
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 3 AS2
temp 25
units mg/l
pe 10
pH 6.98
Cl 678.5
S(6) 427.00
Al 0.00
As 0.1526
Ca 238.3
Cu 0.00
Fe 0.00
K 40.73
Mg 13.69
Mn 0.114
Na 392.9
Zn 2.44
C(4) 153.72
MIX 2
1 1

```

3      1
SELECTED_OUTPUT
file          DAM_AS2
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

CaAl407	-50.90	17.69	68.59	CaAl407
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 3. AS2

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

Elements	Molality	Moles
As	2.041e-006	2.041e-006
C(4)	2.525e-003	2.525e-003

Ca	5.958e-003	5.958e-003
Cl	1.918e-002	1.918e-002
K	1.044e-003	1.044e-003
Mg	5.644e-004	5.644e-004
Mn	2.079e-006	2.079e-006
Na	1.712e-002	1.712e-002
S(6)	4.455e-003	4.455e-003
Zn	3.739e-005	3.739e-005

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

pH	=	6.980
pe	=	10.000
Activity of water	=	0.999
Ionic strength	=	3.800e-002
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	2.128e-003
Total CO2 (mol/kg)	=	2.525e-003
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	1.075e-003
Percent error, 100*(Cat- An)/(Cat+ An)	=	1.86
Iterations	=	4
Total H	=	1.110528e+002
Total O	=	5.555032e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	1.207e-007	1.047e-007	-6.918	-6.980	-0.062
OH-	1.105e-007	9.193e-008	-6.957	-7.037	-0.080
H2O	5.553e+001	9.992e-001	1.744	-0.000	0.000
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-132.370	-132.370	0.000
As(3)	5.398e-026				
HAsO2	2.863e-026	2.863e-026	-25.543	-25.543	0.000
As(OH)3	2.501e-026	2.501e-026	-25.602	-25.602	0.000
H2AsO3-	1.747e-028	1.461e-028	-27.758	-27.835	-0.078
AsO2-	1.672e-028	1.398e-028	-27.777	-27.855	-0.078
AsO2OH-2	2.820e-032	1.363e-032	-31.550	-31.866	-0.316
As(5)	2.041e-006				
HAsO4-2	1.495e-006	7.226e-007	-5.825	-6.141	-0.316
H2AsO4-	5.453e-007	4.559e-007	-6.263	-6.341	-0.078
AsO4-3	9.134e-011	1.770e-011	-10.039	-10.752	-0.713
H3AsO4	8.408e-012	8.408e-012	-11.075	-11.075	0.000
C(4)	2.525e-003				
HCO3-	2.009e-003	1.680e-003	-2.697	-2.775	-0.078
CO2	4.046e-004	4.084e-004	-3.393	-3.389	0.004
CaHCO3+	6.422e-005	5.369e-005	-4.192	-4.270	-0.078
NaHCO3	3.387e-005	3.387e-005	-4.470	-4.470	0.000
MgHCO3+	5.687e-006	4.755e-006	-5.245	-5.323	-0.078
CaCO3	4.449e-006	4.449e-006	-5.352	-5.352	0.000
CO3-2	1.446e-006	7.117e-007	-5.840	-6.148	-0.308
ZnHCO3+	8.088e-007	6.762e-007	-6.092	-6.170	-0.078
MgCO3	1.835e-007	1.835e-007	-6.736	-6.736	0.000
ZnCO3	9.333e-008	9.333e-008	-7.030	-7.030	0.000
NaCO3-	4.199e-008	3.511e-008	-7.377	-7.455	-0.078
MnCO3	2.132e-008	2.132e-008	-7.671	-7.671	0.000
MnHCO3+	1.309e-008	1.095e-008	-7.883	-7.961	-0.078
Ca	5.958e-003				
Ca+2	5.216e-003	2.697e-003	-2.283	-2.569	-0.286
CaSO4	6.619e-004	6.619e-004	-3.179	-3.179	0.000
CaHCO3+	6.422e-005	5.369e-005	-4.192	-4.270	-0.078
CaCl+	1.082e-005	9.048e-006	-4.966	-5.043	-0.078
CaCO3	4.449e-006	4.449e-006	-5.352	-5.352	0.000
CaCl2	1.685e-007	1.685e-007	-6.774	-6.774	0.000

CaOH+	4.348e-009	3.635e-009	-8.362	-8.439	-0.078
Cl(-1)	1.918e-002				
Cl-	1.912e-002	1.583e-002	-1.719	-1.801	-0.082
NaCl	3.922e-005	3.922e-005	-4.407	-4.407	0.000
CaCl+	1.082e-005	9.048e-006	-4.966	-5.043	-0.078
MgCl+	3.602e-006	3.011e-006	-5.443	-5.521	-0.078
ZnCl+	4.967e-007	4.153e-007	-6.304	-6.382	-0.078
KCl	4.530e-007	4.530e-007	-6.344	-6.344	0.000
CaCl2	1.685e-007	1.685e-007	-6.774	-6.774	0.000
Zn(OH)Cl	6.775e-008	6.775e-008	-7.169	-7.169	0.000
MnCl+	3.450e-008	2.885e-008	-7.462	-7.540	-0.078
ZnCl2	7.678e-009	7.678e-009	-8.115	-8.115	0.000
HCl	3.723e-010	3.723e-010	-9.429	-9.429	0.000
ZnCl3-	8.028e-011	6.712e-011	-10.095	-10.173	-0.078
ZnCl4-2	1.666e-011	8.053e-012	-10.778	-11.094	-0.316
MnCl3-	1.888e-012	1.579e-012	-11.724	-11.802	-0.078
Cl(1)	5.707e-026				
HClO	4.363e-026	4.363e-026	-25.360	-25.360	0.000
ClO-	1.344e-026	1.124e-026	-25.872	-25.949	-0.078
Cl(3)	0.000e+000				
ClO2-	0.000e+000	0.000e+000	-42.915	-42.993	-0.078
HClO2	0.000e+000	0.000e+000	-46.803	-46.803	0.000
Cl(5)	0.000e+000				
ClO3-	0.000e+000	0.000e+000	-46.104	-46.184	-0.080
Cl(7)	0.000e+000				
ClO4-	0.000e+000	0.000e+000	-53.597	-53.677	-0.080
ZnClO4+	0.000e+000	0.000e+000	-57.129	-57.207	-0.078
H(0)	1.724e-037				
H2	8.621e-038	8.701e-038	-37.064	-37.060	0.004
K	1.044e-003				
K+	1.029e-003	8.522e-004	-2.987	-3.069	-0.082
KSO4-	1.382e-005	1.156e-005	-4.859	-4.937	-0.078
KCl	4.530e-007	4.530e-007	-6.344	-6.344	0.000
KOH	2.820e-011	2.820e-011	-10.550	-10.550	0.000
KHSO4	1.068e-012	1.068e-012	-11.972	-11.972	0.000
Mg	5.644e-004				
Mg+2	4.456e-004	2.437e-004	-3.351	-3.613	-0.262
MgSO4	1.093e-004	1.093e-004	-3.961	-3.961	0.000
MgHCO3+	5.687e-006	4.755e-006	-5.245	-5.323	-0.078
MgCl+	3.602e-006	3.011e-006	-5.443	-5.521	-0.078
MgCO3	1.835e-007	1.835e-007	-6.736	-6.736	0.000
Mg4(OH)4+4	7.829e-026	5.199e-027	-25.106	-26.284	-1.178
Mn(2)	2.079e-006				
Mn+2	1.655e-006	8.558e-007	-5.781	-6.068	-0.286
MnSO4	3.548e-007	3.548e-007	-6.450	-6.450	0.000
MnCl+	3.450e-008	2.885e-008	-7.462	-7.540	-0.078
MnCO3	2.132e-008	2.132e-008	-7.671	-7.671	0.000
MnHCO3+	1.309e-008	1.095e-008	-7.883	-7.961	-0.078
MnOH+	2.511e-010	2.099e-010	-9.600	-9.678	-0.078
MnCl3-	1.888e-012	1.579e-012	-11.724	-11.802	-0.078
Mn(OH)2	4.917e-015	4.917e-015	-14.308	-14.308	0.000
Mn2(OH)3+	9.583e-016	8.011e-016	-15.019	-15.096	-0.078
Mn2OH+3	9.169e-016	1.925e-016	-15.038	-15.716	-0.678
Mn(OH)3-	5.264e-020	4.400e-020	-19.279	-19.357	-0.078
Mn(OH)4-2	7.358e-027	3.556e-027	-26.133	-26.449	-0.316
Mn(3)	1.087e-021				
Mn+3	1.087e-021	2.283e-022	-20.964	-21.642	-0.678
Mn(6)	4.364e-029				
MnO4-2	4.364e-029	2.109e-029	-28.360	-28.676	-0.316
Mn(7)	1.116e-028				
MnO4-	1.116e-028	9.286e-029	-27.952	-28.032	-0.080
Na	1.712e-002				
Na+	1.686e-002	1.410e-002	-1.773	-1.851	-0.078
NaSO4-	1.872e-004	1.565e-004	-3.728	-3.806	-0.078
NaCl	3.922e-005	3.922e-005	-4.407	-4.407	0.000
NaHCO3	3.387e-005	3.387e-005	-4.470	-4.470	0.000
NaCO3-	4.199e-008	3.511e-008	-7.377	-7.455	-0.078

NaOH	2.236e-010	2.236e-010	-9.651	-9.651	0.000
O(0)	1.664e-018				
O2	8.321e-019	8.398e-019	-18.080	-18.076	0.004
S(6)	4.455e-003				
SO4-2	3.477e-003	1.680e-003	-2.459	-2.775	-0.316
CaSO4	6.619e-004	6.619e-004	-3.179	-3.179	0.000
NaSO4-	1.872e-004	1.565e-004	-3.728	-3.806	-0.078
MgSO4	1.093e-004	1.093e-004	-3.961	-3.961	0.000
KSO4-	1.382e-005	1.156e-005	-4.859	-4.937	-0.078
ZnSO4	5.512e-006	5.512e-006	-5.259	-5.259	0.000
MnSO4	3.548e-007	3.548e-007	-6.450	-6.450	0.000
HSO4-	2.126e-008	1.777e-008	-7.673	-7.750	-0.078
KHSO4	1.068e-012	1.068e-012	-11.972	-11.972	0.000
H2SO4	1.756e-018	1.756e-018	-17.756	-17.756	0.000
Zn	3.739e-005				
Zn+2	3.020e-005	1.561e-005	-4.520	-4.806	-0.286
ZnSO4	5.512e-006	5.512e-006	-5.259	-5.259	0.000
ZnHCO3+	8.088e-007	6.762e-007	-6.092	-6.170	-0.078
ZnCl+	4.967e-007	4.153e-007	-6.304	-6.382	-0.078
ZnOH+	1.955e-007	1.634e-007	-6.709	-6.787	-0.078
ZnCO3	9.333e-008	9.333e-008	-7.030	-7.030	0.000
Zn(OH)Cl	6.775e-008	6.775e-008	-7.169	-7.169	0.000
ZnCl2	7.678e-009	7.678e-009	-8.115	-8.115	0.000
Zn(OH)2	6.677e-009	6.677e-009	-8.175	-8.175	0.000
ZnCl3-	8.028e-011	6.712e-011	-10.095	-10.173	-0.078
ZnCl4-2	1.666e-011	8.053e-012	-10.778	-11.094	-0.316
Zn(OH)3-	2.362e-013	1.975e-013	-12.627	-12.704	-0.078
Zn(OH)4-2	6.648e-019	3.213e-019	-18.177	-18.493	-0.316
ZnClO4+	0.000e+000	0.000e+000	-57.129	-57.207	-0.078

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

Phase	SI	log IAP	log KT	
Anhydrite	-0.99	-5.34	-4.35	CaSO4
Antarcticite	-10.27	-6.17	4.09	CaCl2:6H2O
Aphthitalite	-12.72	-16.61	-3.89	NaK3(SO4)2
Aragonite	-0.33	1.64	1.97	CaCO3
Arcanite	-7.07	-8.91	-1.84	K2SO4
Arsenolite	-49.79	-69.63	-19.84	As2O3
Artinite	-8.69	10.94	19.63	Mg2CO3(OH)2:3H2O
As	-63.94	-21.26	42.68	As
As2O5	-28.78	-26.64	2.14	As2O5
As4O6(cubi)	-99.44	-139.26	-39.82	As4O6
As4O6(mono)	-99.21	-139.26	-40.05	As4O6
Bassanite	-1.64	-5.34	-3.71	CaSO4:0.5H2O
Birnessite	-2.90	-88.45	-85.55	Mn8O14:5H2O
Bischofite	-11.61	-7.22	4.39	MgCl2:6H2O
Bixbyite	-0.44	-1.40	-0.96	Mn2O3
Bloedite	-10.39	-12.87	-2.48	Na2Mg(SO4)2:4H2O
Brucite	-5.94	10.35	16.28	Mg(OH)2
Burkeite	-21.94	-12.45	9.49	Na6CO3(SO4)2
C	-55.82	8.32	64.15	C
C(g)	-173.44	8.32	181.77	C
Ca	-119.40	20.43	139.83	Ca
Ca(g)	-144.64	20.43	165.07	Ca
Ca2Cl2(OH)2:H2O	-21.07	5.22	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-10.27	7.53	17.80	Ca3(AsO4)2
Ca4Cl2(OH)6:13H2O	-40.33	28.00	68.33	Ca4Cl2(OH)6:13H2O
Calcite	-0.19	1.64	1.82	CaCO3
Carnallite	-16.36	-12.09	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.81	-5.34	-3.54	CaSO4:0.5H2O
Chloromagnesite	-29.03	-7.21	21.82	MgCl2
Cl2(g)	-29.59	-26.60	2.99	Cl2
Claudetite	-49.83	-69.63	-19.80	As2O3
CO2(g)	-1.93	-9.75	-7.83	CO2
Dolomite	-0.25	2.23	2.47	CaMg(CO3)2

Dolomite-dis	-1.78	2.23	4.01	CaMg(CO ₃) ₂
Dolomite-ord	-0.24	2.23	2.46	CaMg(CO ₃) ₂
Epsomite	-4.43	-6.39	-1.96	MgSO ₄ :7H ₂ O
Gaylussite	-9.03	2.14	11.16	CaNa ₂ (CO ₃) ₂ :5H ₂ O
Glauberite	-6.35	-11.82	-5.47	Na ₂ Ca(SO ₄) ₂
Gypsum	-0.81	-5.34	-4.53	CaSO ₄ :2H ₂ O
H ₂ (g)	-33.96	-37.06	-3.10	H ₂
H ₂ O(g)	-1.59	-0.00	1.59	H ₂ O
Halite	-5.21	-3.65	1.56	NaCl
Hausmannite	-3.66	6.49	10.14	Mn ₃ O ₄
HCl(g)	-15.08	-8.78	6.30	HCl
Hexahydrate	-4.66	-6.39	-1.73	MgSO ₄ :6H ₂ O
Huntite	-6.81	3.41	10.22	CaMg ₃ (CO ₃) ₄
Hydromagnesite	-18.03	12.71	30.74	Mg ₅ (CO ₃) ₄ (OH) ₂ :4H ₂ O
Hydrophilite	-17.92	-6.17	11.75	CaCl ₂
Hydrozincite	-4.05	26.26	30.31	Zn ₅ (OH) ₆ (CO ₃) ₂
Ice	-0.14	-0.00	0.14	H ₂ O
K	-62.55	8.43	70.98	K
K(g)	-73.15	8.43	81.58	K
K ₂ CO ₃ :1.5H ₂ O	-15.31	-1.93	13.38	K ₂ CO ₃ :1.5H ₂ O
K ₂ O	-76.21	7.82	84.04	K ₂ O
K ₃ H(SO ₄) ₂	-18.11	-21.74	-3.62	K ₃ H(SO ₄) ₂
K ₈ H ₄ (CO ₃) ₆ :3H ₂ O	-54.95	-27.24	27.71	K ₈ H ₄ (CO ₃) ₆ :3H ₂ O
Kainite	-10.95	-11.26	-0.31	KMgClSO ₄ :3H ₂ O
Kaliginite	-6.13	-5.84	0.28	KHCO ₃
Kieserite	-6.12	-6.39	-0.27	MgSO ₄ :H ₂ O
KMgCl ₃	-33.33	-12.08	21.25	KMgCl ₃
KMgCl ₃ :2H ₂ O	-26.05	-12.08	13.96	KMgCl ₃ :2H ₂ O
KNaCO ₃ :6H ₂ O	-10.98	-0.72	10.26	KNaCO ₃ :6H ₂ O
Lansfordite	-4.25	0.59	4.84	MgCO ₃ :5H ₂ O
Leonite	-11.19	-15.30	-4.11	K ₂ Mg(SO ₄) ₂ :4H ₂ O
Lime	-21.18	11.39	32.57	CaO
Magnesite	-1.68	0.59	2.27	MgCO ₃
Manganite	-0.54	-0.70	-0.16	MnO(OH)
Manganosite	-10.02	7.89	17.92	MnO
Mercallite	-11.39	-12.82	-1.44	KHSO ₄
Mg	-103.14	19.38	122.52	Mg
Mg(g)	-122.86	19.38	142.25	Mg
Mg _{1.25} SO ₄ (OH) _{0.5} :0.5H ₂ O	-9.00	-3.80	5.20	Mg _{1.25} SO ₄ (OH) _{0.5} :0.5H ₂ O
Mg _{1.5} SO ₄ (OH)	-10.42	-1.21	9.21	Mg _{1.5} SO ₄ (OH)
MgCl ₂ :2H ₂ O	-19.95	-7.21	12.73	MgCl ₂ :2H ₂ O
MgCl ₂ :4H ₂ O	-14.52	-7.22	7.30	MgCl ₂ :4H ₂ O
MgCl ₂ :H ₂ O	-23.29	-7.21	16.07	MgCl ₂ :H ₂ O
MgOHCl	-14.33	1.57	15.89	MgOHCl
MgSO ₄	-11.22	-6.39	4.83	MgSO ₄
Mirabilite	-5.33	-6.48	-1.15	Na ₂ SO ₄ :10H ₂ O
Misenite	-74.78	-85.86	-11.08	K ₈ H ₆ (SO ₄) ₇
Mn	-66.00	16.93	82.93	Mn
Mn(OH) ₂ (am)	-7.42	7.89	15.31	Mn(OH) ₂
Mn(OH) ₃	-7.04	-0.70	6.34	Mn(OH) ₃
MnCl ₂ :2H ₂ O	-13.67	-9.67	4.00	MnCl ₂ :2H ₂ O
MnCl ₂ :4H ₂ O	-12.42	-9.67	2.75	MnCl ₂ :4H ₂ O
MnCl ₂ :H ₂ O	-15.21	-9.67	5.54	MnCl ₂ :H ₂ O
MnO ₂ (gamma)	-1.25	-17.37	-16.13	MnO ₂
MnSO ₄	-11.45	-8.84	2.61	MnSO ₄
Monohydrocalcite	-1.04	1.64	2.68	CaCO ₃ :H ₂ O
Na	-57.72	9.65	67.37	Na
Na(g)	-71.21	9.65	80.86	Na
Na ₂ CO ₃	-10.66	0.50	11.16	Na ₂ CO ₃
Na ₂ CO ₃ :7H ₂ O	-9.44	0.50	9.94	Na ₂ CO ₃ :7H ₂ O
Na ₂ O	-57.16	10.26	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-17.19	-18.08	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-12.40	-18.30	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
Nahcolite	-4.48	-4.63	-0.14	NaHCO ₃
Natron	-9.09	0.50	9.59	Na ₂ CO ₃ :10H ₂ O
Nesquehonite	-4.70	0.59	5.29	MgCO ₃ :3H ₂ O
O ₂ (g)	-15.18	-18.08	-2.89	O ₂

Oxychloride-Mg	-13.92	11.91	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-5.00	-6.39	-1.39	MgSO4:5H2O
Periclase	-10.98	10.35	21.33	MgO
Picromerite	-10.86	-15.30	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-9.18	2.14	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-11.68	-25.99	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-11.16	11.39	22.55	Ca(OH)2
Pyrolusite	0.29	-17.37	-17.66	MnO2
Rhodochrosite	-1.64	-1.86	-0.22	MnCO3
Scacchite	-18.41	-9.67	8.74	MnCl2
Smithsonite	-1.05	-0.60	0.44	ZnCO3
Starkeyite	-5.39	-6.39	-1.00	MgSO4:4H2O
Sylvite	-5.70	-4.87	0.83	KCl
Syngenite	-6.66	-14.26	-7.60	K2Ca(SO4)2:H2O
Tachyhydrate	-37.75	-20.60	17.14	Mg2CaCl6:12H2O
Thenardite	-6.12	-6.48	-0.36	Na2SO4
Thermonatrite	-10.43	0.50	10.94	Na2CO3:H2O
Todorokite	-1.03	-46.85	-45.82	Mn7O12:3H2O
Trona-K	-18.15	-6.56	11.59	K2NaH(CO3)2:2H2O
Zincite	-2.05	9.15	11.20	ZnO
Zn	-50.60	18.19	68.79	Zn
Zn(ClO4)2:6H2O	-117.80	-112.16	5.63	Zn(ClO4)2:6H2O
Zn(g)	-67.22	18.19	85.41	Zn
Zn(OH)2(beta)	-2.78	9.15	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-2.51	9.15	11.66	Zn(OH)2
Zn(OH)2(gamma)	-2.73	9.15	11.88	Zn(OH)2
Zn2(OH)3Cl	-5.77	9.53	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-6.01	1.57	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-8.49	0.82	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-25.10	-6.01	19.09	Zn3O(SO4)2
ZnCl2	-15.49	-8.41	7.08	ZnCl2
ZnCO3:H2O	-0.74	-0.60	0.14	ZnCO3:H2O
ZnSO4	-11.11	-7.58	3.53	ZnSO4
ZnSO4:6H2O	-5.88	-7.58	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.71	-7.58	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-7.03	-7.58	-0.55	ZnSO4:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using mix 2.

Mixture 2.

1.000e+000 Solution 1 Flujo 2
1.000e+000 Solution 3 AS2

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

Elements	Molality	Moles
Al	1.558e-004	3.117e-004
As	3.025e-006	6.049e-006
C	1.262e-003	2.525e-003
Ca	3.415e-003	6.829e-003
Cl	1.023e-002	2.045e-002
Cu	7.877e-007	1.575e-006
Fe	3.890e-004	7.780e-004
K	7.242e-004	1.448e-003
Mg	5.190e-004	1.038e-003
Mn	5.571e-005	1.114e-004
Na	8.871e-003	1.774e-002
S	7.164e-003	1.433e-002
Zn	3.018e-005	6.035e-005

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

pH	=	3.515	Charge balance
pe	=	16.210	Adjusted to redox equilibrium
Activity of water	=	0.999	
Ionic strength	=	2.918e-002	
Mass of water (kg)	=	2.000e+000	
Total alkalinity (eq/kg)	=	-7.202e-004	
Total CO2 (mol/kg)	=	1.262e-003	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	-1.069e-002	
Percent error, 100*(Cat- An)/(Cat+ An)	=	-13.61	
Iterations	=	9	
Total H	=	2.221067e+002	
Total O	=	1.111158e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	3.483e-004	3.056e-004	-3.458	-3.515	-0.057
OH-	3.718e-011	3.151e-011	-10.430	-10.502	-0.072
H2O	5.553e+001	9.995e-001	1.744	-0.000	0.000
Al	1.558e-004				
AlSO4+	7.221e-005	6.144e-005	-4.141	-4.212	-0.070
Al+3	6.509e-005	1.961e-005	-4.186	-4.707	-0.521
Al(SO4)2-	1.716e-005	1.460e-005	-4.765	-4.836	-0.070
AlOH+2	1.362e-006	7.186e-007	-5.866	-6.144	-0.278
Al(OH)2+	6.414e-009	5.457e-009	-8.193	-8.263	-0.070
Al2(OH)2+4	9.788e-010	8.397e-011	-9.009	-10.076	-1.067
HALO2	2.599e-011	2.599e-011	-10.585	-10.585	0.000
Al3(OH)4+5	4.875e-013	1.137e-014	-12.312	-13.944	-1.632
AlO2-	3.424e-014	2.913e-014	-13.465	-13.536	-0.070
NaAlO2	4.107e-017	4.107e-017	-16.387	-16.387	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-44.258	-47.458	-3.200
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-150.133	-150.133	0.000
As(3)	2.732e-027				
HAsO2	1.458e-027	1.458e-027	-26.836	-26.836	0.000
As(OH)3	1.274e-027	1.274e-027	-26.895	-26.895	0.000
H2AsO3-	2.996e-033	2.549e-033	-32.523	-32.594	-0.070
AsO2-	2.866e-033	2.438e-033	-32.543	-32.613	-0.070
AsO2OH-2	1.568e-040	0.000e+000	-39.805	-40.089	-0.284
HAsS2	0.000e+000	0.000e+000	-272.897	-272.897	0.000
As(5)	3.025e-006				
H2AsO4-	2.890e-006	2.459e-006	-5.539	-5.609	-0.070
H3AsO4	1.324e-007	1.324e-007	-6.878	-6.878	0.000
HAsO4-2	2.569e-009	1.336e-009	-8.590	-8.874	-0.284
AsO4-3	4.903e-017	1.121e-017	-16.310	-16.950	-0.641
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-251.654	-251.654	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-222.217	-222.217	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-139.162	-139.162	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-47.388	-47.388	0.000
C(4)	1.262e-003				
CO2	1.260e-003	1.269e-003	-2.900	-2.896	0.003
HCO3-	2.103e-006	1.790e-006	-5.677	-5.747	-0.070
CaHCO3+	3.750e-008	3.190e-008	-7.426	-7.496	-0.070
NaHCO3	1.891e-008	1.891e-008	-7.723	-7.723	0.000
FeCO3+	9.480e-009	8.067e-009	-8.023	-8.093	-0.070
MgHCO3+	4.947e-009	4.209e-009	-8.306	-8.376	-0.070
ZnHCO3+	6.594e-010	5.611e-010	-9.181	-9.251	-0.070

MnHCO3+	3.435e-010	2.922e-010	-9.464	-9.534	-0.070
FeHCO3+	3.815e-012	3.246e-012	-11.418	-11.489	-0.070
CaCO3	9.059e-013	9.059e-013	-12.043	-12.043	0.000
CuCO3	7.656e-013	7.656e-013	-12.116	-12.116	0.000
CO3-2	4.925e-013	2.598e-013	-12.308	-12.585	-0.278
MnCO3	1.951e-013	1.951e-013	-12.710	-12.710	0.000
MgCO3	5.566e-014	5.566e-014	-13.254	-13.254	0.000
ZnCO3	2.654e-014	2.654e-014	-13.576	-13.576	0.000
NaCO3-	7.894e-015	6.717e-015	-14.103	-14.173	-0.070
FeCO3	5.099e-017	5.099e-017	-16.293	-16.293	0.000
Cu(CO3)2-2	6.816e-022	3.544e-022	-21.166	-21.451	-0.284
CuCO3(OH)2-2	1.339e-025	6.963e-026	-24.873	-25.157	-0.284
Ca	3.415e-003				
Ca+2	2.739e-003	1.504e-003	-2.562	-2.823	-0.260
CaSO4	6.728e-004	6.728e-004	-3.172	-3.172	0.000
CaCl+	3.230e-006	2.748e-006	-5.491	-5.561	-0.070
CaHCO3+	3.750e-008	3.190e-008	-7.426	-7.496	-0.070
CaCl2	2.786e-008	2.786e-008	-7.555	-7.555	0.000
CaCO3	9.059e-013	9.059e-013	-12.043	-12.043	0.000
CaOH+	8.168e-013	6.950e-013	-12.088	-12.158	-0.070
Cl(-1)	1.023e-002				
Cl-	1.021e-002	8.619e-003	-1.991	-2.065	-0.074
NaCl	1.119e-005	1.119e-005	-4.951	-4.951	0.000
CaCl+	3.230e-006	2.748e-006	-5.491	-5.561	-0.070
MgCl+	1.601e-006	1.363e-006	-5.795	-5.866	-0.070
HCl	5.916e-007	5.916e-007	-6.228	-6.228	0.000
MnCl+	4.626e-007	3.936e-007	-6.335	-6.405	-0.070
ZnCl+	2.070e-007	1.761e-007	-6.684	-6.754	-0.070
KCl	1.727e-007	1.727e-007	-6.763	-6.763	0.000
FeCl2+	6.331e-008	5.387e-008	-7.199	-7.269	-0.070
CaCl2	2.786e-008	2.786e-008	-7.555	-7.555	0.000
FeCl+2	1.463e-008	7.720e-009	-7.835	-8.112	-0.278
CuCl+	8.560e-009	7.283e-009	-8.068	-8.138	-0.070
ZnCl2	1.773e-009	1.773e-009	-8.751	-8.751	0.000
CuCl2	3.306e-011	3.306e-011	-10.481	-10.481	0.000
FeCl+	2.551e-011	2.170e-011	-10.593	-10.663	-0.070
ZnCl3-	9.920e-012	8.440e-012	-11.004	-11.074	-0.070
Zn(OH)Cl	9.850e-012	9.850e-012	-11.007	-11.007	0.000
MnCl3-	7.507e-012	6.388e-012	-11.125	-11.195	-0.070
ZnCl4-2	1.061e-012	5.514e-013	-11.974	-12.259	-0.284
FeCl4-	5.654e-015	4.811e-015	-14.248	-14.318	-0.070
FeCl2	1.004e-015	1.004e-015	-14.998	-14.998	0.000
FeCl4-2	4.145e-019	2.155e-019	-18.383	-18.667	-0.284
CuCl4-2	8.865e-020	4.609e-020	-19.052	-19.336	-0.284
CuCl2-	6.030e-020	5.131e-020	-19.220	-19.290	-0.070
CuCl3-2	5.463e-021	2.840e-021	-20.263	-20.547	-0.284
Cl(1)	2.143e-017				
HClO	2.143e-017	2.143e-017	-16.669	-16.669	0.000
ClO-	2.222e-021	1.891e-021	-20.653	-20.723	-0.070
Cl(3)	8.602e-033				
ClO2-	6.214e-033	5.287e-033	-32.207	-32.277	-0.070
HClO2	2.389e-033	2.389e-033	-32.622	-32.622	0.000
Cl(5)	1.241e-030				
ClO3-	1.241e-030	1.052e-030	-29.906	-29.978	-0.072
Cl(7)	1.233e-032				
ClO4-	1.233e-032	1.045e-032	-31.909	-31.981	-0.072
ZnClO4+	2.825e-036	2.404e-036	-35.549	-35.619	-0.070
Cu(1)	7.802e-020				
CuCl2-	6.030e-020	5.131e-020	-19.220	-19.290	-0.070
Cu+	1.225e-020	1.043e-020	-19.912	-19.982	-0.070
CuCl3-2	5.463e-021	2.840e-021	-20.263	-20.547	-0.284
Cu(2)	7.877e-007				
Cu+2	5.624e-007	3.089e-007	-6.250	-6.510	-0.260
CuSO4	2.167e-007	2.167e-007	-6.664	-6.664	0.000
CuCl+	8.560e-009	7.283e-009	-8.068	-8.138	-0.070
CuOH+	6.126e-011	5.212e-011	-10.213	-10.283	-0.070
CuCl2	3.306e-011	3.306e-011	-10.481	-10.481	0.000

CuCO3	7.656e-013	7.656e-013	-12.116	-12.116	0.000
CuCl4-2	8.865e-020	4.609e-020	-19.052	-19.336	-0.284
Cu(CO3)2-2	6.816e-022	3.544e-022	-21.166	-21.451	-0.284
CuCO3(OH)2-2	1.339e-025	6.963e-026	-24.873	-25.157	-0.284
CuO2-2	2.417e-032	1.257e-032	-31.617	-31.901	-0.284
Fe(2)	7.998e-009				
Fe+2	6.292e-009	3.456e-009	-8.201	-8.461	-0.260
FeSO4	1.677e-009	1.677e-009	-8.775	-8.775	0.000
FeCl+	2.551e-011	2.170e-011	-10.593	-10.663	-0.070
FeHCO3+	3.815e-012	3.246e-012	-11.418	-11.489	-0.070
FeOH+	4.201e-015	3.575e-015	-14.377	-14.447	-0.070
FeCl2	1.004e-015	1.004e-015	-14.998	-14.998	0.000
FeCO3	5.099e-017	5.099e-017	-16.293	-16.293	0.000
FeCl4-2	4.145e-019	2.155e-019	-18.383	-18.667	-0.284
Fe(OH)2	9.287e-023	9.287e-023	-22.032	-22.032	0.000
Fe(OH)3-	1.421e-029	1.209e-029	-28.847	-28.917	-0.070
Fe(OH)4-2	0.000e+000	0.000e+000	-40.119	-40.403	-0.284
Fe(3)	3.890e-004				
FeOH+2	2.152e-004	1.135e-004	-3.667	-3.945	-0.278
Fe(OH)2+	1.445e-004	1.229e-004	-3.840	-3.910	-0.070
Fe+3	1.784e-005	5.376e-006	-4.749	-5.270	-0.521
Fe2(OH)2+4	4.043e-006	3.469e-007	-5.393	-6.460	-1.067
FeSO4+	1.871e-006	1.592e-006	-5.728	-5.798	-0.070
Fe3(OH)4+5	3.820e-007	8.910e-009	-6.418	-8.050	-1.632
Fe(OH)3	1.881e-007	1.881e-007	-6.726	-6.726	0.000
Fe(SO4)2-	9.686e-008	8.242e-008	-7.014	-7.084	-0.070
FeCl2+	6.331e-008	5.387e-008	-7.199	-7.269	-0.070
FeCl+2	1.463e-008	7.720e-009	-7.835	-8.112	-0.278
FeCO3+	9.480e-009	8.067e-009	-8.023	-8.093	-0.070
Fe(OH)4-	1.816e-013	1.545e-013	-12.741	-12.811	-0.070
FeCl4-	5.654e-015	4.811e-015	-14.248	-14.318	-0.070
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-42.553	-42.550	0.003
K	7.242e-004				
K+	7.067e-004	5.965e-004	-3.151	-3.224	-0.074
KSO4-	1.733e-005	1.474e-005	-4.761	-4.831	-0.070
KCl	1.727e-007	1.727e-007	-6.763	-6.763	0.000
KHSO4	3.975e-009	3.975e-009	-8.401	-8.401	0.000
KOH	6.765e-015	6.765e-015	-14.170	-14.170	0.000
Mg	5.190e-004				
Mg+2	3.518e-004	2.025e-004	-3.454	-3.694	-0.240
MgSO4	1.656e-004	1.656e-004	-3.781	-3.781	0.000
MgCl+	1.601e-006	1.363e-006	-5.795	-5.866	-0.070
MgHCO3+	4.947e-009	4.209e-009	-8.306	-8.376	-0.070
MgCO3	5.566e-014	5.566e-014	-13.254	-13.254	0.000
Mg4(OH)4+4	3.990e-040	0.000e+000	-39.399	-40.466	-1.067
Mn(2)	5.571e-005				
Mn+2	3.904e-005	2.145e-005	-4.408	-4.669	-0.260
MnSO4	1.620e-005	1.620e-005	-4.790	-4.790	0.000
MnCl+	4.626e-007	3.936e-007	-6.335	-6.405	-0.070
MnHCO3+	3.435e-010	2.922e-010	-9.464	-9.534	-0.070
MnCl3-	7.507e-012	6.388e-012	-11.125	-11.195	-0.070
MnOH+	2.119e-012	1.803e-012	-11.674	-11.744	-0.070
MnCO3	1.951e-013	1.951e-013	-12.710	-12.710	0.000
Mn2OH+3	1.698e-016	4.144e-017	-15.770	-16.383	-0.613
Mn(OH)2	1.448e-020	1.448e-020	-19.839	-19.839	0.000
Mn2(OH)3+	2.381e-023	2.026e-023	-22.623	-22.693	-0.070
Mn(OH)3-	5.219e-029	4.441e-029	-28.282	-28.353	-0.070
Mn(OH)4-2	2.366e-039	1.230e-039	-38.626	-38.910	-0.284
Mn(3)	3.803e-014				
Mn+3	3.803e-014	9.280e-015	-13.420	-14.032	-0.613
Mn(6)	1.340e-030				
MnO4-2	1.340e-030	6.964e-031	-29.873	-30.157	-0.284
Mn(7)	5.869e-024				
MnO4-	5.869e-024	4.974e-024	-23.231	-23.303	-0.072
Na	8.871e-003				
Na+	8.684e-003	7.389e-003	-2.061	-2.131	-0.070

NaSO4-	1.757e-004	1.495e-004	-3.755	-3.825	-0.070
NaCl	1.119e-005	1.119e-005	-4.951	-4.951	0.000
NaHCO3	1.891e-008	1.891e-008	-7.723	-7.723	0.000
NaOH	4.017e-014	4.017e-014	-13.396	-13.396	0.000
NaCO3-	7.894e-015	6.717e-015	-14.103	-14.173	-0.070
NaAlO2	4.107e-017	4.107e-017	-16.387	-16.387	0.000
O(0)	1.593e-007				
O2	7.965e-008	8.022e-008	-7.099	-7.096	0.003
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-126.625	-126.625	0.000
HS-	0.000e+000	0.000e+000	-130.048	-130.120	-0.072
S-2	0.000e+000	0.000e+000	-139.260	-139.531	-0.272
S2-2	0.000e+000	0.000e+000	-230.246	-230.530	-0.284
HAsS2	0.000e+000	0.000e+000	-272.897	-272.897	0.000
S3-2	0.000e+000	0.000e+000	-321.286	-321.570	-0.284
S4-2	0.000e+000	0.000e+000	-412.554	-412.838	-0.284
S5-2	0.000e+000	0.000e+000	-504.038	-504.322	-0.284
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-131.056	-131.340	-0.284
HS2O3-	0.000e+000	0.000e+000	-133.771	-133.841	-0.070
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-119.544	-119.816	-0.272
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-41.797	-41.867	-0.070
H2SO3	0.000e+000	0.000e+000	-43.401	-43.401	0.000
SO2	0.000e+000	0.000e+000	-43.501	-43.501	0.000
SO3-2	0.000e+000	0.000e+000	-45.306	-45.584	-0.278
S2O6-2	0.000e+000	0.000e+000	-59.594	-59.878	-0.284
S3O6-2	0.000e+000	0.000e+000	-153.117	-153.401	-0.284
S4O6-2	0.000e+000	0.000e+000	-230.735	-231.019	-0.284
S5O6-2	0.000e+000	0.000e+000	-337.232	-337.516	-0.284
S(5)	0.000e+000				
S2O5-2	0.000e+000	0.000e+000	-88.280	-88.565	-0.284
S(6)	7.164e-003				
SO4-2	5.889e-003	3.062e-003	-2.230	-2.514	-0.284
CaSO4	6.728e-004	6.728e-004	-3.172	-3.172	0.000
NaSO4-	1.757e-004	1.495e-004	-3.755	-3.825	-0.070
MgSO4	1.656e-004	1.656e-004	-3.781	-3.781	0.000
HSO4-	1.111e-004	9.450e-005	-3.954	-4.025	-0.070
AlSO4+	7.221e-005	6.144e-005	-4.141	-4.212	-0.070
KSO4-	1.733e-005	1.474e-005	-4.761	-4.831	-0.070
Al(SO4)2-	1.716e-005	1.460e-005	-4.765	-4.836	-0.070
MnSO4	1.620e-005	1.620e-005	-4.790	-4.790	0.000
ZnSO4	7.825e-006	7.825e-006	-5.107	-5.107	0.000
FeSO4+	1.871e-006	1.592e-006	-5.728	-5.798	-0.070
CuSO4	2.167e-007	2.167e-007	-6.664	-6.664	0.000
Fe(SO4)2-	9.686e-008	8.242e-008	-7.014	-7.084	-0.070
KHSO4	3.975e-009	3.975e-009	-8.401	-8.401	0.000
FeSO4	1.677e-009	1.677e-009	-8.775	-8.775	0.000
H2SO4	2.725e-011	2.725e-011	-10.565	-10.565	0.000
S(7)	3.347e-038				
S2O8-2	1.673e-038	8.699e-039	-37.776	-38.061	-0.284
S(8)	1.709e-027				
HSO5-	1.709e-027	1.454e-027	-26.767	-26.837	-0.070
Zn	3.018e-005				
Zn+2	2.214e-005	1.216e-005	-4.655	-4.915	-0.260
ZnSO4	7.825e-006	7.825e-006	-5.107	-5.107	0.000
ZnCl+	2.070e-007	1.761e-007	-6.684	-6.754	-0.070
ZnCl2	1.773e-009	1.773e-009	-8.751	-8.751	0.000
ZnHCO3+	6.594e-010	5.611e-010	-9.181	-9.251	-0.070
ZnOH+	5.127e-011	4.363e-011	-10.290	-10.360	-0.070
ZnCl3-	9.920e-012	8.440e-012	-11.004	-11.074	-0.070
Zn(OH)Cl	9.850e-012	9.850e-012	-11.007	-11.007	0.000
ZnCl4-2	1.061e-012	5.514e-013	-11.974	-12.259	-0.284
ZnCO3	2.654e-014	2.654e-014	-13.576	-13.576	0.000
Zn(OH)2	6.111e-016	6.111e-016	-15.214	-15.214	0.000
Zn(OH)3-	7.281e-024	6.195e-024	-23.138	-23.208	-0.070

Zn(OH)4-2	6.645e-033	3.455e-033	-32.177	-32.462	-0.284
ZnClO4+	2.825e-036	2.404e-036	-35.549	-35.619	-0.070

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

Phase	SI	log IAP	log KT	
Al	-138.75	11.16	149.91	Al
Al(g)	-189.46	11.16	200.62	Al
Al2(SO4)3	-35.86	-16.96	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-18.51	-16.96	1.56	Al2(SO4)3:6H2O
Alabandite	-130.85	-131.27	-0.42	MnS
Alum-K	-7.99	-12.96	-4.97	KAl(SO4)2:12H2O
Alunite	-0.82	-1.29	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.99	-5.34	-4.35	CaSO4
Antarcticite	-11.05	-6.95	4.09	CaCl2:6H2O
Antlerite	-16.72	-7.99	8.73	Cu3(SO4)(OH)4
Aphthitalite	-12.94	-16.83	-3.89	NaK3(SO4)2
Aragonite	-7.03	-5.06	1.97	CaCO3
Arcanite	-7.12	-8.96	-1.84	K2SO4
Arsenolite	-52.37	-72.22	-19.84	As2O3
Arsenopyrite	-213.74	-228.19	-14.45	FeAsS
Artinite	-22.22	-2.59	19.63	Mg2CO3(OH)2:3H2O
As	-73.47	-30.79	42.68	As
As2O5	-20.38	-18.25	2.14	As2O5
As4O6(cubi)	-104.61	-144.43	-39.82	As4O6
As4O6(mono)	-104.38	-144.43	-40.05	As4O6
Atacamite	-23.35	-9.08	14.26	Cu4Cl2(OH)6
Azurite	-26.08	-16.97	9.12	Cu3(CO3)2(OH)2
Bassanite	-1.63	-5.34	-3.71	CaSO4:0.5H2O
Birnessite	-14.21	-99.76	-85.55	Mn8O14:5H2O
Bischofite	-12.22	-7.82	4.39	MgCl2:6H2O
Bixbyite	-6.01	-6.98	-0.96	Mn2O3
Bloedite	-10.51	-12.99	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-1.71	5.84	7.55	AlO2H
Bornite	-498.79	-601.32	-102.53	Cu5FeS4
Brochantite	-22.89	-7.47	15.42	Cu4(SO4)(OH)6
Brucite	-12.95	3.34	16.28	Mg(OH)2
Burkeite	-29.54	-20.05	9.49	Na6CO3(SO4)2
C	-66.31	-2.17	64.15	C
C(g)	-183.93	-2.17	181.77	C
Ca	-132.08	7.75	139.83	Ca
Ca(g)	-157.32	7.75	165.07	Ca
Ca2Al2O5:8H2O	-39.48	20.09	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-29.04	-2.75	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-23.43	-5.63	17.80	Ca3(AsO4)2
Ca3Al2O6	-88.74	24.29	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-101.43	39.05	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-78.76	28.50	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-75.18	28.50	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-62.66	5.67	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-31.03	15.88	46.91	CaAl2O4
CaAl2O4:10H2O	-22.12	15.88	37.99	CaAl2O4:10H2O
CaAl4O7	-41.04	27.55	68.59	CaAl4O7
Calcite	-6.88	-5.06	1.82	CaCO3
Carnallite	-17.39	-13.11	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.80	-5.34	-3.54	CaSO4:0.5H2O
CH4(g)	-136.32	-139.16	-2.84	CH4
Chalcanthite	-6.40	-9.03	-2.63	CuSO4:5H2O
Chalcocite	-131.83	-166.57	-34.74	Cu2S
Chalcocyanite	-11.94	-9.02	2.91	CuSO4
Chalcopyrite	-235.58	-268.18	-32.60	CuFeS2
Chloromagnesite	-29.64	-7.82	21.82	MgCl2
Cl2(g)	-17.70	-14.71	2.99	Cl2
Claudetite	-52.42	-72.22	-19.80	As2O3
CO(g)	-44.39	-47.39	-3.00	CO
CO2(g)	-1.43	-9.26	-7.83	CO2

Corundum	-6.62	11.67	18.29	Al ₂ O ₃
Covellite	-110.26	-133.12	-22.86	CuS
Cu	-27.43	4.07	31.50	Cu
Cu(g)	-79.59	4.07	83.66	Cu
CuCl ₂	-14.36	-10.64	3.72	CuCl ₂
Cuprite	-31.03	-32.93	-1.91	Cu ₂ O
Dawsonite	-6.38	-2.04	4.34	NaAlCO ₃ (OH) ₂
Delafossite	-4.76	-11.19	-6.44	CuFeO ₂
Diaspore	-1.31	5.84	7.15	AlHO ₂
Dolomite	-13.45	-10.98	2.47	CaMg(CO ₃) ₂
Dolomite-dis	-14.99	-10.98	4.01	CaMg(CO ₃) ₂
Dolomite-ord	-13.45	-10.98	2.46	CaMg(CO ₃) ₂
Epsomite	-4.25	-6.21	-1.96	MgSO ₄ ·7H ₂ O
Ettringite	-54.19	8.28	62.46	Ca ₆ Al ₂ (SO ₄) ₃ (OH) ₁₂ ·26H ₂ O
Fe	-56.90	2.12	59.02	Fe
Fe(OH) ₂	-15.33	-1.43	13.89	Fe(OH) ₂
Fe(OH) ₃	-0.37	5.27	5.64	Fe(OH) ₃
Fe ₂ (SO ₄) ₃	-21.13	-18.08	3.05	Fe ₂ (SO ₄) ₃
FeO	-14.95	-1.43	13.52	FeO
Ferrite-Ca	-6.74	14.76	21.50	CaFe ₂ O ₄
Ferrite-Cu	0.79	11.07	10.28	CuFe ₂ O ₄
Ferrite-Dicalcium	-37.84	18.96	56.80	Ca ₂ Fe ₂ O ₅
Ferrite-Mg	-7.14	13.89	21.02	MgFe ₂ O ₄
Ferrite-Zn	0.96	12.66	11.70	ZnFe ₂ O ₄
FeSO ₄	-13.58	-10.98	2.61	FeSO ₄
Gaylussite	-22.72	-11.55	11.16	CaNa ₂ (CO ₃) ₂ ·5H ₂ O
Gibbsite	-1.90	5.84	7.74	Al(OH) ₃
Glauberite	-6.64	-12.11	-5.47	Na ₂ Ca(SO ₄) ₂
Goethite	4.74	5.27	0.53	FeOOH
Gypsum	-0.81	-5.34	-4.53	CaSO ₄ ·2H ₂ O
H ₂ (g)	-39.45	-42.55	-3.10	H ₂
H ₂ O(g)	-1.59	-0.00	1.59	H ₂ O
H ₂ S(g)	-125.64	-133.63	-7.99	H ₂ S
Halite	-5.76	-4.20	1.56	NaCl
Hausmannite	-14.76	-4.62	10.14	Mn ₃ O ₄
HCl(g)	-11.88	-5.58	6.30	HCl
Hematite	10.47	10.55	0.08	Fe ₂ O ₃
Hercynite	-18.56	10.24	28.80	FeAl ₂ O ₄
Hexahydrite	-4.48	-6.21	-1.73	MgSO ₄ ·6H ₂ O
Huntite	-33.05	-22.83	10.22	CaMg ₃ (CO ₃) ₄
Hydromagnesite	-51.11	-20.37	30.74	Mg ₅ (CO ₃) ₄ (OH) ₂ ·4H ₂ O
Hydrophilite	-18.70	-6.95	11.75	CaCl ₂
Hydrozincite	-38.26	-7.95	30.31	Zn ₅ (OH) ₆ (CO ₃) ₂
Ice	-0.14	-0.00	0.14	H ₂ O
Jarosite	6.44	-2.97	-9.41	KFe ₃ (SO ₄) ₂ (OH) ₆
Jarosite-Na	3.57	-1.88	-5.45	NaFe ₃ (SO ₄) ₂ (OH) ₆
K	-68.91	2.06	70.98	K
K(g)	-79.51	2.06	81.58	K
K ₂ CO ₃ ·1.5H ₂ O	-22.06	-8.68	13.38	K ₂ CO ₃ ·1.5H ₂ O
K ₂ O	-83.45	0.58	84.04	K ₂ O
K ₃ H(SO ₄) ₂	-14.59	-18.22	-3.62	K ₃ H(SO ₄) ₂
K ₈ H ₄ (CO ₃) ₆ ·3H ₂ O	-80.96	-53.25	27.71	K ₈ H ₄ (CO ₃) ₆ ·3H ₂ O
Kainite	-11.19	-11.50	-0.31	KMgClSO ₄ ·3H ₂ O
KAl(SO ₄) ₂	-16.23	-12.96	3.27	KAl(SO ₄) ₂
Kalinite	-9.26	-8.97	0.28	KHCO ₃
Katoite	-54.65	24.29	78.94	Ca ₃ Al ₂ H ₁₂ O ₁₂
Kieserite	-5.94	-6.21	-0.27	MgSO ₄ ·H ₂ O
KMgCl ₃	-34.36	-13.11	21.25	KMgCl ₃
KMgCl ₃ ·2H ₂ O	-27.07	-13.11	13.96	KMgCl ₃ ·2H ₂ O
KNaCO ₃ ·6H ₂ O	-17.85	-7.59	10.26	KNaCO ₃ ·6H ₂ O
Lammerite	-18.24	-16.69	1.55	Cu ₃ (AsO ₄) ₂
Lansfordite	-10.77	-5.93	4.84	MgCO ₃ ·5H ₂ O
Lawrencite	-21.65	-12.59	9.05	FeCl ₂
Leonite	-11.06	-15.17	-4.11	K ₂ Mg(SO ₄) ₂ ·4H ₂ O
Lime	-28.36	4.21	32.57	CaO
Magnesite	-8.20	-5.93	2.27	MgCO ₃
Magnetite	-1.30	9.12	10.42	Fe ₃ O ₄

Malachite	-14.12	-8.22	5.90	Cu ₂ CO ₃ (OH) ₂
Manganite	-3.32	-3.49	-0.16	MnO(OH)
Manganosite	-15.56	2.36	17.92	MnO
Mayenite	-361.95	132.20	494.15	Ca ₁₂ Al ₁₄ O ₃₃
Melanterite	-8.58	-10.98	-2.40	FeSO ₄ ·7H ₂ O
Mercallite	-7.81	-9.25	-1.44	KHSO ₄
Mg	-115.64	6.88	122.52	Mg
Mg(g)	-135.36	6.88	142.25	Mg
Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O	-10.57	-5.37	5.20	Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O
Mg _{1.5} SO ₄ (OH)	-13.75	-4.54	9.21	Mg _{1.5} SO ₄ (OH)
MgCl ₂ :2H ₂ O	-20.55	-7.82	12.73	MgCl ₂ :2H ₂ O
MgCl ₂ :4H ₂ O	-15.13	-7.82	7.30	MgCl ₂ :4H ₂ O
MgCl ₂ :H ₂ O	-23.89	-7.82	16.07	MgCl ₂ :H ₂ O
MgOHCl	-18.13	-2.24	15.89	MgOHCl
MgSO ₄	-11.04	-6.21	4.83	MgSO ₄
Mirabilite	-5.62	-6.78	-1.15	Na ₂ SO ₄ :10H ₂ O
Misenite	-53.41	-64.48	-11.08	K ₈ H ₆ (SO ₄) ₇
Mn	-77.02	5.91	82.93	Mn
Mn(OH) ₂ (am)	-12.95	2.36	15.31	Mn(OH) ₂
Mn(OH) ₃	-9.83	-3.49	6.34	Mn(OH) ₃
MnCl ₂ :2H ₂ O	-12.80	-8.80	4.00	MnCl ₂ :2H ₂ O
MnCl ₂ :4H ₂ O	-11.55	-8.80	2.75	MnCl ₂ :4H ₂ O
MnCl ₂ :H ₂ O	-14.34	-8.80	5.54	MnCl ₂ :H ₂ O
MnO ₂ (gamma)	-1.29	-17.41	-16.13	MnO ₂
MnSO ₄	-9.79	-7.18	2.61	MnSO ₄
Molysite	-24.93	-11.46	13.47	FeCl ₃
Monohydrocalcite	-7.73	-5.06	2.68	CaCO ₃ :H ₂ O
Na	-64.21	3.16	67.37	Na
Na(g)	-77.70	3.16	80.86	Na
Na ₂ CO ₃	-17.66	-6.50	11.16	Na ₂ CO ₃
Na ₂ CO ₃ :7H ₂ O	-16.44	-6.50	9.94	Na ₂ CO ₃ :7H ₂ O
Na ₂ O	-64.65	2.77	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-14.05	-14.94	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-13.00	-18.89	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
NaFeO ₂	-13.23	6.66	19.88	NaFeO ₂
Nahcolite	-7.74	-7.88	-0.14	NaHCO ₃
Nantokite	-15.28	-22.05	-6.77	CuCl
Natron	-16.09	-6.50	9.59	Na ₂ CO ₃ :10H ₂ O
Nesquehonite	-11.22	-5.93	5.29	MgCO ₃ :3H ₂ O
O ₂ (g)	-4.20	-7.10	-2.89	O ₂
Orpiment	-393.63	-473.12	-79.49	As ₂ S ₃
Oxychloride-Mg	-24.74	1.09	25.83	Mg ₂ Cl(OH) ₃ :4H ₂ O
Pentahydrite	-4.82	-6.21	-1.39	MgSO ₄ :5H ₂ O
Periclase	-17.99	3.34	21.33	MgO
Picromerite	-10.73	-15.17	-4.44	K ₂ Mg(SO ₄) ₂ :6H ₂ O
Pirssonite	-22.87	-11.55	11.32	Na ₂ Ca(CO ₃) ₂ :2H ₂ O
Polyhalite	-11.53	-25.84	-14.31	K ₂ MgCa ₂ (SO ₄) ₄ :2H ₂ O
Portlandite	-18.34	4.21	22.55	Ca(OH) ₂
Pyrite	-212.98	-237.68	-24.70	FeS ₂
Pyrolusite	0.25	-17.41	-17.66	MnO ₂
Pyrrhotite	-131.33	-135.07	-3.74	FeS
Realgar	-153.28	-213.56	-60.28	AsS
Rhodochrosite	-6.68	-6.90	-0.22	MnCO ₃
S	-92.07	-137.18	-45.11	S
S ₂ (g)	-198.04	-205.22	-7.19	S ₂
Scacchite	-17.54	-8.80	8.74	MnCl ₂
Siderite	-10.48	-10.69	-0.22	FeCO ₃
Smithsonite	-7.59	-7.15	0.44	ZnCO ₃
SO ₂ (g)	-43.68	-43.50	0.18	SO ₂
Sphalerite	-120.05	-131.52	-11.47	ZnS
Spinel	-22.60	15.01	37.61	Al ₂ MgO ₄
Starkeyite	-5.21	-6.21	-1.00	MgSO ₄ :4H ₂ O
Sylvite	-6.12	-5.29	0.83	KCl
Syngenite	-6.70	-14.30	-7.60	K ₂ Ca(SO ₄) ₂ :H ₂ O
Tachyhydrite	-39.74	-22.60	17.14	Mg ₂ CaCl ₆ :12H ₂ O
Tenorite	-7.13	0.52	7.65	CuO
Thenardite	-6.42	-6.78	-0.36	Na ₂ SO ₄

Thermonatrite	-17.43	-6.50	10.94	Na ₂ CO ₃ :H ₂ O
Todorokite	-12.29	-58.12	-45.82	Mn ₇ O ₁₂ :3H ₂ O
Troilite	-131.22	-135.07	-3.84	FeS
Trona-K	-28.15	-16.56	11.59	K ₂ NaH(CO ₃) ₂ :2H ₂ O
Wurtzite	-122.35	-131.52	-9.17	ZnS
Wustite	-13.05	-0.65	12.40	Fe.947O
Zincite	-9.08	2.11	11.20	ZnO
Zn	-63.13	5.66	68.79	Zn
Zn(ClO ₄) ₂ :6H ₂ O	-74.51	-68.88	5.63	Zn(ClO ₄) ₂ :6H ₂ O
Zn(g)	-79.75	5.66	85.41	Zn
Zn(OH) ₂ (beta)	-9.82	2.11	11.93	Zn(OH) ₂
Zn(OH) ₂ (epsilon)	-9.55	2.11	11.66	Zn(OH) ₂
Zn(OH) ₂ (gamma)	-9.77	2.11	11.88	Zn(OH) ₂
Zn ₂ (OH) ₃ Cl	-16.64	-1.35	15.29	Zn ₂ (OH) ₃ Cl
Zn ₂ SO ₄ (OH) ₂	-12.90	-5.31	7.58	Zn ₂ SO ₄ (OH) ₂
Zn ₃ (AsO ₄) ₂	-21.22	-11.90	9.31	Zn ₃ (AsO ₄) ₂
Zn ₃ O(SO ₄) ₂	-31.83	-12.74	19.09	Zn ₃ O(SO ₄) ₂
ZnCl ₂	-16.12	-9.04	7.08	ZnCl ₂
ZnCO ₃ :H ₂ O	-7.29	-7.15	0.14	ZnCO ₃ :H ₂ O
ZnSO ₄	-10.96	-7.43	3.53	ZnSO ₄
ZnSO ₄ :6H ₂ O	-5.73	-7.43	-1.70	ZnSO ₄ :6H ₂ O
ZnSO ₄ :7H ₂ O	-5.55	-7.43	-1.88	ZnSO ₄ :7H ₂ O
ZnSO ₄ :H ₂ O	-6.88	-7.43	-0.55	ZnSO ₄ :H ₂ O

End of simulation.

Reading input data for simulation 2.

End of run.
