-4.39	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.49	-9.76	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.06	-9.76	7.30	MgCl2:4H2O
MgCl2:H2O	-25.83	-9.76	16.07	MgCl2:H2O
MgOHCl	-19.01	-3.12	15.89	MgOHCl
MgSO4	-10.97	-6.15	4.83	MgSO4
Mirabilite	-7.14	-8.29	-1.15	Na2SO4:10H2O
Misenite	-55.44	-66.52	-11.08	K8H6(SO4)7
Mn	-76.60	6.33	82.93	Mn
Mn(OH)2(am)	-12.66	2.65	15.31	Mn(OH)2
Mn(OH)3	-9.61	-3.27	6.34	Mn(OH)3
MnCl2:2H2O	-14.62	-10.62	4.00	MnCl2:2H2O

MnCl2:4H2O	-13.37	-10.62	2.75	MnCl2:4H2O
MnCl2:H2O	-16.16	-10.62	5.54	MnCl2:H2O
MnO2(gamma)	-1.14	-17.27	-16.13	MnO2
MnSO4	-9.62	-7.01	2.61	MnSO4
Molysite	-27.80	-14.32	13.47	FeCl3
N2(g)	-1.29	-4.47	-3.18	N2
Na	-64.84	2.53	67.37	Na
Na(g)	-78.33	2.53	80.86	Na
Na2O	-66.05	1.37	67.42	Na2O
Na3H(SO4)2	-16.37	-17.26	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.17	-22.07	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-13.62	6.26	19.88	NaFeO2
Nantokite	-13.97	-20.74	-6.77	CuCl
NH3(g)	-56.73	-54.93	1.80	NH3
Niter	-7.26	-7.48	-0.22	KNO3
NO(g)	-18.06	-17.32	0.74	NO
NO2(g)	-14.12	-5.77	8.35	NO2
O2(g)	-4.48	-7.38	-2.89	O2
Orpiment	-391.14	-470.63	-79.49	As2S3
Oxychloride-Mg	-25.45	0.39	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.76	-6.15	-1.39	MgSO4:5H2O
Periclase	-17.81	3.51	21.33	MgO
Picromerite	-11.09	-15.53	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-12.20	-26.51	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-18.38	4.17	22.55	Ca(OH)2
Pyrite	-211.86	-236.55	-24.70	FeS2
Pyrolusite	0.39	-17.27	-17.66	MnO2
Pyrrhotite	-130.51	-134.25	-3.74	FeS
Realgar	-152.18	-212.46	-60.28	AsS
S	-91.77	-136.88	-45.11	S
S2(g)	-197.42	-204.61	-7.19	S2
Scacchite	-19.36	-10.62	8.74	MnCl2
Sellaite	-79.04	-88.48	-9.44	MgF2
SO2(g)	-43.65	-43.47	0.18	SO2
Sphalerite	-119.20	-130.67	-11.47	ZnS
Spinel	-21.87	15.73	37.61	Al2MgO4
Starkeyite	-5.15	-6.15	-1.00	MgSO4:4H2O
Sylvite	-7.33	-6.50	0.83	KCl
Syngenite	-7.28	-14.88	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-45.76	-28.61	17.14	Mg2CaCl6:12H2O
Tenorite	-4.83	2.81	7.65	CuO
Thenardite	-7.93	-8.29	-0.36	Na2SO4
Todorokite	-11.00	-56.82	-45.82	Mn7O12:3H2O
Troilite	-130.41	-134.25	-3.84	FeS
Wurtzite	-121.50	-130.67	-9.17	ZnS
Wustite	-12.70	-0.30	12.40	Fe.947O
Zincite	-8.68	2.52	11.20	ZnO
Zn	-62.58	6.20	68.79	Zn
Zn(ClO4)2:6H2O	-77.34	-71.70	5.63	Zn(ClO4)2:6H2O
Zn(g)	-79.20	6.20	85.41	Zn
Zn(NO3)2:6H2O	-16.12	-12.72	3.40	Zn(NO3)2:6H2O
Zn(OH)2(beta)	-9.42	2.52	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-9.14	2.52	11.66	Zn(OH)2
Zn(OH)2(gamma)	-9.37	2.52	11.88	Zn(OH)2
Zn2(OH)3Cl	-16.89	-1.60	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-12.21	-4.62	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-19.13	-9.82	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-30.85	-11.76	19.09	Zn3O(SO4)2
Zn5(NO3)2(OH)8	-45.32	-2.65	42.67	Zn5(NO3)2(OH)8
ZnCl2	-17.83	-10.75	7.08	ZnCl2
ZnCl2(NH3)2	-113.61	-120.62	-7.01	ZnCl2(NH3)2
ZnCl2(NH3)4	-223.78	-230.49	-6.71	ZnCl2(NH3)4
ZnCl2(NH3)6	-335.62	-340.36	-4.74	ZnCl2(NH3)6
ZnF2	-88.98	-89.48	-0.49	ZnF2
ZnSO4	-10.67	-7.14	3.53	ZnSO4
ZnSO4:6H2O	-5.44	-7.14	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.26	-7.14	-1.88	ZnSO4:7H2O

ZnSO4:H2O -6.59 -7.14 -0.55 ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
