
Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
NAMED_EXPRESSIONS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

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

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

```

Beginning of initial solution calculations.

Initial solution 1. Flujo 2

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

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

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

```

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

```

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

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

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

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

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

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

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

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

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

Initial solution 2. AS1

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

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

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

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

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

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

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

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

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

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

Antlerite	-0.42	8.31	8.73	Cu 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 2
1.000e+000 Solution 2 AS1

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

Elements	Molality	Moles
Al	1.558e-004	3.117e-004
As	2.649e-006	5.299e-006
Ca	1.519e-003	3.039e-003
Cl	9.810e-004	1.962e-003
Cu	1.677e-006	3.354e-006
F	6.582e-006	1.316e-005
Fe	3.890e-004	7.780e-004
K	2.416e-004	4.831e-004
Mg	5.696e-004	1.139e-003
Mn	5.632e-005	1.126e-004
N	1.036e-004	2.071e-004
Na	1.245e-003	2.490e-003
S	6.203e-003	1.241e-002
Zn	1.297e-005	2.595e-005

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

pH	=	3.025	Charge balance
pe	=	16.947	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	1.670e-002	
Mass of water (kg)	=	2.000e+000	
Total alkalinity (eq/kg)	=	-1.783e-003	
Total carbon (mol/kg)	=	0.000e+000	
Total CO2 (mol/kg)	=	0.000e+000	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	-1.011e-002	
Percent error, 100*(Cat- An)/(Cat+ An)	=	-27.21	
Iterations	=	13	
Total H	=	2.221046e+002	
Total O	=	1.111015e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	1.051e-003	9.433e-004	-2.978	-3.025	-0.047
OH-	1.164e-011	1.021e-011	-10.934	-10.991	-0.057
H2O	5.553e+001	9.998e-001	1.744	-0.000	0.000
Al	1.558e-004				
AlSO4+	7.616e-005	6.698e-005	-4.118	-4.174	-0.056
Al+3	5.717e-005	2.126e-005	-4.243	-4.672	-0.430
Al(SO4)2-	1.820e-005	1.600e-005	-4.740	-4.796	-0.056
AlF+2	3.875e-006	2.329e-006	-5.412	-5.633	-0.221
AlOH+2	4.202e-007	2.525e-007	-6.377	-6.598	-0.221
AlF2+	1.154e-008	1.015e-008	-7.938	-7.993	-0.056
Al(OH)2+	7.066e-010	6.214e-010	-9.151	-9.207	-0.056
Al2(OH)2+4	7.448e-011	1.037e-011	-10.128	-10.984	-0.856
AlF3	1.399e-012	1.399e-012	-11.854	-11.854	0.000
HAlo2	9.588e-013	9.588e-013	-12.018	-12.018	0.000
Al3(OH)4+5	3.308e-015	1.599e-016	-14.480	-15.796	-1.316
AlO2-	3.959e-016	3.482e-016	-15.402	-15.458	-0.056
AlF4-	4.377e-018	3.849e-018	-17.359	-17.415	-0.056
NaAlO2	7.127e-020	7.127e-020	-19.147	-19.147	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-60.082	-62.661	-2.580
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-186.775	-186.775	0.000

As(3)	0.000e+000					
HAsO2	0.000e+000	0.000e+000	0.000e+000	-61.995	-61.995	0.000
As(OH)3	0.000e+000	0.000e+000	0.000e+000	-62.054	-62.054	0.000
H2AsO3-	0.000e+000	0.000e+000	0.000e+000	-68.186	-68.242	-0.056
AsO2-	0.000e+000	0.000e+000	0.000e+000	-68.206	-68.262	-0.056
AsO2OH-2	0.000e+000	0.000e+000	0.000e+000	-76.002	-76.227	-0.225
HAsS2	0.000e+000	0.000e+000	0.000e+000	-310.048	-310.048	0.000
As(5)	2.649e-006					
HAsO3F-	2.644e-006	2.325e-006		-5.578	-5.634	-0.056
AsO3F-2	5.576e-009	3.320e-009		-8.254	-8.479	-0.225
H2AsO4-	0.000e+000	0.000e+000		-40.708	-40.764	-0.056
H3AsO4	0.000e+000	0.000e+000		-41.543	-41.543	0.000
HAsO4-2	0.000e+000	0.000e+000		-44.293	-44.518	-0.225
AsO4-3	0.000e+000	0.000e+000		-52.576	-53.084	-0.508
Ca	1.519e-003					
Ca+2	1.189e-003	7.333e-004		-2.925	-3.135	-0.210
CaSO4	3.297e-004	3.297e-004		-3.482	-3.482	0.000
CaNO3+	3.752e-007	3.300e-007		-6.426	-6.482	-0.056
CaCl+	1.516e-007	1.333e-007		-6.819	-6.875	-0.056
CaCl2	1.345e-010	1.345e-010		-9.871	-9.871	0.000
CaF+	4.642e-011	4.082e-011		-10.333	-10.389	-0.056
CaOH+	1.248e-013	1.098e-013		-12.904	-12.959	-0.056
Cl(-1)	9.810e-004					
Cl-	9.803e-004	8.579e-004		-3.009	-3.067	-0.058
HCl	1.817e-007	1.817e-007		-6.741	-6.741	0.000
MgCl+	1.811e-007	1.593e-007		-6.742	-6.798	-0.056
NaCl	1.618e-007	1.618e-007		-6.791	-6.791	0.000
CaCl+	1.516e-007	1.333e-007		-6.819	-6.875	-0.056
MnCl+	4.908e-008	4.316e-008		-7.309	-7.365	-0.056
ZnCl+	9.367e-009	8.238e-009		-8.028	-8.084	-0.056
KCl	5.943e-009	5.943e-009		-8.226	-8.226	0.000
FeCl+2	5.261e-009	3.161e-009		-8.279	-8.500	-0.221
FeCl2+	2.497e-009	2.196e-009		-8.603	-8.658	-0.056
CuCl+	1.921e-009	1.689e-009		-8.716	-8.772	-0.056
CaCl2	1.345e-010	1.345e-010		-9.871	-9.871	0.000
ZnCl2	8.255e-012	8.255e-012		-11.083	-11.083	0.000
FeCl+	1.854e-012	1.630e-012		-11.732	-11.788	-0.056
CuCl2	7.633e-013	7.633e-013		-12.117	-12.117	0.000
Zn(OH)Cl	1.493e-013	1.493e-013		-12.826	-12.826	0.000
MnCl3-	7.891e-015	6.939e-015		-14.103	-14.159	-0.056
ZnCl3-	4.447e-015	3.911e-015		-14.352	-14.408	-0.056
ZnCl4-2	4.272e-017	2.543e-017		-16.369	-16.595	-0.225
FeCl2	7.504e-018	7.504e-018		-17.125	-17.125	0.000
FeCl4-	2.209e-018	1.943e-018		-17.656	-17.712	-0.056
CuCl2-	2.471e-022	2.173e-022		-21.607	-21.663	-0.056
FeCl4-2	2.681e-023	1.596e-023		-22.572	-22.797	-0.225
CuCl4-2	1.771e-023	1.054e-023		-22.752	-22.977	-0.225
CuCl3-2	2.011e-024	1.197e-024		-23.697	-23.922	-0.225
Cl(1)	2.054e-017					
HClO	2.054e-017	2.054e-017		-16.687	-16.687	0.000
ClO-	6.678e-022	5.872e-022		-21.175	-21.231	-0.056
Cl(3)	1.297e-032					
HClO2	7.146e-033	7.146e-033		-32.146	-32.146	0.000
ClO2-	5.827e-033	5.124e-033		-32.235	-32.290	-0.056
Cl(5)	3.626e-030					
ClO3-	3.626e-030	3.182e-030		-29.441	-29.497	-0.057
Cl(7)	1.124e-031					
ClO4-	1.124e-031	9.860e-032		-30.949	-31.006	-0.057
ZnClO4+	1.212e-035	1.066e-035		-34.916	-34.972	-0.056
Cu(1)	5.317e-021					
Cu+	5.068e-021	4.457e-021		-20.295	-20.351	-0.056
CuCl2-	2.471e-022	2.173e-022		-21.607	-21.663	-0.056
CuCl3-2	2.011e-024	1.197e-024		-23.697	-23.922	-0.225
Cu(2)	1.677e-006					
Cu+2	1.168e-006	7.200e-007		-5.933	-6.143	-0.210
CuSO4	5.077e-007	5.077e-007		-6.294	-6.294	0.000
CuCl+	1.921e-009	1.689e-009		-8.716	-8.772	-0.056

	CuOH+	4.476e-011	3.936e-011	-10.349	-10.405	-0.056
	CuCl2	7.633e-013	7.633e-013	-12.117	-12.117	0.000
	CuF+	1.421e-013	1.250e-013	-12.847	-12.903	-0.056
	CuNO2+	5.093e-021	4.479e-021	-20.293	-20.349	-0.056
	CuCl4-2	1.771e-023	1.054e-023	-22.752	-22.977	-0.225
	CuO2-2	5.422e-034	3.228e-034	-33.266	-33.491	-0.225
	Cu(NO2)2	2.722e-036	2.722e-036	-35.565	-35.565	0.000
	CuNH3+2	0.000e+000	0.000e+000	-58.807	-59.028	-0.221
	Cu(NH3)2+2	0.000e+000	0.000e+000	-112.299	-112.521	-0.221
	Cu(NH3)3+2	0.000e+000	0.000e+000	-166.405	-166.626	-0.221
F		6.582e-006				
	AlF+2	3.875e-006	2.329e-006	-5.412	-5.633	-0.221
	HAsO3F-	2.644e-006	2.325e-006	-5.578	-5.634	-0.056
	HF	1.586e-008	1.586e-008	-7.800	-7.800	0.000
	F-	1.248e-008	1.095e-008	-7.904	-7.961	-0.057
	AlF2+	1.154e-008	1.015e-008	-7.938	-7.993	-0.056
	FeF+2	6.045e-009	3.632e-009	-8.219	-8.440	-0.221
	AsO3F-2	5.576e-009	3.320e-009	-8.254	-8.479	-0.225
	MgF+	7.147e-011	6.285e-011	-10.146	-10.202	-0.056
	CaF+	4.642e-011	4.082e-011	-10.333	-10.389	-0.056
	MnF+	7.919e-012	6.964e-012	-11.101	-11.157	-0.056
	AlF3	1.399e-012	1.399e-012	-11.854	-11.854	0.000
	NaF	1.257e-012	1.257e-012	-11.901	-11.901	0.000
	ZnF+	1.005e-012	8.841e-013	-11.998	-12.054	-0.056
	FeF2+	7.318e-013	6.436e-013	-12.136	-12.191	-0.056
	CuF+	1.421e-013	1.250e-013	-12.847	-12.903	-0.056
	FeF+	7.440e-016	6.543e-016	-15.128	-15.184	-0.056
	H2F2	6.254e-016	6.254e-016	-15.204	-15.204	0.000
	HF2-	4.783e-017	4.206e-017	-16.320	-16.376	-0.056
	AlF4-	4.377e-018	3.849e-018	-17.359	-17.415	-0.056
Fe(2)		5.504e-009				
	Fe+2	4.230e-009	2.608e-009	-8.374	-8.584	-0.210
	FeSO4	1.272e-009	1.272e-009	-8.895	-8.895	0.000
	FeCl+	1.854e-012	1.630e-012	-11.732	-11.788	-0.056
	FeOH+	9.941e-016	8.743e-016	-15.003	-15.058	-0.056
	FeF+	7.440e-016	6.543e-016	-15.128	-15.184	-0.056
	FeCl2	7.504e-018	7.504e-018	-17.125	-17.125	0.000
	FeCl4-2	2.681e-023	1.596e-023	-22.572	-22.797	-0.225
	Fe(OH)2	7.361e-024	7.361e-024	-23.133	-23.133	0.000
	Fe(OH)3-	3.532e-031	3.106e-031	-30.452	-30.508	-0.056
	Fe(OH)4-2	0.000e+000	0.000e+000	-42.257	-42.483	-0.225
Fe(3)		3.890e-004				
	FeOH+2	2.519e-004	1.513e-004	-3.599	-3.820	-0.221
	Fe(OH)2+	6.040e-005	5.312e-005	-4.219	-4.275	-0.056
	Fe+3	5.947e-005	2.212e-005	-4.226	-4.655	-0.430
	FeSO4+	7.489e-006	6.586e-006	-5.126	-5.181	-0.056
	Fe2(OH)2+4	4.430e-006	6.165e-007	-5.354	-6.210	-0.856
	Fe(SO4)2-	3.897e-007	3.427e-007	-6.409	-6.465	-0.056
	Fe3(OH)4+5	1.416e-007	6.843e-009	-6.849	-8.165	-1.316
	FeNO3+2	3.304e-008	1.986e-008	-7.481	-7.702	-0.221
	Fe(OH)3	2.634e-008	2.634e-008	-7.579	-7.579	0.000
	FeF+2	6.045e-009	3.632e-009	-8.219	-8.440	-0.221
	FeCl+2	5.261e-009	3.161e-009	-8.279	-8.500	-0.221
	FeCl2+	2.497e-009	2.196e-009	-8.603	-8.658	-0.056
	FeF2+	7.318e-013	6.436e-013	-12.136	-12.191	-0.056
	Fe(OH)4-	7.973e-015	7.012e-015	-14.098	-14.154	-0.056
	FeNO2+2	3.089e-018	1.856e-018	-17.510	-17.731	-0.221
	FeCl4-	2.209e-018	1.943e-018	-17.656	-17.712	-0.056
H(0)		0.000e+000				
	H2	0.000e+000	0.000e+000	-43.046	-43.044	0.002
K		2.416e-004				
	K+	2.357e-004	2.063e-004	-3.628	-3.686	-0.058
	KSO4-	5.828e-006	5.125e-006	-5.234	-5.290	-0.056
	KCl	5.943e-009	5.943e-009	-8.226	-8.226	0.000
	KHSO4	4.265e-009	4.265e-009	-8.370	-8.370	0.000
	KOH	7.581e-016	7.581e-016	-15.120	-15.120	0.000
Mg		5.696e-004				

Mg+2	3.740e-004	2.378e-004	-3.427	-3.624	-0.197
MgSO4	1.955e-004	1.955e-004	-3.709	-3.709	0.000
MgCl+	1.811e-007	1.593e-007	-6.742	-6.798	-0.056
MgF+	7.147e-011	6.285e-011	-10.146	-10.202	-0.056
Mg4(OH)4+4	0.000e+000	0.000e+000	-41.288	-42.144	-0.856
Mn(2)	5.632e-005				
Mn+2	3.832e-005	2.363e-005	-4.417	-4.627	-0.210
MnSO4	1.795e-005	1.795e-005	-4.746	-4.746	0.000
MnCl+	4.908e-008	4.316e-008	-7.309	-7.365	-0.056
MnNO3+	3.823e-009	3.362e-009	-8.418	-8.473	-0.056
MnF+	7.919e-012	6.964e-012	-11.101	-11.157	-0.056
Mn(NO3)2	7.582e-013	7.582e-013	-12.120	-12.120	0.000
MnOH+	7.320e-013	6.438e-013	-12.135	-12.191	-0.056
MnCl3-	7.891e-015	6.939e-015	-14.103	-14.159	-0.056
Mn2OH+3	5.036e-017	1.630e-017	-16.298	-16.788	-0.490
Mn(OH)2	1.675e-021	1.675e-021	-20.776	-20.776	0.000
Mn2(OH)3+	9.518e-025	8.370e-025	-24.021	-24.077	-0.056
Mn(OH)3-	1.894e-030	1.665e-030	-29.723	-29.779	-0.056
Mn(OH)4-2	0.000e+000	0.000e+000	-40.600	-40.825	-0.225
Mn(3)	1.722e-013				
Mn+3	1.722e-013	5.574e-014	-12.764	-13.254	-0.490
Mn(6)	1.383e-031				
MnO4-2	1.383e-031	8.234e-032	-30.859	-31.084	-0.225
Mn(7)	3.655e-024				
MnO4-	3.655e-024	3.206e-024	-23.437	-23.494	-0.057
N(-03)	0.000e+000				
HN3	0.000e+000	0.000e+000	-81.343	-81.343	0.000
N3-	0.000e+000	0.000e+000	-82.964	-83.020	-0.056
ZnN3+	0.000e+000	0.000e+000	-87.765	-87.821	-0.056
Zn(N3)2	0.000e+000	0.000e+000	-170.087	-170.087	0.000
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-50.652	-50.711	-0.059
NH3	0.000e+000	0.000e+000	-56.926	-56.926	0.000
CuNH3+2	0.000e+000	0.000e+000	-58.807	-59.028	-0.221
Zn(NH3)+2	0.000e+000	0.000e+000	-59.895	-60.116	-0.221
NH4SO4-	0.000e+000	0.000e+000	-61.467	-61.523	-0.056
Cu(NH3)2+2	0.000e+000	0.000e+000	-112.299	-112.521	-0.221
Zn(NH3)2+2	0.000e+000	0.000e+000	-114.614	-114.835	-0.221
Cu(NH3)3+2	0.000e+000	0.000e+000	-166.405	-166.626	-0.221
Zn(NH3)3+2	0.000e+000	0.000e+000	-169.334	-169.555	-0.221
Zn(NH3)4+2	0.000e+000	0.000e+000	-224.327	-224.548	-0.221
N(0)	5.591e-007				
N2	2.796e-007	2.796e-007	-6.554	-6.554	0.000
N(3)	1.666e-016				
HNO2	9.563e-017	9.563e-017	-16.019	-16.019	0.000
NO2-	6.788e-017	5.940e-017	-16.168	-16.226	-0.058
FeNO2+2	3.089e-018	1.856e-018	-17.510	-17.731	-0.221
CuNO2+	5.093e-021	4.479e-021	-20.293	-20.349	-0.056
Cu(NO2)2	2.722e-036	2.722e-036	-35.565	-35.565	0.000
N(5)	1.030e-004				
NO3-	1.026e-004	8.978e-005	-3.989	-4.047	-0.058
CaNO3+	3.752e-007	3.300e-007	-6.426	-6.482	-0.056
FeNO3+2	3.304e-008	1.986e-008	-7.481	-7.702	-0.221
HNO3	4.429e-009	4.429e-009	-8.354	-8.354	0.000
MnNO3+	3.823e-009	3.362e-009	-8.418	-8.473	-0.056
Mn(NO3)2	7.582e-013	7.582e-013	-12.120	-12.120	0.000
Na	1.245e-003				
Na+	1.220e-003	1.073e-003	-2.914	-2.969	-0.056
NaSO4-	2.481e-005	2.182e-005	-4.605	-4.661	-0.056
NaCl	1.618e-007	1.618e-007	-6.791	-6.791	0.000
NaF	1.257e-012	1.257e-012	-11.901	-11.901	0.000
NaOH	1.890e-015	1.890e-015	-14.723	-14.723	0.000
NaAlO2	7.127e-020	7.127e-020	-19.147	-19.147	0.000
O(0)	1.556e-006				
O2	7.779e-007	7.811e-007	-6.109	-6.107	0.002
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-127.621	-127.621	0.000

HS-	0.000e+000	0.000e+000	-131.548	-131.605	-0.057
S-2	0.000e+000	0.000e+000	-141.288	-141.506	-0.217
S2-2	0.000e+000	0.000e+000	-232.781	-233.006	-0.225
HAsS2	0.000e+000	0.000e+000	-310.048	-310.048	0.000
S3-2	0.000e+000	0.000e+000	-324.323	-324.548	-0.225
S4-2	0.000e+000	0.000e+000	-416.091	-416.317	-0.225
S5-2	0.000e+000	0.000e+000	-508.077	-508.302	-0.225
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-132.108	-132.333	-0.225
HS2O3-	0.000e+000	0.000e+000	-134.289	-134.345	-0.056
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-120.098	-120.315	-0.217
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-41.814	-41.870	-0.056
H2SO3	0.000e+000	0.000e+000	-42.913	-42.913	0.000
SO2	0.000e+000	0.000e+000	-43.014	-43.014	0.000
SO3-2	0.000e+000	0.000e+000	-45.855	-46.076	-0.221
S2O6-2	0.000e+000	0.000e+000	-59.164	-59.389	-0.225
S3O6-2	0.000e+000	0.000e+000	-153.188	-153.414	-0.225
S4O6-2	0.000e+000	0.000e+000	-231.307	-231.533	-0.225
S5O6-2	0.000e+000	0.000e+000	-338.306	-338.531	-0.225
S(5)	0.000e+000				
S2O5-2	0.000e+000	0.000e+000	-88.344	-88.569	-0.225
S(6)	6.203e-003				
SO4-2	5.171e-003	3.078e-003	-2.286	-2.512	-0.225
HSO4-	3.335e-004	2.933e-004	-3.477	-3.533	-0.056
CaSO4	3.297e-004	3.297e-004	-3.482	-3.482	0.000
MgSO4	1.955e-004	1.955e-004	-3.709	-3.709	0.000
AlSO4+	7.616e-005	6.698e-005	-4.118	-4.174	-0.056
NaSO4-	2.481e-005	2.182e-005	-4.605	-4.661	-0.056
Al(SO4)2-	1.820e-005	1.600e-005	-4.740	-4.796	-0.056
MnSO4	1.795e-005	1.795e-005	-4.746	-4.746	0.000
FeSO4+	7.489e-006	6.586e-006	-5.126	-5.181	-0.056
KSO4-	5.828e-006	5.125e-006	-5.234	-5.290	-0.056
ZnSO4	3.697e-006	3.697e-006	-5.432	-5.432	0.000
CuSO4	5.077e-007	5.077e-007	-6.294	-6.294	0.000
Fe(SO4)2-	3.897e-007	3.427e-007	-6.409	-6.465	-0.056
KHSO4	4.265e-009	4.265e-009	-8.370	-8.370	0.000
FeSO4	1.272e-009	1.272e-009	-8.895	-8.895	0.000
H2SO4	2.610e-010	2.610e-010	-9.583	-9.583	0.000
NH4SO4-	0.000e+000	0.000e+000	-61.467	-61.523	-0.056
S(7)	8.780e-037				
S2O8-2	4.390e-037	2.613e-037	-36.358	-36.583	-0.225
S(8)	1.601e-026				
HSO5-	1.601e-026	1.408e-026	-25.796	-25.851	-0.056
Zn	1.297e-005				
Zn+2	9.268e-006	5.715e-006	-5.033	-5.243	-0.210
ZnSO4	3.697e-006	3.697e-006	-5.432	-5.432	0.000
ZnCl+	9.367e-009	8.238e-009	-8.028	-8.084	-0.056
ZnCl2	8.255e-012	8.255e-012	-11.083	-11.083	0.000
ZnOH+	7.554e-012	6.644e-012	-11.122	-11.178	-0.056
ZnF+	1.005e-012	8.841e-013	-11.998	-12.054	-0.056
Zn(OH)Cl	1.493e-013	1.493e-013	-12.826	-12.826	0.000
ZnCl3-	4.447e-015	3.911e-015	-14.352	-14.408	-0.056
ZnCl4-2	4.272e-017	2.543e-017	-16.369	-16.595	-0.225
Zn(OH)2	3.016e-017	3.016e-017	-16.521	-16.521	0.000
Zn(OH)3-	1.127e-025	9.908e-026	-24.948	-25.004	-0.056
Zn(OH)4-2	3.008e-035	1.790e-035	-34.522	-34.747	-0.225
ZnClO4+	1.212e-035	1.066e-035	-34.916	-34.972	-0.056
Zn(NH3)+2	0.000e+000	0.000e+000	-59.895	-60.116	-0.221
ZnN3+	0.000e+000	0.000e+000	-87.765	-87.821	-0.056
Zn(NH3)2+2	0.000e+000	0.000e+000	-114.614	-114.835	-0.221
Zn(NH3)3+2	0.000e+000	0.000e+000	-169.334	-169.555	-0.221
Zn(N3)2	0.000e+000	0.000e+000	-170.087	-170.087	0.000
Zn(NH3)4+2	0.000e+000	0.000e+000	-224.327	-224.548	-0.221

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

Phase	SI	log IAP	log KT	
Al	-140.93	8.98	149.91	Al
Al(g)	-191.63	8.98	200.62	Al
Al2(SO4)3	-35.78	-16.88	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-18.44	-16.88	1.56	Al2(SO4)3:6H2O
Alabandite	-132.79	-133.21	-0.42	MnS
AlF3	-11.29	-28.55	-17.27	AlF3
Alum-K	-8.41	-13.38	-4.97	KAl(SO4)2:12H2O
Alunite	-4.10	-4.57	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.30	-5.65	-4.35	CaSO4
Antarcticite	-13.36	-9.27	4.09	CaCl2:6H2O
Antlerite	-17.57	-8.84	8.73	Cu3(SO4)(OH)4
Aphthitalite	-15.16	-19.05	-3.89	NaK3(SO4)2
Arcanite	-8.04	-9.88	-1.84	K2SO4
Arsenolite	-122.69	-142.53	-19.84	As2O3
Arsenopyrite	-251.74	-266.18	-14.45	FeAsS
As	-109.37	-66.69	42.68	As
As2O5	-89.71	-87.58	2.14	As2O5
As4O6(cubi)	-245.25	-285.07	-39.82	As4O6
As4O6(mono)	-245.02	-285.07	-40.05	As4O6
Atacamite	-26.82	-12.55	14.26	Cu4Cl2(OH)6
Bassanite	-1.94	-5.65	-3.71	CaSO4:0.5H2O
Birnessite	-18.74	-104.29	-85.55	Mn8O14:5H2O
Bischofite	-14.15	-9.76	4.39	MgCl2:6H2O
Bixbyite	-7.39	-8.36	-0.96	Mn2O3
Bloedite	-12.11	-14.59	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-3.15	4.40	7.55	AlO2H
Bornite	-507.92	-610.45	-102.53	Cu5FeS4
Brochantite	-24.35	-8.93	15.42	Cu4(SO4)(OH)6
Brucite	-13.86	2.43	16.28	Mg(OH)2
Ca	-133.86	5.97	139.83	Ca
Ca(g)	-159.10	5.97	165.07	Ca
Ca2Al2O5:8H2O	-44.93	14.64	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-32.64	-6.35	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-96.63	-78.83	17.80	Ca3(AsO4)2
Ca3Al2O6	-95.48	17.56	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-111.17	29.31	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-86.78	20.47	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-83.21	20.47	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-68.85	-0.52	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-35.18	11.72	46.91	CaAl2O4
CaAl2O4:10H2O	-26.27	11.72	37.99	CaAl2O4:10H2O
CaAl4O7	-48.06	20.53	68.59	CaAl4O7
Carnallite	-20.78	-16.51	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-2.11	-5.65	-3.54	CaSO4:0.5H2O
Chalcanthite	-6.03	-8.65	-2.63	CuSO4:5H2O
Chalcocite	-134.54	-169.28	-34.74	Cu2S
Chalcocyanite	-11.57	-8.65	2.91	CuSO4
Chalcopyrite	-239.28	-271.89	-32.60	CuFeS2
Chloromagnesite	-31.57	-9.76	21.82	MgCl2
Cl2(g)	-18.23	-15.24	2.99	Cl2
Claudetite	-122.74	-142.53	-19.80	As2O3
Corundum	-9.48	8.81	18.29	Al2O3
Covellite	-111.86	-134.72	-22.86	CuS
Cu	-28.53	2.96	31.50	Cu
Cu(g)	-80.69	2.96	83.66	Cu
CuCl2	-16.00	-12.28	3.72	CuCl2
CuF	-35.39	-28.31	7.08	CuF
CuF2	-21.44	-22.06	-0.62	CuF2
CuF2:2H2O	-17.51	-22.06	-4.55	CuF2:2H2O
Cuprite	-32.74	-34.65	-1.91	Cu2O
Delafossite	-6.47	-12.90	-6.44	CuFeO2
Diaspore	-2.74	4.40	7.15	AlHO2
Epsomite	-4.17	-6.14	-1.96	MgSO4:7H2O
Ettringite	-61.85	0.61	62.46	Ca6Al2(SO4)3(OH)12:26H2O

F2(g)	-80.74	-25.03	55.71	F2
Fe	-58.50	0.52	59.02	Fe
Fe(OH)2	-16.43	-2.53	13.89	Fe(OH)2
Fe(OH)3	-1.22	4.42	5.64	Fe(OH)3
Fe2(SO4)3	-19.89	-16.85	3.05	Fe2(SO4)3
FeF2	-22.08	-24.50	-2.42	FeF2
FeF3	-9.28	-28.54	-19.26	FeF3
FeO	-16.06	-2.53	13.52	FeO
Ferrite-Ca	-9.74	11.76	21.50	CaFe2O4
Ferrite-Cu	-1.53	8.75	10.28	CuFe2O4
Ferrite-Dicalcium	-42.13	14.67	56.80	Ca2Fe2O5
Ferrite-Mg	-9.75	11.27	21.02	MgFe2O4
Ferrite-Zn	-2.05	9.65	11.70	ZnFe2O4
FeSO4	-13.70	-11.10	2.61	FeSO4
Fluorite	-8.99	-19.06	-10.07	CaF2
Gibbsite	-3.34	4.40	7.74	Al(OH)3
Glauberite	-8.63	-14.10	-5.47	Na2Ca(SO4)2
Goethite	3.89	4.42	0.53	FeOOH
Gypsum	-1.12	-5.65	-4.53	CaSO4:2H2O
H2(g)	-39.94	-43.04	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-126.64	-134.63	-7.99	H2S
Halite	-7.60	-6.04	1.56	NaCl
Hausmannite	-17.08	-6.93	10.14	Mn3O4
HCl(g)	-12.39	-6.09	6.30	HCl
Hematite	8.77	8.84	0.08	Fe2O3
Hercynite	-22.53	6.27	28.80	FeAl2O4
Hexahydrite	-4.41	-6.14	-1.73	MgSO4:6H2O
Hydrophilite	-21.01	-9.27	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	4.89	-4.52	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	1.64	-3.81	-5.45	NaFe3(SO4)2(OH)6
K	-70.11	0.87	70.98	K
K(g)	-80.71	0.87	81.58	K
K2O	-85.36	-1.32	84.04	K2O
K3H(SO4)2	-15.48	-19.11	-3.62	K3H(SO4)2
Kainite	-12.58	-12.89	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-16.65	-13.38	3.27	KAl(SO4)2
Katoite	-61.39	17.55	78.94	Ca3Al2H12O12
Kieserite	-5.87	-6.14	-0.27	MgSO4:H2O
KMgCl3	-37.76	-16.51	21.25	KMgCl3
KMgCl3:2H2O	-30.47	-16.51	13.96	KMgCl3:2H2O
Lammerite	-89.41	-87.85	1.55	Cu3(AsO4)2
Lawrencite	-23.77	-14.72	9.05	FeCl2
Leonite	-11.91	-16.02	-4.11	K2Mg(SO4)2:4H2O
Lime	-29.65	2.92	32.57	CaO
Magnetite	-4.11	6.31	10.42	Fe3O4
Manganite	-4.01	-4.18	-0.16	MnO(OH)
Manganosite	-16.49	1.42	17.92	MnO
Mayenite	-397.51	96.64	494.15	Ca12Al14O33
Melanterite	-8.70	-11.10	-2.40	FeSO4:7H2O
Mercallite	-7.78	-9.22	-1.44	KHSO4
Mg	-117.04	5.48	122.52	Mg
Mg(g)	-136.76	5.48	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.72	-5.53	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-14.13	-4.92	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	-19.56	-3.67	15.89	MgOHCl
MgSO4	-10.96	-6.14	4.83	MgSO4
Mirabilite	-7.30	-8.45	-1.15	Na2SO4:10H2O
Misenite	-54.14	-65.22	-11.08	K8H6(SO4)7
Mn	-78.46	4.48	82.93	Mn
Mn(OH)2(am)	-13.88	1.42	15.31	Mn(OH)2
Mn(OH)3	-10.52	-4.18	6.34	Mn(OH)3
MnCl2:2H2O	-14.76	-10.76	4.00	MnCl2:2H2O

MnCl2:4H2O	-13.51	-10.76	2.75	MnCl2:4H2O
MnCl2:H2O	-16.30	-10.76	5.54	MnCl2:H2O
MnO2 (gamma)	-1.73	-17.86	-16.13	MnO2
MnSO4	-9.75	-7.14	2.61	MnSO4
Molysite	-27.33	-13.86	13.47	FeCl3
N2(g)	-3.37	-6.55	-3.18	N2
Na	-65.79	1.58	67.37	Na
Na(g)	-79.28	1.58	80.86	Na
Na2O	-67.31	0.11	67.42	Na2O
Na3H(SO4)2	-16.07	-16.96	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.65	-22.55	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-15.41	4.48	19.88	NaFeO2
Nantokite	-16.65	-23.42	-6.77	CuCl
NH3(g)	-58.72	-56.93	1.80	NH3
Niter	-7.51	-7.73	-0.22	KNO3
NO(g)	-18.46	-17.72	0.74	NO
NO2(g)	-13.89	-5.55	8.35	NO2
O2(g)	-3.21	-6.11	-2.89	O2
Orpiment	-466.94	-546.43	-79.49	As2S3
Oxychloride-Mg	-27.07	-1.24	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.75	-6.14	-1.39	MgSO4:5H2O
Periclase	-18.90	2.43	21.33	MgO
Picromerite	-11.58	-16.02	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-13.00	-27.31	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-19.63	2.92	22.55	Ca(OH)2
Pyrite	-215.58	-240.28	-24.70	FeS2
Pyrolusite	-0.19	-17.86	-17.66	MnO2
Pyrrhotite	-133.42	-137.16	-3.74	FeS
Realgar	-189.68	-249.96	-60.28	AsS
S	-92.57	-137.68	-45.11	S
S2(g)	-199.04	-206.23	-7.19	S2
Scacchite	-19.50	-10.76	8.74	MnCl2
Sellaite	-10.10	-19.54	-9.44	MgF2
SO2(g)	-43.19	-43.01	0.18	SO2
Sphalerite	-122.35	-133.82	-11.47	ZnS
Spinel	-26.37	11.23	37.61	Al2MgO4
Starkeyite	-5.14	-6.14	-1.00	MgSO4:4H2O
Sylvite	-7.58	-6.75	0.83	KCl
Syngenite	-7.93	-15.53	-7.60	K2Ca(SO4)2:H2O
Tachyhydrate	-45.93	-28.78	17.14	Mg2CaCl6:12H2O
Tenorite	-7.74	-0.09	7.65	CuO
Thenardite	-8.09	-8.45	-0.36	Na2SO4
Todorokite	-16.38	-62.20	-45.82	Mn7O12:3H2O
Troilite	-133.32	-137.16	-3.84	FeS
Wurtzite	-124.65	-133.82	-9.17	ZnS
Wustite	-14.06	-1.66	12.40	Fe.947O
Zincite	-10.39	0.81	11.20	ZnO
Zn	-64.93	3.86	68.79	Zn
Zn(ClO4)2:6H2O	-72.89	-67.26	5.63	Zn(ClO4)2:6H2O
Zn(g)	-81.55	3.86	85.41	Zn
Zn(NO3)2:6H2O	-16.74	-13.34	3.40	Zn(NO3)2:6H2O
Zn(OH)2(beta)	-11.12	0.81	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-10.85	0.81	11.66	Zn(OH)2
Zn(OH)2(gamma)	-11.08	0.81	11.88	Zn(OH)2
Zn2(OH)3Cl	-19.77	-4.48	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-14.53	-6.95	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-94.47	-85.15	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-33.79	-14.70	19.09	Zn3O(SO4)2
Zn5(NO3)2(OH)8	-52.77	-10.11	42.67	Zn5(NO3)2(OH)8
ZnCl2	-18.45	-11.38	7.08	ZnCl2
ZnCl2(NH3)2	-118.22	-125.23	-7.01	ZnCl2(NH3)2
ZnCl2(NH3)4	-232.37	-239.08	-6.71	ZnCl2(NH3)4
ZnCl2(NH3)6	-348.19	-352.93	-4.74	ZnCl2(NH3)6
ZnF2	-20.67	-21.16	-0.49	ZnF2
ZnSO4	-11.29	-7.75	3.53	ZnSO4
ZnSO4:6H2O	-6.06	-7.76	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.88	-7.76	-1.88	ZnSO4:7H2O

ZnSO4:H2O -7.20 -7.75 -0.55 ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
