
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 4 AS3
temp 25
units mg/l
pe 10
pH 7.74
Cl 24.2
S(6) 243.00
Al 0.00
As 0.0966
Ca 86.82
Cu 0.113
Fe 0.00
K 3.07
Mg 16.17
Mn 0.181
Na 43.01
Zn 0.195
C(4) 115.9
MIX 4
1 1

```

4      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
Delafoosite	-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
Hexahydrite	-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
Tachyhydrate	-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.9470
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 4. AS3

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

Elements	Molality	Moles
As	1.290e-006	1.290e-006
C(4)	1.901e-003	1.901e-003

Ca	2.167e-003	2.167e-003
Cl	6.830e-004	6.830e-004
Cu	1.779e-006	1.779e-006
K	7.856e-005	7.856e-005
Mg	6.656e-004	6.656e-004
Mn	3.296e-006	3.296e-006
Na	1.872e-003	1.872e-003
S(6)	2.531e-003	2.531e-003
Zn	2.984e-006	2.984e-006

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

pH	=	7.740
pe	=	10.000
Activity of water	=	1.000
Ionic strength	=	1.132e-002
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	1.857e-003
Total CO2 (mol/kg)	=	1.901e-003
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	2.892e-005
Percent error, 100*(Cat- An)/(Cat+ An)	=	0.21
Iterations	=	4
Total H	=	1.110525e+002
Total O	=	5.554109e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	5.913e-007	5.294e-007	-6.228	-6.276	-0.048
H+	1.999e-008	1.820e-008	-7.699	-7.740	-0.041
H2O	5.553e+001	9.998e-001	1.744	-0.000	0.000
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-139.943	-139.943	0.000
As(3)	5.393e-029				
HAsO2	2.782e-029	2.782e-029	-28.556	-28.556	0.000
As(OH)3	2.432e-029	2.432e-029	-28.614	-28.614	0.000
H2AsO3-	9.114e-031	8.174e-031	-30.040	-30.088	-0.047
AsO2-	8.714e-031	7.815e-031	-30.060	-30.107	-0.047
AsO2OH-2	6.804e-034	4.389e-034	-33.167	-33.358	-0.190
As(5)	1.290e-006				
HAsO4-2	1.195e-006	7.711e-007	-5.922	-6.113	-0.190
H2AsO4-	9.424e-008	8.452e-008	-7.026	-7.073	-0.047
AsO4-3	2.920e-010	1.087e-010	-9.535	-9.964	-0.429
H3AsO4	2.709e-013	2.709e-013	-12.567	-12.567	0.000
C(4)	1.901e-003				
HCO3-	1.776e-003	1.593e-003	-2.751	-2.798	-0.047
CO2	6.706e-005	6.724e-005	-4.174	-4.172	0.001
CaHCO3+	2.618e-005	2.348e-005	-4.582	-4.629	-0.047
CaCO3	1.119e-005	1.119e-005	-4.951	-4.951	0.000
MgHCO3+	7.342e-006	6.584e-006	-5.134	-5.181	-0.047
CO3-2	5.981e-006	3.883e-006	-5.223	-5.411	-0.188
NaHCO3	3.782e-006	3.782e-006	-5.422	-5.422	0.000
CuCO3	1.553e-006	1.553e-006	-5.809	-5.809	0.000
MgCO3	1.462e-006	1.462e-006	-5.835	-5.835	0.000
MnCO3	2.237e-007	2.237e-007	-6.650	-6.650	0.000
ZnHCO3+	6.961e-008	6.243e-008	-7.157	-7.205	-0.047
ZnCO3	4.958e-008	4.958e-008	-7.305	-7.305	0.000
NaCO3-	2.515e-008	2.256e-008	-7.599	-7.647	-0.047
MnHCO3+	2.225e-008	1.996e-008	-7.653	-7.700	-0.047
Cu(CO3)2-2	1.666e-008	1.075e-008	-7.778	-7.969	-0.190
CuCO3(OH)2-2	6.181e-011	3.987e-011	-10.209	-10.399	-0.190
Ca	2.167e-003				
Ca+2	1.880e-003	1.244e-003	-2.726	-2.905	-0.179
CaSO4	2.499e-004	2.499e-004	-3.602	-3.602	0.000

CaHCO ₃ ⁺	2.618e-005	2.348e-005	-4.582	-4.629	-0.047
CaCO ₃	1.119e-005	1.119e-005	-4.951	-4.951	0.000
CaCl ⁺	1.793e-007	1.608e-007	-6.746	-6.794	-0.047
CaOH ⁺	1.076e-008	9.653e-009	-7.968	-8.015	-0.047
CaCl ₂	1.153e-010	1.153e-010	-9.938	-9.938	0.000
Cl(-1)	6.830e-004				
Cl ⁻	6.824e-004	6.099e-004	-3.166	-3.215	-0.049
MgCl ⁺	1.890e-007	1.695e-007	-6.724	-6.771	-0.047
CaCl ⁺	1.793e-007	1.608e-007	-6.746	-6.794	-0.047
NaCl	1.780e-007	1.780e-007	-6.750	-6.750	0.000
MnCl ⁺	2.383e-009	2.137e-009	-8.623	-8.670	-0.047
ZnCl ⁺	1.737e-009	1.558e-009	-8.760	-8.807	-0.047
Zn(OH)Cl	1.464e-009	1.464e-009	-8.835	-8.835	0.000
KCl	1.422e-009	1.422e-009	-8.847	-8.847	0.000
CaCl ₂	1.153e-010	1.153e-010	-9.938	-9.938	0.000
CuCl ⁺	7.800e-011	6.996e-011	-10.108	-10.155	-0.047
HCl	2.493e-012	2.493e-012	-11.603	-11.603	0.000
ZnCl ₂	1.110e-012	1.110e-012	-11.955	-11.955	0.000
CuCl ₂	2.247e-014	2.247e-014	-13.648	-13.648	0.000
ZnCl ₃ ⁻	4.169e-016	3.739e-016	-15.380	-15.427	-0.047
MnCl ₃ ⁻	1.936e-016	1.737e-016	-15.713	-15.760	-0.047
CuCl ₂ ⁻	6.308e-017	5.658e-017	-16.200	-16.247	-0.047
ZnCl ₄ ⁻²	2.680e-018	1.729e-018	-17.572	-17.762	-0.190
CuCl ₃ ⁻²	3.436e-019	2.216e-019	-18.464	-18.654	-0.190
CuCl ₄ ⁻²	2.432e-025	1.569e-025	-24.614	-24.804	-0.190
Cl(1)	2.568e-026				
ClO ⁻	1.599e-026	1.435e-026	-25.796	-25.843	-0.047
HClO	9.681e-027	9.681e-027	-26.014	-26.014	0.000
Cl(3)	0.000e+000				
ClO ₂ ⁻	0.000e+000	0.000e+000	-41.319	-41.366	-0.047
HClO ₂	0.000e+000	0.000e+000	-45.937	-45.937	0.000
Cl(5)	0.000e+000				
ClO ₃ ⁻	0.000e+000	0.000e+000	-42.989	-43.037	-0.048
Cl(7)	0.000e+000				
ClO ₄ ⁻	0.000e+000	0.000e+000	-48.962	-49.010	-0.048
ZnClO ₄ ⁺	0.000e+000	0.000e+000	-53.504	-53.551	-0.047
Cu(1)	2.623e-015				
Cu ⁺	2.560e-015	2.296e-015	-14.592	-14.639	-0.047
CuCl ₂ ⁻	6.308e-017	5.658e-017	-16.200	-16.247	-0.047
CuCl ₃ ⁻²	3.436e-019	2.216e-019	-18.464	-18.654	-0.190
Cu(2)	1.779e-006				
CuCO ₃	1.553e-006	1.553e-006	-5.809	-5.809	0.000
CuOH ⁺	1.325e-007	1.189e-007	-6.878	-6.925	-0.047
Cu ²	6.339e-008	4.193e-008	-7.198	-7.377	-0.179
Cu(CO ₃) ₂ ⁻²	1.666e-008	1.075e-008	-7.778	-7.969	-0.190
CuSO ₄	1.321e-008	1.321e-008	-7.879	-7.879	0.000
CuCl ⁺	7.800e-011	6.996e-011	-10.108	-10.155	-0.047
CuCO ₃ (OH) ₂ ⁻²	6.181e-011	3.987e-011	-10.209	-10.399	-0.190
CuCl ₂	2.247e-014	2.247e-014	-13.648	-13.648	0.000
CuO ₂ ⁻²	2.105e-016	1.357e-016	-15.677	-15.867	-0.190
CuCl ₄ ⁻²	2.432e-025	1.569e-025	-24.614	-24.804	-0.190
H(0)	5.241e-039				
H ₂	2.620e-039	2.628e-039	-38.582	-38.580	0.001
K	7.856e-005				
K ⁺	7.770e-005	6.945e-005	-4.110	-4.158	-0.049
KSO ₄ ⁻	8.595e-007	7.709e-007	-6.066	-6.113	-0.047
KCl	1.422e-009	1.422e-009	-8.847	-8.847	0.000
KOH	1.323e-011	1.323e-011	-10.878	-10.878	0.000
KHSO ₄	1.238e-014	1.238e-014	-13.907	-13.907	0.000
Mg	6.656e-004				
Mg ²	5.259e-004	3.559e-004	-3.279	-3.449	-0.170
MgSO ₄	1.307e-004	1.307e-004	-3.884	-3.884	0.000
MgHCO ₃ ⁺	7.342e-006	6.584e-006	-5.134	-5.181	-0.047
MgCO ₃	1.462e-006	1.462e-006	-5.835	-5.835	0.000
MgCl ⁺	1.890e-007	1.695e-007	-6.724	-6.771	-0.047
Mg ₄ (OH) ₄ ⁴⁺	1.396e-022	2.601e-023	-21.855	-22.585	-0.730
Mn(2)	3.296e-006				

Mn+2	2.487e-006	1.645e-006	-5.604	-5.784	-0.179
MnSO4	5.583e-007	5.583e-007	-6.253	-6.253	0.000
MnCO3	2.237e-007	2.237e-007	-6.650	-6.650	0.000
MnHCO3+	2.225e-008	1.996e-008	-7.653	-7.700	-0.047
MnOH+	2.591e-009	2.324e-009	-8.587	-8.634	-0.047
MnCl+	2.383e-009	2.137e-009	-8.623	-8.670	-0.047
Mn2(OH)3+	6.304e-013	5.654e-013	-12.200	-12.248	-0.047
Mn(OH)2	3.134e-013	3.134e-013	-12.504	-12.504	0.000
Mn2OH+3	1.069e-014	4.097e-015	-13.971	-14.388	-0.416
MnCl3-	1.936e-016	1.737e-016	-15.713	-15.760	-0.047
Mn(OH)3-	1.801e-017	1.615e-017	-16.744	-16.792	-0.047
Mn(OH)4-2	1.165e-023	7.516e-024	-22.934	-23.124	-0.190
Mn(3)	1.145e-021				
Mn+3	1.145e-021	4.389e-022	-20.941	-21.358	-0.416
Mn(6)	7.578e-023				
MnO4-2	7.578e-023	4.888e-023	-22.120	-22.311	-0.190
Mn(7)	2.404e-022				
MnO4-	2.404e-022	2.152e-022	-21.619	-21.667	-0.048
Na	1.872e-003				
Na+	1.851e-003	1.660e-003	-2.733	-2.780	-0.047
NaSO4-	1.682e-005	1.508e-005	-4.774	-4.821	-0.047
NaHCO3	3.782e-006	3.782e-006	-5.422	-5.422	0.000
NaCl	1.780e-007	1.780e-007	-6.750	-6.750	0.000
NaCO3-	2.515e-008	2.256e-008	-7.599	-7.647	-0.047
NaOH	1.516e-010	1.516e-010	-9.819	-9.819	0.000
O(0)	1.839e-015				
O2	9.196e-016	9.221e-016	-15.036	-15.035	0.001
S(6)	2.531e-003				
SO4-2	2.132e-003	1.375e-003	-2.671	-2.862	-0.190
CaSO4	2.499e-004	2.499e-004	-3.602	-3.602	0.000
MgSO4	1.307e-004	1.307e-004	-3.884	-3.884	0.000
NaSO4-	1.682e-005	1.508e-005	-4.774	-4.821	-0.047
KSO4-	8.595e-007	7.709e-007	-6.066	-6.113	-0.047
MnSO4	5.583e-007	5.583e-007	-6.253	-6.253	0.000
ZnSO4	4.394e-007	4.394e-007	-6.357	-6.357	0.000
CuSO4	1.321e-008	1.321e-008	-7.879	-7.879	0.000
HSO4-	2.818e-009	2.528e-009	-8.550	-8.597	-0.047
KHSO4	1.238e-014	1.238e-014	-13.907	-13.907	0.000
H2SO4	4.340e-020	4.340e-020	-19.363	-19.363	0.000
Zn	2.984e-006				
Zn+2	2.298e-006	1.520e-006	-5.639	-5.818	-0.179
ZnSO4	4.394e-007	4.394e-007	-6.357	-6.357	0.000
ZnOH+	1.022e-007	9.162e-008	-6.991	-7.038	-0.047
ZnHCO3+	6.961e-008	6.243e-008	-7.157	-7.205	-0.047
ZnCO3	4.958e-008	4.958e-008	-7.305	-7.305	0.000
Zn(OH)2	2.156e-008	2.156e-008	-7.666	-7.666	0.000
ZnCl+	1.737e-009	1.558e-009	-8.760	-8.807	-0.047
Zn(OH)Cl	1.464e-009	1.464e-009	-8.835	-8.835	0.000
Zn(OH)3-	4.094e-012	3.672e-012	-11.388	-11.435	-0.047
ZnCl2	1.110e-012	1.110e-012	-11.955	-11.955	0.000
ZnCl3-	4.169e-016	3.739e-016	-15.380	-15.427	-0.047
Zn(OH)4-2	5.333e-017	3.439e-017	-16.273	-16.464	-0.190
ZnCl4-2	2.680e-018	1.729e-018	-17.572	-17.762	-0.190
ZnClO4+	0.000e+000	0.000e+000	-53.504	-53.551	-0.047

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

Phase	SI	log IAP	log KT	
Anhydrite	-1.42	-5.77	-4.35	CaSO4
Antarcticite	-13.43	-9.34	4.09	CaCl2:6H2O
Antlerite	-2.76	5.97	8.73	Cu3(SO4)(OH)4
Aphthitalite	-17.09	-20.98	-3.89	NaK3(SO4)2
Aragonite	0.07	2.04	1.97	CaCO3
Arcanite	-9.33	-11.18	-1.84	K2SO4
Arsenolite	-55.81	-75.65	-19.84	As2O3
Artinite	-6.10	13.52	19.63	Mg2CO3(OH)2:3H2O

As	-69.23	-26.55	42.68	As
As2O5	-31.76	-29.63	2.14	As2O5
As4O6(cubi)	-111.49	-151.31	-39.82	As4O6
As4O6(mono)	-111.26	-151.31	-40.05	As4O6
Atacamite	-3.76	10.50	14.26	Cu4Cl2(OH)6
Azurite	-5.88	3.23	9.12	Cu3(CO3)2(OH)2
Bassanite	-2.06	-5.77	-3.71	CaSO4:0.5H2O
Birnessite	20.65	-64.89	-85.55	Mn8O14:5H2O
Bischofite	-14.27	-9.88	4.39	MgCl2:6H2O
Bixbyite	4.69	3.72	-0.96	Mn2O3
Bloedite	-12.25	-14.73	-2.48	Na2Mg(SO4)2:4H2O
Brochantite	-1.35	14.07	15.42	Cu4(SO4)(OH)6
Brucite	-4.25	12.03	16.28	Mg(OH)2
Burkeite	-26.95	-17.46	9.49	Na6CO3(SO4)2
C	-59.65	4.50	64.15	C
C(g)	-177.27	4.50	181.77	C
Ca	-119.74	20.09	139.83	Ca
Ca(g)	-144.98	20.09	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.05	3.24	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-9.70	8.10	17.80	Ca3(AsO4)2
Ca4Cl2(OH)6:13H2O	-39.94	28.39	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.21	2.04	1.82	CaCO3
Carnallite	-21.52	-17.25	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-2.23	-5.77	-3.54	CaSO4:0.5H2O
Chalcanthite	-7.61	-10.24	-2.63	CuSO4:5H2O
Chalcocyanite	-13.15	-10.24	2.91	CuSO4
Chloromagnesite	-31.69	-9.88	21.82	MgCl2
Cl2(g)	-32.42	-29.43	2.99	Cl2
Claudetite	-55.86	-75.65	-19.80	As2O3
CO2(g)	-2.71	-10.54	-7.83	CO2
Cu	-15.88	15.62	31.50	Cu
Cu(g)	-68.04	15.62	83.66	Cu
CuCl2	-17.53	-13.81	3.72	CuCl2
Cuprite	-11.89	-13.80	-1.91	Cu2O
Dolomite	1.06	3.53	2.47	CaMg(CO3)2
Dolomite-dis	-0.48	3.53	4.01	CaMg(CO3)2
Dolomite-ord	1.07	3.53	2.46	CaMg(CO3)2
Epsomite	-4.35	-6.31	-1.96	MgSO4:7H2O
Gaylussite	-9.75	1.42	11.16	CaNa2(CO3)2:5H2O
Glauberite	-8.72	-14.19	-5.47	Na2Ca(SO4)2
Gypsum	-1.24	-5.77	-4.53	CaSO4:2H2O
H2(g)	-35.48	-38.58	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.56	-5.99	1.56	NaCl
Hausmannite	3.28	13.42	10.14	Mn3O4
HCl(g)	-17.26	-10.95	6.30	HCl
Hexahydrate	-4.58	-6.31	-1.73	MgSO4:6H2O
Huntite	-3.70	6.52	10.22	CaMg3(CO3)4
Hydromagnesite	-12.73	18.01	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-21.08	-9.33	11.75	CaCl2
Hydrozincite	-3.07	27.23	30.31	Zn5(OH)6(CO3)2
Ice	-0.14	-0.00	0.14	H2O
K	-63.64	7.34	70.98	K
K(g)	-74.24	7.34	81.58	K
K2CO3:1.5H2O	-16.75	-3.37	13.38	K2CO3:1.5H2O
K2O	-76.87	7.16	84.04	K2O
K3H(SO4)2	-22.32	-25.94	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-62.28	-34.57	27.71	K8H4(CO3)6:3H2O
Kainite	-13.37	-13.68	-0.31	KMgClSO4:3H2O
Kaliginite	-7.24	-6.96	0.28	KHCO3
Kieserite	-6.04	-6.31	-0.27	MgSO4:H2O
KMgCl3	-38.50	-17.25	21.25	KMgCl3
KMgCl3:2H2O	-31.21	-17.25	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-12.26	-2.00	10.26	KNaCO3:6H2O
Lammerite	-6.87	-5.32	1.55	Cu3(AsO4)2
Lansfordite	-3.35	1.49	4.84	MgCO3:5H2O
Leonite	-13.38	-17.49	-4.11	K2Mg(SO4)2:4H2O

Lime	-19.99	12.57	32.57	CaO
Magnesite	-0.78	1.49	2.27	MgCO ₃
Malachite	-0.23	5.67	5.90	Cu ₂ CO ₃ (OH) ₂
Manganite	2.03	1.86	-0.16	MnO(OH)
Manganosite	-8.22	9.70	17.92	MnO
Mercallite	-13.32	-14.76	-1.44	KHSO ₄
Mg	-102.97	19.55	122.52	Mg
Mg(g)	-122.70	19.55	142.25	Mg
Mg1.25SO ₄ (OH)0.5:0.5H ₂ O	-8.50	-3.30	5.20	Mg1.25SO ₄ (OH)0.5:0.5H ₂ O
Mg1.5SO ₄ (OH)	-9.50	-0.29	9.21	Mg1.5SO ₄ (OH)
MgCl ₂ :2H ₂ O	-22.61	-9.88	12.73	MgCl ₂ :2H ₂ O
MgCl ₂ :4H ₂ O	-17.18	-9.88	7.30	MgCl ₂ :4H ₂ O
MgCl ₂ :H ₂ O	-25.95	-9.88	16.07	MgCl ₂ :H ₂ O
MgOHCl	-14.81	1.08	15.89	MgOHCl
MgSO ₄	-11.14	-6.31	4.83	MgSO ₄
Mirabilite	-7.27	-8.42	-1.15	Na ₂ SO ₄ :10H ₂ O
Misenite	-88.66	-99.74	-11.08	K ₈ H ₆ (SO ₄) ₇
Mn	-65.72	17.21	82.93	Mn
Mn(OH) ₂ (am)	-5.61	9.70	15.31	Mn(OH) ₂
Mn(OH) ₃	-4.48	1.86	6.34	Mn(OH) ₃
MnCl ₂ :2H ₂ O	-16.21	-12.21	4.00	MnCl ₂ :2H ₂ O
MnCl ₂ :4H ₂ O	-14.97	-12.21	2.75	MnCl ₂ :4H ₂ O
MnCl ₂ :H ₂ O	-17.76	-12.21	5.54	MnCl ₂ :H ₂ O
MnO ₂ (gamma)	2.08	-14.05	-16.13	MnO ₂
MnSO ₄	-11.25	-8.65	2.61	MnSO ₄
Monohydrocalcite	-0.64	2.04	2.68	CaCO ₃ :H ₂ O
Na	-58.65	8.72	67.37	Na
Na(g)	-72.14	8.72	80.86	Na
Na ₂ CO ₃	-11.78	-0.62	11.16	Na ₂ CO ₃
Na ₂ CO ₃ :7H ₂ O	-10.56	-0.62	9.94	Na ₂ CO ₃ :7H ₂ O
Na ₂ O	-57.50	9.92	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-20.91	-21.80	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-16.72	-22.61	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
Nahcolite	-5.44	-5.58	-0.14	NaHCO ₃
Nantokite	-11.09	-17.85	-6.77	CuCl
Natron	-10.21	-0.62	9.59	Na ₂ CO ₃ :10H ₂ O
Nesquehonite	-3.80	1.49	5.29	MgCO ₃ :3H ₂ O
O ₂ (g)	-12.14	-15.04	-2.89	O ₂
Oxychloride-Mg	-12.72	13.11	25.83	Mg ₂ Cl(OH) ₃ :4H ₂ O
Pentahydrate	-4.92	-6.31	-1.39	MgSO ₄ :5H ₂ O
Periclase	-9.29	12.03	21.33	MgO
Picromerite	-13.05	-17.49	-4.44	K ₂ Mg(SO ₄) ₂ :6H ₂ O
Pirssonite	-9.90	1.42	11.32	Na ₂ Ca(CO ₃) ₂ :2H ₂ O
Polyhalite	-14.71	-29.02	-14.31	K ₂ MgCa ₂ (SO ₄) ₄ :2H ₂ O
Portlandite	-9.97	12.57	22.55	Ca(OH) ₂
Pyrolusite	3.61	-14.05	-17.66	MnO ₂
Rhodochrosite	-0.62	-0.84	-0.22	MnCO ₃
Scacchite	-20.95	-12.21	8.74	MnCl ₂
Smithsonite	-1.32	-0.88	0.44	ZnCO ₃
Starkeyite	-5.31	-6.31	-1.00	MgSO ₄ :4H ₂ O
Sylvite	-8.20	-7.37	0.83	KCl
Syngenite	-9.35	-16.95	-7.60	K ₂ Ca(SO ₄) ₂ :H ₂ O
Tachyhydrite	-46.24	-29.09	17.14	Mg ₂ CaCl ₆ :12H ₂ O
Tenorite	0.46	8.10	7.65	CuO
Thenardite	-8.06	-8.42	-0.36	Na ₂ SO ₄
Thermonatrite	-11.55	-0.62	10.94	Na ₂ CO ₃ :H ₂ O
Todorokite	19.21	-26.62	-45.82	Mn ₇ O ₁₂ :3H ₂ O
Trona-K	-20.54	-8.95	11.59	K ₂ NaH(CO ₃) ₂ :2H ₂ O
Zincite	-1.54	9.66	11.20	ZnO
Zn	-51.61	17.18	68.79	Zn
Zn(ClO ₄) ₂ :6H ₂ O	-109.47	-103.84	5.63	Zn(ClO ₄) ₂ :6H ₂ O
Zn(g)	-68.23	17.18	85.41	Zn
Zn(OH) ₂ (beta)	-2.27	9.66	11.93	Zn(OH) ₂
Zn(OH) ₂ (epsilon)	-2.00	9.66	11.66	Zn(OH) ₂
Zn(OH) ₂ (gamma)	-2.22	9.66	11.88	Zn(OH) ₂
Zn ₂ (OH) ₃ Cl	-6.92	8.37	15.29	Zn ₂ (OH) ₃ Cl
Zn ₂ SO ₄ (OH) ₂	-6.60	0.98	7.58	Zn ₂ SO ₄ (OH) ₂

Zn3(AsO4)2	-9.95	-0.64	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-26.79	-7.70	19.09	Zn3O(SO4)2
ZnCl2	-19.33	-12.25	7.08	ZnCl2
ZnCO3:H2O	-1.02	-0.88	0.14	ZnCO3:H2O
ZnSO4	-12.21	-8.68	3.53	ZnSO4
ZnSO4:6H2O	-6.98	-8.68	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-6.80	-8.68	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-8.13	-8.68	-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 4 AS3

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

Elements	Molality	Moles
Al	1.558e-004	3.117e-004
As	2.649e-006	5.299e-006
C	9.505e-004	1.901e-003
Ca	1.520e-003	3.039e-003
Cl	9.811e-004	1.962e-003
Cu	1.677e-006	3.355e-006
Fe	3.890e-004	7.780e-004
K	2.416e-004	4.831e-004
Mg	5.697e-004	1.139e-003
Mn	5.632e-005	1.126e-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	=	3.410	Charge balance
pe	=	16.315	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	1.635e-002	
Mass of water (kg)	=	2.000e+000	
Total alkalinity (eq/kg)	=	-8.560e-004	
Total CO2 (mol/kg)	=	9.505e-004	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	-1.174e-002	
Percent error, 100*(Cat- An)/(Cat+ An)	=	-32.87	
Iterations	=	12	
Total H	=	2.221064e+002	
Total O	=	1.111065e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	4.333e-004	3.891e-004	-3.363	-3.410	-0.047
OH-	2.819e-011	2.476e-011	-10.550	-10.606	-0.056
H2O	5.553e+001	9.998e-001	1.744	-0.000	0.000
Al	1.558e-004				
AlSO4+	7.872e-005	6.931e-005	-4.104	-4.159	-0.055
Al+3	5.657e-005	2.120e-005	-4.247	-4.674	-0.426

Al(SO4)2-	1.953e-005	1.719e-005	-4.709	-4.765	-0.055
AlOH+2	1.011e-006	6.102e-007	-5.995	-6.215	-0.219
Al(OH)2+	4.136e-009	3.641e-009	-8.383	-8.439	-0.055
Al2(OH)2+4	4.278e-010	6.054e-011	-9.369	-10.218	-0.849
HALO2	1.362e-011	1.362e-011	-10.866	-10.866	0.000
Al3(OH)4+5	1.104e-013	5.470e-015	-12.957	-14.262	-1.305
AlO2-	1.362e-014	1.199e-014	-13.866	-13.921	-0.055
NaAlO2	2.455e-018	2.455e-018	-17.610	-17.610	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-47.814	-50.372	-2.558
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-150.076	-150.076	0.000
As(3)	3.110e-027				
HAsO2	1.659e-027	1.659e-027	-26.780	-26.780	0.000
As(OH)3	1.451e-027	1.451e-027	-26.838	-26.838	0.000
H2AsO3-	2.590e-033	2.280e-033	-32.587	-32.642	-0.055
AsO2-	2.476e-033	2.180e-033	-32.606	-32.661	-0.055
AsO2OH-2	0.000e+000	0.000e+000	-40.019	-40.242	-0.223
HAsS2	0.000e+000	0.000e+000	-272.383	-272.383	0.000
As(5)	2.649e-006				
H2AsO4-	2.497e-006	2.198e-006	-5.603	-5.658	-0.055
H3AsO4	1.507e-007	1.507e-007	-6.822	-6.822	0.000
HAsO4-2	1.568e-009	9.380e-010	-8.805	-9.028	-0.223
AsO4-3	1.970e-017	6.185e-018	-16.705	-17.209	-0.503
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-251.902	-251.902	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-222.465	-222.465	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-139.286	-139.286	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-47.512	-47.512	0.000
C(4)	9.505e-004				
CO2	9.493e-004	9.530e-004	-3.023	-3.021	0.002
HCO3-	1.199e-006	1.056e-006	-5.921	-5.976	-0.055
CaHCO3+	1.037e-008	9.131e-009	-7.984	-8.039	-0.055
FeCO3+	6.464e-009	5.691e-009	-8.190	-8.245	-0.055
MgHCO3+	3.277e-009	2.885e-009	-8.485	-8.540	-0.055
NaHCO3	1.621e-009	1.621e-009	-8.790	-8.790	0.000
MnHCO3+	2.137e-010	1.882e-010	-9.670	-9.725	-0.055
ZnHCO3+	1.753e-010	1.543e-010	-9.756	-9.812	-0.055
FeHCO3+	2.602e-012	2.291e-012	-11.585	-11.640	-0.055
CuCO3	8.196e-013	8.196e-013	-12.086	-12.086	0.000
CaCO3	2.036e-013	2.036e-013	-12.691	-12.691	0.000
CO3-2	1.995e-013	1.204e-013	-12.700	-12.919	-0.219
MnCO3	9.867e-014	9.867e-014	-13.006	-13.006	0.000
MgCO3	2.997e-014	2.997e-014	-13.523	-13.523	0.000
ZnCO3	5.733e-015	5.733e-015	-14.242	-14.242	0.000
NaCO3-	5.136e-016	4.522e-016	-15.289	-15.345	-0.055
FeCO3	2.826e-017	2.826e-017	-16.549	-16.549	0.000
Cu(CO3)2-2	2.939e-022	1.758e-022	-21.532	-21.755	-0.223
CuCO3(OH)2-2	7.694e-026	4.601e-026	-25.114	-25.337	-0.223
Ca	1.520e-003				
Ca+2	1.179e-003	7.298e-004	-2.929	-3.137	-0.208
CaSO4	3.407e-004	3.407e-004	-3.468	-3.468	0.000
CaCl+	1.509e-007	1.329e-007	-6.821	-6.877	-0.055
CaHCO3+	1.037e-008	9.131e-009	-7.984	-8.039	-0.055
CaCl2	1.343e-010	1.343e-010	-9.872	-9.872	0.000
CaOH+	3.009e-013	2.649e-013	-12.522	-12.577	-0.055
CaCO3	2.036e-013	2.036e-013	-12.691	-12.691	0.000
Cl(-1)	9.811e-004				
Cl-	9.804e-004	8.590e-004	-3.009	-3.066	-0.057
MgCl+	1.792e-007	1.578e-007	-6.747	-6.802	-0.055
NaCl	1.621e-007	1.621e-007	-6.790	-6.790	0.000
CaCl+	1.509e-007	1.329e-007	-6.821	-6.877	-0.055
HCl	7.507e-008	7.507e-008	-7.125	-7.125	0.000
MnCl+	4.863e-008	4.282e-008	-7.313	-7.368	-0.055
ZnCl+	9.295e-009	8.183e-009	-8.032	-8.087	-0.055

KCl	5.953e-009	5.953e-009	-8.225	-8.225	0.000
FeCl+2	1.941e-009	1.171e-009	-8.712	-8.931	-0.219
CuCl+	1.905e-009	1.677e-009	-8.720	-8.775	-0.055
FeCl2+	9.254e-010	8.147e-010	-9.034	-9.089	-0.055
CaCl2	1.343e-010	1.343e-010	-9.872	-9.872	0.000
ZnCl2	8.212e-012	8.212e-012	-11.086	-11.086	0.000
FeCl+	2.939e-012	2.587e-012	-11.532	-11.587	-0.055
CuCl2	7.587e-013	7.587e-013	-12.120	-12.120	0.000
Zn(OH)Cl	3.596e-013	3.596e-013	-12.444	-12.444	0.000
MnCl3-	7.841e-015	6.903e-015	-14.106	-14.161	-0.055
ZnCl3-	4.425e-015	3.896e-015	-14.354	-14.409	-0.055
ZnCl4-2	4.242e-017	2.537e-017	-16.372	-16.596	-0.223
FeCl2	1.193e-017	1.193e-017	-16.923	-16.923	0.000
FeCl4-	8.210e-019	7.228e-019	-18.086	-18.141	-0.055
CuCl2-	1.051e-021	9.252e-022	-20.978	-21.034	-0.055
FeCl4-2	4.253e-023	2.543e-023	-22.371	-22.595	-0.223
CuCl4-2	1.757e-023	1.051e-023	-22.755	-22.979	-0.223
CuCl3-2	8.536e-024	5.105e-024	-23.069	-23.292	-0.223
Cl(1)	2.718e-018				
HClO	2.718e-018	2.718e-018	-17.566	-17.566	0.000
ClO-	2.140e-022	1.884e-022	-21.670	-21.725	-0.055
Cl(3)	9.011e-034				
ClO2-	5.981e-034	5.266e-034	-33.223	-33.279	-0.055
HClO2	3.029e-034	3.029e-034	-33.519	-33.519	0.000
Cl(5)	1.193e-031				
ClO3-	1.193e-031	1.048e-031	-30.923	-30.980	-0.056
Cl(7)	1.184e-033				
ClO4-	1.184e-033	1.040e-033	-32.927	-32.983	-0.056
ZnClO4+	1.267e-037	1.115e-037	-36.897	-36.953	-0.055
Cu(1)	2.255e-020				
Cu+	2.149e-020	1.892e-020	-19.668	-19.723	-0.055
CuCl2-	1.051e-021	9.252e-022	-20.978	-21.034	-0.055
CuCl3-2	8.536e-024	5.105e-024	-23.069	-23.292	-0.223
Cu(2)	1.677e-006				
Cu+2	1.153e-006	7.137e-007	-5.938	-6.146	-0.208
CuSO4	5.225e-007	5.225e-007	-6.282	-6.282	0.000
CuCl+	1.905e-009	1.677e-009	-8.720	-8.775	-0.055
CuOH+	1.075e-010	9.461e-011	-9.969	-10.024	-0.055
CuCO3	8.196e-013	8.196e-013	-12.086	-12.086	0.000
CuCl2	7.587e-013	7.587e-013	-12.120	-12.120	0.000
Cu(CO3)2-2	2.939e-022	1.758e-022	-21.532	-21.755	-0.223
CuCl4-2	1.757e-023	1.051e-023	-22.755	-22.979	-0.223
CuCO3(OH)2-2	7.694e-026	4.601e-026	-25.114	-25.337	-0.223
CuO2-2	1.849e-032	1.106e-032	-31.733	-31.956	-0.223
Fe(2)	8.777e-009				
Fe+2	6.678e-009	4.134e-009	-8.175	-8.384	-0.208
FeSO4	2.094e-009	2.094e-009	-8.679	-8.679	0.000
FeCl+	2.939e-012	2.587e-012	-11.532	-11.587	-0.055
FeHCO3+	2.602e-012	2.291e-012	-11.585	-11.640	-0.055
FeOH+	3.816e-015	3.360e-015	-14.418	-14.474	-0.055
FeCO3	2.826e-017	2.826e-017	-16.549	-16.549	0.000
FeCl2	1.193e-017	1.193e-017	-16.923	-16.923	0.000
Fe(OH)2	6.858e-023	6.858e-023	-22.164	-22.164	0.000
FeCl4-2	4.253e-023	2.543e-023	-22.371	-22.595	-0.223
Fe(OH)3-	7.969e-030	7.016e-030	-29.099	-29.154	-0.055
Fe(OH)4-2	0.000e+000	0.000e+000	-40.521	-40.744	-0.223
Fe(3)	3.890e-004				
FeOH+2	2.250e-004	1.358e-004	-3.648	-3.867	-0.219
Fe(OH)2+	1.312e-004	1.155e-004	-3.882	-3.937	-0.055
Fe+3	2.184e-005	8.184e-006	-4.661	-5.087	-0.426
Fe2(OH)2+4	3.507e-006	4.963e-007	-5.455	-6.304	-0.849
FeSO4+	2.874e-006	2.530e-006	-5.542	-5.597	-0.055
Fe3(OH)4+5	2.418e-007	1.198e-008	-6.617	-7.922	-1.305
Fe(SO4)2-	1.553e-007	1.367e-007	-6.809	-6.864	-0.055
Fe(OH)3	1.389e-007	1.389e-007	-6.857	-6.857	0.000
FeCO3+	6.464e-009	5.691e-009	-8.190	-8.245	-0.055
FeCl+2	1.941e-009	1.171e-009	-8.712	-8.931	-0.219

FeCl2+	9.254e-010	8.147e-010	-9.034	-9.089	-0.055
Fe(OH)4-	1.018e-013	8.965e-014	-12.992	-13.047	-0.055
FeCl4-	8.210e-019	7.228e-019	-18.086	-18.141	-0.055
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-42.552	-42.550	0.002
K	2.416e-004				
K+	2.355e-004	2.063e-004	-3.628	-3.685	-0.057
KSO4-	6.045e-006	5.322e-006	-5.219	-5.274	-0.055
KCl	5.953e-009	5.953e-009	-8.225	-8.225	0.000
KHSO4	1.827e-009	1.827e-009	-8.738	-8.738	0.000
KOH	1.839e-015	1.839e-015	-14.736	-14.736	0.000
Mg	5.697e-004				
Mg+2	3.687e-004	2.353e-004	-3.433	-3.628	-0.195
MgSO4	2.008e-004	2.008e-004	-3.697	-3.697	0.000
MgCl+	1.792e-007	1.578e-007	-6.747	-6.802	-0.055
MgHCO3+	3.277e-009	2.885e-009	-8.485	-8.540	-0.055
MgCO3	2.997e-014	2.997e-014	-13.523	-13.523	0.000
Mg4(OH)4+4	1.679e-040	0.000e+000	-39.775	-40.624	-0.849
Mn(2)	5.632e-005				
Mn+2	3.781e-005	2.341e-005	-4.422	-4.631	-0.208
MnSO4	1.846e-005	1.846e-005	-4.734	-4.734	0.000
MnCl+	4.863e-008	4.282e-008	-7.313	-7.368	-0.055
MnHCO3+	2.137e-010	1.882e-010	-9.670	-9.725	-0.055
MnOH+	1.756e-012	1.546e-012	-11.755	-11.811	-0.055
MnCO3	9.867e-014	9.867e-014	-13.006	-13.006	0.000
MnCl3-	7.841e-015	6.903e-015	-14.106	-14.161	-0.055
Mn2OH+3	1.187e-016	3.879e-017	-15.926	-16.411	-0.486
Mn(OH)2	9.754e-021	9.754e-021	-20.011	-20.011	0.000
Mn2(OH)3+	1.330e-023	1.171e-023	-22.876	-22.932	-0.055
Mn(OH)3-	2.670e-029	2.351e-029	-28.573	-28.629	-0.055
Mn(OH)4-2	8.555e-040	5.116e-040	-39.068	-39.291	-0.223
Mn(3)	3.944e-014				
Mn+3	3.944e-014	1.289e-014	-13.404	-13.890	-0.486
Mn(6)	4.837e-031				
MnO4-2	4.837e-031	2.893e-031	-30.315	-30.539	-0.223
Mn(7)	2.994e-024				
MnO4-	2.994e-024	2.630e-024	-23.524	-23.580	-0.056
Na	1.245e-003				
Na+	1.219e-003	1.073e-003	-2.914	-2.969	-0.055
NaSO4-	2.574e-005	2.266e-005	-4.589	-4.645	-0.055
NaCl	1.621e-007	1.621e-007	-6.790	-6.790	0.000
NaHCO3	1.621e-009	1.621e-009	-8.790	-8.790	0.000
NaOH	4.585e-015	4.585e-015	-14.339	-14.339	0.000
NaCO3-	5.136e-016	4.522e-016	-15.289	-15.345	-0.055
NaAlO2	2.455e-018	2.455e-018	-17.610	-17.610	0.000
O(0)	1.597e-007				
O2	7.985e-008	8.017e-008	-7.098	-7.096	0.002
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-126.396	-126.396	0.000
HS-	0.000e+000	0.000e+000	-129.940	-129.996	-0.056
S-2	0.000e+000	0.000e+000	-139.297	-139.512	-0.215
S2-2	0.000e+000	0.000e+000	-230.059	-230.282	-0.223
HAsS2	0.000e+000	0.000e+000	-272.383	-272.383	0.000
S3-2	0.000e+000	0.000e+000	-320.871	-321.094	-0.223
S4-2	0.000e+000	0.000e+000	-411.909	-412.133	-0.223
S5-2	0.000e+000	0.000e+000	-503.165	-503.388	-0.223
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-130.869	-131.092	-0.223
HS2O3-	0.000e+000	0.000e+000	-133.433	-133.489	-0.055
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-119.353	-119.569	-0.215
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-41.688	-41.744	-0.055
H2SO3	0.000e+000	0.000e+000	-43.172	-43.172	0.000
SO2	0.000e+000	0.000e+000	-43.272	-43.272	0.000
SO3-2	0.000e+000	0.000e+000	-45.346	-45.565	-0.219
S2O6-2	0.000e+000	0.000e+000	-59.408	-59.631	-0.223

S306-2	0.000e+000	0.000e+000	-152.703	-152.926	-0.223
S406-2	0.000e+000	0.000e+000	-230.091	-230.315	-0.223
S506-2	0.000e+000	0.000e+000	-336.360	-336.583	-0.223
S(5)	0.000e+000				
S205-2	0.000e+000	0.000e+000	-88.094	-88.317	-0.223
S(6)	6.203e-003				
SO4-2	5.343e-003	3.196e-003	-2.272	-2.495	-0.223
CaSO4	3.407e-004	3.407e-004	-3.468	-3.468	0.000
MgSO4	2.008e-004	2.008e-004	-3.697	-3.697	0.000
HSO4-	1.426e-004	1.256e-004	-3.846	-3.901	-0.055
AlSO4+	7.872e-005	6.931e-005	-4.104	-4.159	-0.055
NaSO4-	2.574e-005	2.266e-005	-4.589	-4.645	-0.055
Al(SO4)2-	1.953e-005	1.719e-005	-4.709	-4.765	-0.055
MnSO4	1.846e-005	1.846e-005	-4.734	-4.734	0.000
KSO4-	6.045e-006	5.322e-006	-5.219	-5.274	-0.055
ZnSO4	3.807e-006	3.807e-006	-5.419	-5.419	0.000
FeSO4+	2.874e-006	2.530e-006	-5.542	-5.597	-0.055
CuSO4	5.225e-007	5.225e-007	-6.282	-6.282	0.000
Fe(SO4)2-	1.553e-007	1.367e-007	-6.809	-6.864	-0.055
FeSO4	2.094e-009	2.094e-009	-8.679	-8.679	0.000
KHSO4	1.827e-009	1.827e-009	-8.738	-8.738	0.000
H2SO4	4.610e-011	4.610e-011	-10.336	-10.336	0.000
S(7)	5.134e-038				
S208-2	2.567e-038	1.535e-038	-37.591	-37.814	-0.223
S(8)	2.194e-027				
HSO5-	2.194e-027	1.932e-027	-26.659	-26.714	-0.055
Zn	1.297e-005				
Zn+2	9.158e-006	5.670e-006	-5.038	-5.246	-0.208
ZnSO4	3.807e-006	3.807e-006	-5.419	-5.419	0.000
ZnCl+	9.295e-009	8.183e-009	-8.032	-8.087	-0.055
ZnHCO3+	1.753e-010	1.543e-010	-9.756	-9.812	-0.055
ZnOH+	1.815e-011	1.598e-011	-10.741	-10.796	-0.055
ZnCl2	8.212e-012	8.212e-012	-11.086	-11.086	0.000
Zn(OH)Cl	3.596e-013	3.596e-013	-12.444	-12.444	0.000
ZnCO3	5.733e-015	5.733e-015	-14.242	-14.242	0.000
ZnCl3-	4.425e-015	3.896e-015	-14.354	-14.409	-0.055
Zn(OH)2	1.759e-016	1.759e-016	-15.755	-15.755	0.000
ZnCl4-2	4.242e-017	2.537e-017	-16.372	-16.596	-0.223
Zn(OH)3-	1.591e-024	1.401e-024	-23.798	-23.854	-0.055
Zn(OH)4-2	1.026e-033	6.137e-034	-32.989	-33.212	-0.223
ZnClO4+	1.267e-037	1.115e-037	-36.897	-36.953	-0.055

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

Phase	SI	log IAP	log KT	
Al	-139.04	10.88	149.91	Al
Al(g)	-189.74	10.88	200.62	Al
Al2(SO4)3	-35.73	-16.83	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-18.39	-16.83	1.56	Al2(SO4)3:6H2O
Alabandite	-130.80	-131.22	-0.42	MnS
Alum-K	-8.38	-13.35	-4.97	KAl(SO4)2:12H2O
Alunite	-1.77	-2.24	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.28	-5.63	-4.35	CaSO4
Antarcticite	-13.36	-9.27	4.09	CaCl2:6H2O
Antlerite	-16.03	-7.30	8.73	Cu3(SO4)(OH)4
Aphthitalite	-15.13	-19.02	-3.89	NaK3(SO4)2
Aragonite	-7.67	-5.70	1.97	CaCO3
Arcanite	-8.02	-9.87	-1.84	K2SO4
Arsenolite	-52.26	-72.10	-19.84	As2O3
Arsenopyrite	-213.59	-228.03	-14.45	FeAsS
Artinite	-22.63	-3.00	19.63	Mg2CO3(OH)2:3H2O
As	-73.41	-30.73	42.68	As
As2O5	-20.27	-18.14	2.14	As2O5
As4O6(cubi)	-104.38	-144.21	-39.82	As4O6
As4O6(mono)	-104.16	-144.21	-40.05	As4O6
Atacamite	-24.52	-10.26	14.26	Cu4Cl2(OH)6

Azurite	-25.87	-16.75	9.12	$\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$
Bassanite	-1.93	-5.63	-3.71	$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$
Birnessite	-15.58	-101.13	-85.55	$\text{Mn}_8\text{O}_{14} \cdot 5\text{H}_2\text{O}$
Bischofite	-14.15	-9.76	4.39	$\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$
Bixbyite	-6.36	-7.32	-0.96	Mn_2O_3
Bloedite	-12.08	-14.56	-2.48	$\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$
Boehmite	-1.99	5.56	7.55	AlO_2H
Bornite	-497.23	-599.77	-102.53	Cu_5FeS_4
Brochantite	-22.04	-6.62	15.42	$\text{Cu}_4(\text{SO}_4)(\text{OH})_6$
Brucite	-13.09	3.19	16.28	$\text{Mg}(\text{OH})_2$
Burkeite	-34.86	-25.37	9.49	$\text{Na}_6\text{CO}_3(\text{SO}_4)_2$
C	-66.44	-2.29	64.15	C
C(g)	-184.06	-2.29	181.77	C
Ca	-132.60	7.23	139.83	Ca
Ca(g)	-157.84	7.23	165.07	Ca
$\text{Ca}_2\text{Al}_2\text{O}_5 \cdot 8\text{H}_2\text{O}$	-41.09	18.48	59.57	$\text{Ca}_2\text{Al}_2\text{O}_5 \cdot 8\text{H}_2\text{O}$
$\text{Ca}_2\text{Cl}_2(\text{OH})_2 \cdot \text{H}_2\text{O}$	-31.88	-5.59	26.29	$\text{Ca}_2\text{Cl}_2(\text{OH})_2 \cdot \text{H}_2\text{O}$
$\text{Ca}_3(\text{AsO}_4)_2$	-24.89	-7.09	17.80	$\text{Ca}_3(\text{AsO}_4)_2$
$\text{Ca}_3\text{Al}_2\text{O}_6$	-90.87	22.16	113.03	$\text{Ca}_3\text{Al}_2\text{O}_6$
$\text{Ca}_4\text{Al}_2\text{Fe}_2\text{O}_{10}$	-104.35	36.13	140.48	$\text{Ca}_4\text{Al}_2\text{Fe}_2\text{O}_{10}$
$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 13\text{H}_2\text{O}$	-81.41	25.84	107.25	$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 13\text{H}_2\text{O}$
$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 19\text{H}_2\text{O}$	-77.84	25.84	103.68	$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 19\text{H}_2\text{O}$
$\text{Ca}_4\text{Cl}_2(\text{OH})_6 \cdot 13\text{H}_2\text{O}$	-66.55	1.78	68.33	$\text{Ca}_4\text{Cl}_2(\text{OH})_6 \cdot 13\text{H}_2\text{O}$
CaAl_2O_4	-32.11	14.80	46.91	CaAl_2O_4
$\text{CaAl}_2\text{O}_4 \cdot 10\text{H}_2\text{O}$	-23.20	14.79	37.99	$\text{CaAl}_2\text{O}_4 \cdot 10\text{H}_2\text{O}$
CaAl_4O_7	-42.68	25.91	68.59	CaAl_4O_7
Calcite	-7.53	-5.70	1.82	CaCO_3
Carnallite	-20.78	-16.51	4.27	$\text{KMgCl}_3 \cdot 6\text{H}_2\text{O}$
$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}(\text{beta})$	-2.10	-5.63	-3.54	$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$
$\text{CH}_4(\text{g})$	-136.44	-139.29	-2.84	CH_4
Chalcanthite	-6.01	-8.64	-2.63	$\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$
Chalcocite	-131.29	-166.03	-34.74	Cu_2S
Chalcocyanite	-11.55	-8.64	2.91	CuSO_4
Chalcopyrite	-235.10	-267.70	-32.60	CuFeS_2
Chloromagnesite	-31.58	-9.76	21.82	MgCl_2
$\text{Cl}_2(\text{g})$	-19.49	-16.50	2.99	Cl_2
Claudetite	-52.31	-72.10	-19.80	As_2O_3
$\text{CO}(\text{g})$	-44.51	-47.51	-3.00	CO
$\text{CO}_2(\text{g})$	-1.56	-9.39	-7.83	CO_2
Corundum	-7.18	11.11	18.29	Al_2O_3
Covellite	-109.87	-132.73	-22.86	CuS
Cu	-27.28	4.22	31.50	Cu
Cu(g)	-79.43	4.22	83.66	Cu
CuCl_2	-16.00	-12.28	3.72	CuCl_2
Cuprite	-30.72	-32.63	-1.91	Cu_2O
Dawsonite	-7.73	-3.39	4.34	$\text{NaAlCO}_3(\text{OH})_2$
Delafossite	-4.73	-11.17	-6.44	CuFeO_2
Diaspore	-1.59	5.56	7.15	AlHO_2
Dolomite	-14.37	-11.90	2.47	$\text{CaMg}(\text{CO}_3)_2$
Dolomite-dis	-15.91	-11.90	4.01	$\text{CaMg}(\text{CO}_3)_2$
Dolomite-ord	-14.36	-11.90	2.46	$\text{CaMg}(\text{CO}_3)_2$
Epsomite	-4.16	-6.12	-1.96	$\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$
Ettringite	-57.20	5.26	62.46	$\text{Ca}_6\text{Al}_2(\text{SO}_4)_3(\text{OH})_{12} \cdot 26\text{H}_2\text{O}$
Fe	-57.03	1.98	59.02	Fe
$\text{Fe}(\text{OH})_2$	-15.46	-1.56	13.89	$\text{Fe}(\text{OH})_2$
$\text{Fe}(\text{OH})_3$	-0.50	5.14	5.64	$\text{Fe}(\text{OH})_3$
$\text{Fe}_2(\text{SO}_4)_3$	-20.71	-17.66	3.05	$\text{Fe}_2(\text{SO}_4)_3$
FeO	-15.09	-1.56	13.52	FeO
Ferrite-Ca	-7.53	13.97	21.50	CaFe_2O_4
Ferrite-Cu	0.68	10.96	10.28	CuFe_2O_4
Ferrite-Dicalcium	-39.15	17.65	56.80	$\text{Ca}_2\text{Fe}_2\text{O}_5$
Ferrite-Mg	-7.54	13.48	21.02	MgFe_2O_4
Ferrite-Zn	0.16	11.86	11.70	ZnFe_2O_4
FeSO_4	-13.49	-10.88	2.61	FeSO_4
Gaylussite	-25.37	-14.21	11.16	$\text{CaNa}_2(\text{CO}_3)_2 \cdot 5\text{H}_2\text{O}$
Gibbsite	-2.18	5.56	7.74	$\text{Al}(\text{OH})_3$
Glauberite	-8.60	-14.07	-5.47	$\text{Na}_2\text{Ca}(\text{SO}_4)_2$

Goethite	4.61	5.14	0.53	FeOOH
Gypsum	-1.10	-5.63	-4.53	CaSO4:2H2O
H2(g)	-39.45	-42.55	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-125.41	-133.41	-7.99	H2S
Halite	-7.60	-6.04	1.56	NaCl
Hausmannite	-15.28	-5.13	10.14	Mn3O4
HCl(g)	-12.78	-6.48	6.30	HCl
Hematite	10.21	10.29	0.08	Fe2O3
Hercynite	-19.25	9.55	28.80	FeAl2O4
Hexahydrite	-4.40	-6.12	-1.73	MgSO4:6H2O
Huntite	-34.51	-24.29	10.22	CaMg3(CO3)4
Hydromagnesite	-52.33	-21.59	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-21.01	-9.27	11.75	CaCl2
Hydrozincite	-41.21	-10.91	30.31	Zn5(OH)6(CO3)2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	5.93	-3.48	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	2.69	-2.76	-5.45	NaFe3(SO4)2(OH)6
K	-69.48	1.50	70.98	K
K(g)	-80.08	1.50	81.58	K
K2CO3:1.5H2O	-23.32	-9.94	13.38	K2CO3:1.5H2O
K2O	-84.59	-0.55	84.04	K2O
K3H(SO4)2	-15.83	-19.46	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-86.23	-58.52	27.71	K8H4(CO3)6:3H2O
Kainite	-12.56	-12.88	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-16.62	-13.35	3.27	KAl(SO4)2
Kalinite	-9.95	-9.66	0.28	KHCO3
Katoite	-56.78	22.16	78.94	Ca3Al2H12O12
Kieserite	-5.86	-6.12	-0.27	MgSO4:H2O
KMgCl3	-37.76	-16.51	21.25	KMgCl3
KMgCl3:2H2O	-30.47	-16.51	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-19.48	-9.22	10.26	KNaCO3:6H2O
Lammerite	-17.67	-16.12	1.55	Cu3(AsO4)2
Lansfordite	-11.04	-6.20	4.84	MgCO3:5H2O
Lawrencite	-23.57	-14.52	9.05	FeCl2
Leonite	-11.88	-15.99	-4.11	K2Mg(SO4)2:4H2O
Lime	-28.89	3.68	32.57	CaO
Magnesite	-8.47	-6.19	2.27	MgCO3
Magnetite	-1.70	8.72	10.42	Fe3O4
Malachite	-13.94	-8.04	5.90	Cu2CO3(OH)2
Manganite	-3.50	-3.66	-0.16	MnO(OH)
Manganosite	-15.73	2.19	17.92	MnO
Mayenite	-372.17	121.98	494.15	Ca12Al14O33
Melanterite	-8.48	-10.88	-2.40	FeSO4:7H2O
Mercallite	-8.15	-9.59	-1.44	KHSO4
Mg	-115.78	6.74	122.52	Mg
Mg(g)	-135.51	6.74	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.52	-5.33	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-13.74	-4.53	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	-19.18	-3.28	15.89	MgOHCl
MgSO4	-10.95	-6.12	4.83	MgSO4
Mirabilite	-7.28	-8.43	-1.15	Na2SO4:10H2O
Misenite	-56.34	-67.41	-11.08	K8H6(SO4)7
Mn	-77.20	5.74	82.93	Mn
Mn(OH)2(am)	-13.12	2.19	15.31	Mn(OH)2
Mn(OH)3	-10.00	-3.66	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)	-1.46	-17.58	-16.13	MnO2
MnSO4	-9.73	-7.13	2.61	MnSO4
Molysite	-27.76	-14.28	13.47	FeCl3
Monohydrocalcite	-8.38	-5.70	2.68	CaCO3:H2O
Na	-65.16	2.21	67.37	Na

Na(g)	-78.64	2.21	80.86	Na
Na2CO3	-19.67	-8.50	11.16	Na2CO3
Na2CO3:7H2O	-18.44	-8.51	9.94	Na2CO3:7H2O
Na2O	-66.54	0.88	67.42	Na2O
Na3H(SO4)2	-16.42	-17.31	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.61	-22.50	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-14.30	5.58	19.88	NaFeO2
Nahcolite	-8.80	-8.95	-0.14	NaHCO3
Nantokite	-16.02	-22.79	-6.77	CuCl
Natron	-18.09	-8.51	9.59	Na2CO3:10H2O
Nesquehonite	-11.48	-6.20	5.29	MgCO3:3H2O
O2(g)	-4.20	-7.10	-2.89	O2
Orpiment	-392.84	-472.32	-79.49	As2S3
Oxychloride-Mg	-25.93	-0.09	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.74	-6.12	-1.39	MgSO4:5H2O
Periclase	-18.13	3.19	21.33	MgO
Picromerite	-11.55	-15.99	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-25.53	-14.21	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-12.94	-27.25	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-18.86	3.68	22.55	Ca(OH)2
Pyrite	-212.65	-237.35	-24.70	FeS2
Pyrolusite	0.08	-17.58	-17.66	MnO2
Pyrrhotite	-131.23	-134.97	-3.74	FeS
Realgar	-152.99	-213.27	-60.28	AsS
Rhodochrosite	-6.98	-7.20	-0.22	MnCO3
S	-91.84	-136.95	-45.11	S
S2(g)	-197.58	-204.77	-7.19	S2
Scacchite	-19.50	-10.76	8.74	MnCl2
Siderite	-10.73	-10.95	-0.22	FeCO3
Smithsonite	-8.26	-7.81	0.44	ZnCO3
SO2(g)	-43.45	-43.27	0.18	SO2
Sphalerite	-120.36	-131.83	-11.47	ZnS
Spinel	-23.30	14.30	37.61	Al2MgO4
Starkeyite	-5.12	-6.12	-1.00	MgSO4:4H2O
Sylvite	-7.58	-6.75	0.83	KCl
Syngenite	-7.90	-15.50	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-45.93	-28.79	17.14	Mg2CaCl6:12H2O
Tenorite	-6.97	0.67	7.65	CuO
Thenardite	-8.08	-8.43	-0.36	Na2SO4
Thermonatrite	-19.44	-8.50	10.94	Na2CO3:H2O
Todorokite	-13.49	-59.32	-45.82	Mn7O12:3H2O
Troilite	-131.13	-134.97	-3.84	FeS
Trona-K	-30.47	-18.88	11.59	K2NaH(CO3)2:2H2O
Wurtzite	-122.66	-131.83	-9.17	ZnS
Wustite	-13.17	-0.77	12.40	Fe.947O
Zincite	-9.63	1.57	11.20	ZnO
Zn	-63.67	5.12	68.79	Zn
Zn(ClO4)2:6H2O	-76.85	-71.21	5.63	Zn(ClO4)2:6H2O
Zn(g)	-80.29	5.12	85.41	Zn
Zn(OH)2(beta)	-10.36	1.57	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-10.09	1.57	11.66	Zn(OH)2
Zn(OH)2(gamma)	-10.31	1.57	11.88	Zn(OH)2
Zn2(OH)3Cl	-18.62	-3.33	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-13.75	-6.17	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-22.73	-13.42	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-33.00	-13.91	19.09	Zn3O(SO4)2
ZnCl2	-18.46	-11.38	7.08	ZnCl2
ZnCO3:H2O	-7.95	-7.81	0.14	ZnCO3:H2O
ZnSO4	-11.27	-7.74	3.53	ZnSO4
ZnSO4:6H2O	-6.04	-7.74	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.86	-7.74	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-7.19	-7.74	-0.55	ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
