
Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
NAMED_EXPRESSIONS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\llnl.dat
SOLUTION 1 Flujo 2
temp 25
pH 2.80
pe 17
redox pe
units mg/l
density 1
Cl 45.3
S(6) 947.3
Al 8.4
As 0.3
Ca 34.9
Cu 0.1
Fe 43.4
K 15.8
Mg 11.5
Mn 6.0
Na 14.2
Zn 1.5
C(4) 0
water 1 # kg
SOLUTION 2 Inter 3
temp 25
units mg/l
pe 12
pH 2.29
Cl 39.1
S(6) 1113.00
Al 34.60
As 0.01
Ca 305.00
Cu 0.13
Fe 12.16
K 8.67
Mg 29.67
Mn 13.97
Na 65.26
Zn 0.02
C(4) 0
MIX 1
1 1

```

2      3
SELECTED_OUTPUT
file          DAM_AGUASUP
ph            true
percent_error true
totals        Al  As  Cu  Fe  Mg  Mn  Zn
              S(6)

```

Beginning of initial solution calculations.

Initial solution 1. Flujo 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 2. Inter 3

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

Elements	Molality	Moles
Al	1.284e-003	1.284e-003
As	1.337e-007	1.337e-007

Ca	7.623e-003	7.623e-003
Cl	1.105e-003	1.105e-003
Cu	2.049e-006	2.049e-006
Fe	2.181e-004	2.181e-004
K	2.221e-004	2.221e-004
Mg	1.223e-003	1.223e-003
Mn	2.547e-004	2.547e-004
Na	2.843e-003	2.843e-003
S(6)	1.161e-002	1.161e-002
Zn	3.064e-007	3.064e-007

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

pH	=	2.290
pe	=	12.000
Activity of water	=	1.000
Ionic strength	=	3.680e-002
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	-7.977e-003
Total carbon (mol/kg)	=	0.000e+000
Total CO2 (mol/kg)	=	0.000e+000
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	9.172e-003
Percent error, 100*(Cat- An)/(Cat+ An)	=	21.65
Iterations	=	8
Total H	=	1.110586e+002
Total O	=	5.557178e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	5.903e-003	5.129e-003	-2.229	-2.290	-0.061
OH-	2.252e-012	1.878e-012	-11.648	-11.726	-0.079
H2O	5.553e+001	9.995e-001	1.744	-0.000	0.000
Al	1.284e-003				
AlSO4+	5.907e-004	4.949e-004	-3.229	-3.305	-0.077
Al+3	5.446e-004	1.494e-004	-3.264	-3.826	-0.562
Al(SO4)2-	1.484e-004	1.244e-004	-3.828	-3.905	-0.077
AlOH+2	6.571e-007	3.262e-007	-6.182	-6.487	-0.304
Al2(OH)2+4	2.524e-010	1.730e-011	-9.598	-10.762	-1.164
Al(OH)2+	1.762e-010	1.476e-010	-9.754	-9.831	-0.077
HALO2	4.189e-014	4.189e-014	-13.378	-13.378	0.000
Al3(OH)4+5	3.800e-015	6.338e-017	-14.420	-16.198	-1.778
AlO2-	3.339e-018	2.798e-018	-17.476	-17.553	-0.077
NaAlO2	1.245e-021	1.245e-021	-20.905	-20.905	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-71.703	-75.189	-3.486
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-107.015	-107.015	0.000
As(3)	8.809e-017				
HAsO2	4.701e-017	4.701e-017	-16.328	-16.328	0.000
As(OH)3	4.108e-017	4.108e-017	-16.386	-16.386	0.000
H2AsO3-	5.847e-024	4.899e-024	-23.233	-23.310	-0.077
AsO2-	5.592e-024	4.686e-024	-23.252	-23.329	-0.077
AsO2OH-2	1.914e-032	9.333e-033	-31.718	-32.030	-0.312
As(5)	1.337e-007				
H2AsO4-	7.609e-008	6.375e-008	-7.119	-7.195	-0.077
H3AsO4	5.759e-008	5.759e-008	-7.240	-7.240	0.000
HAsO4-2	4.231e-012	2.064e-012	-11.374	-11.685	-0.312
AsO4-3	5.216e-021	1.032e-021	-20.283	-20.986	-0.704
Ca	7.623e-003				
Ca+2	6.115e-003	3.186e-003	-2.214	-2.497	-0.283
CaSO4	1.507e-003	1.507e-003	-2.822	-2.822	0.000
CaCl+	7.369e-007	6.174e-007	-6.133	-6.209	-0.077
CaCl2	6.641e-010	6.641e-010	-9.178	-9.178	0.000
CaOH+	1.047e-013	8.770e-014	-12.980	-13.057	-0.077

Cl(-1)	1.105e-003					
Cl-	1.102e-003	9.144e-004	-2.958	-3.039	-0.081	
HCl	1.053e-006	1.053e-006	-5.977	-5.977	0.000	
CaCl+	7.369e-007	6.174e-007	-6.133	-6.209	-0.077	
MgCl+	3.884e-007	3.254e-007	-6.411	-6.488	-0.077	
NaCl	3.748e-007	3.748e-007	-6.426	-6.426	0.000	
MnCl+	2.176e-007	1.823e-007	-6.662	-6.739	-0.077	
FeCl+	5.641e-008	4.726e-008	-7.249	-7.325	-0.077	
KCl	5.516e-009	5.516e-009	-8.258	-8.258	0.000	
CuCl+	2.296e-009	1.924e-009	-8.639	-8.716	-0.077	
FeCl+2	2.088e-009	1.036e-009	-8.680	-8.984	-0.304	
FeCl2+	9.157e-010	7.673e-010	-9.038	-9.115	-0.077	
CaCl2	6.641e-010	6.641e-010	-9.178	-9.178	0.000	
ZnCl+	2.159e-010	1.809e-010	-9.666	-9.743	-0.077	
CuCl2	9.263e-013	9.263e-013	-12.033	-12.033	0.000	
FeCl2	2.319e-013	2.319e-013	-12.635	-12.635	0.000	
ZnCl2	1.932e-013	1.932e-013	-12.714	-12.714	0.000	
MnCl3-	3.974e-014	3.329e-014	-13.401	-13.478	-0.077	
Zn(OH)Cl	6.029e-016	6.029e-016	-15.220	-15.220	0.000	
ZnCl3-	1.165e-016	9.758e-017	-15.934	-16.011	-0.077	
CuCl2-	2.784e-017	2.332e-017	-16.555	-16.632	-0.077	
ZnCl4-2	1.387e-018	6.763e-019	-17.858	-18.170	-0.312	
FeCl4-2	1.149e-018	5.603e-019	-17.940	-18.252	-0.312	
FeCl4-	9.205e-019	7.713e-019	-18.036	-18.113	-0.077	
CuCl3-2	2.809e-019	1.370e-019	-18.552	-18.863	-0.312	
CuCl4-2	2.980e-023	1.454e-023	-22.526	-22.838	-0.312	
Cl(1)	5.148e-028					
HClO	5.148e-028	5.148e-028	-27.288	-27.288	0.000	
ClO-	3.230e-033	2.707e-033	-32.491	-32.568	-0.077	
Cl(3)	0.000e+000					
HClO2	0.000e+000	0.000e+000	-54.111	-54.111	0.000	
ClO2-	0.000e+000	0.000e+000	-54.914	-54.991	-0.077	
Cl(5)	0.000e+000					
ClO3-	0.000e+000	0.000e+000	-63.483	-63.562	-0.079	
Cl(7)	0.000e+000					
ClO4-	0.000e+000	0.000e+000	-76.356	-76.435	-0.079	
ZnClO4+	0.000e+000	0.000e+000	-82.010	-82.087	-0.077	
Cu(1)	5.307e-016					
Cu+	5.025e-016	4.211e-016	-15.299	-15.376	-0.077	
CuCl2-	2.784e-017	2.332e-017	-16.555	-16.632	-0.077	
CuCl3-2	2.809e-019	1.370e-019	-18.552	-18.863	-0.312	
Cu(2)	2.049e-006					
Cu+2	1.476e-006	7.692e-007	-5.831	-6.114	-0.283	
CuSO4	5.704e-007	5.704e-007	-6.244	-6.244	0.000	
CuCl+	2.296e-009	1.924e-009	-8.639	-8.716	-0.077	
CuOH+	9.229e-012	7.732e-012	-11.035	-11.112	-0.077	
CuCl2	9.263e-013	9.263e-013	-12.033	-12.033	0.000	
CuCl4-2	2.980e-023	1.454e-023	-22.526	-22.838	-0.312	
CuO2-2	8.086e-037	3.944e-037	-36.092	-36.404	-0.312	
Fe(2)	1.726e-004					
Fe+2	1.362e-004	7.095e-005	-3.866	-4.149	-0.283	
FeSO4	3.640e-005	3.640e-005	-4.439	-4.439	0.000	
FeCl+	5.641e-008	4.726e-008	-7.249	-7.325	-0.077	
FeOH+	5.219e-012	4.373e-012	-11.282	-11.359	-0.077	
FeCl2	2.319e-013	2.319e-013	-12.635	-12.635	0.000	
FeCl4-2	1.149e-018	5.603e-019	-17.940	-18.252	-0.312	
Fe(OH)2	6.769e-021	6.769e-021	-20.169	-20.169	0.000	
Fe(OH)3-	6.268e-029	5.252e-029	-28.203	-28.280	-0.077	
Fe(OH)4-2	0.000e+000	0.000e+000	-40.678	-40.990	-0.312	
Fe(3)	4.544e-005					
Fe+3	2.480e-005	6.803e-006	-4.606	-5.167	-0.562	
FeOH+2	1.724e-005	8.560e-006	-4.763	-5.068	-0.304	
FeSO4+	2.543e-006	2.131e-006	-5.595	-5.671	-0.077	
Fe(OH)2+	6.593e-007	5.524e-007	-6.181	-6.258	-0.077	
Fe(SO4)2-	1.392e-007	1.166e-007	-6.856	-6.933	-0.077	
Fe2(OH)2+4	2.876e-008	1.972e-009	-7.541	-8.705	-1.164	
FeCl+2	2.088e-009	1.036e-009	-8.680	-8.984	-0.304	

	FeCl ₂ +	9.157e-010	7.673e-010	-9.038	-9.115	-0.077
	Fe(OH) ₃	5.035e-011	5.035e-011	-10.298	-10.298	0.000
	Fe ₃ (OH) ₄₊₅	1.365e-011	2.276e-013	-10.865	-12.643	-1.778
	Fe(OH) ₄₋	2.942e-018	2.465e-018	-17.531	-17.608	-0.077
	FeCl ₄₋	9.205e-019	7.713e-019	-18.036	-18.113	-0.077
H(0)		4.137e-032				
	H ₂	2.069e-032	2.087e-032	-31.684	-31.680	0.004
K		2.221e-004				
	K+	2.165e-004	1.797e-004	-3.665	-3.746	-0.081
	KSO ₄₋	5.603e-006	4.694e-006	-5.252	-5.328	-0.077
	KHSO ₄	2.124e-008	2.124e-008	-7.673	-7.673	0.000
	KCl	5.516e-009	5.516e-009	-8.258	-8.258	0.000
	KOH	1.214e-016	1.214e-016	-15.916	-15.916	0.000
Mg		1.223e-003				
	Mg+2	8.282e-004	4.559e-004	-3.082	-3.341	-0.259
	MgSO ₄	3.941e-004	3.941e-004	-3.404	-3.404	0.000
	MgCl+	3.884e-007	3.254e-007	-6.411	-6.488	-0.077
	Mg ₄ (OH) ₄₊₄	0.000e+000	0.000e+000	-42.792	-43.955	-1.164
Mn(2)		2.547e-004				
	Mn+2	1.797e-004	9.362e-005	-3.745	-4.029	-0.283
	MnSO ₄	7.478e-005	7.478e-005	-4.126	-4.126	0.000
	MnCl+	2.176e-007	1.823e-007	-6.662	-6.739	-0.077
	MnOH+	5.598e-013	4.690e-013	-12.252	-12.329	-0.077
	MnCl ₃₋	3.974e-014	3.329e-014	-13.401	-13.478	-0.077
	Mn ₂ OH+3	2.199e-016	4.705e-017	-15.658	-16.327	-0.670
	Mn(OH) ₂	2.244e-022	2.244e-022	-21.649	-21.649	0.000
	Mn ₂ (OH) ₃₊	9.749e-026	8.168e-026	-25.011	-25.088	-0.077
	Mn(OH) ₃₋	4.895e-032	4.101e-032	-31.310	-31.387	-0.077
	Mn(OH) ₄₋₂	0.000e+000	0.000e+000	-42.858	-43.169	-0.312
Mn(3)		1.167e-017				
	Mn+3	1.167e-017	2.497e-018	-16.933	-17.603	-0.670
Mn(6)		0.000e+000				
	MnO ₄₋₂	0.000e+000	0.000e+000	-55.845	-56.156	-0.312
Mn(7)		0.000e+000				
	MnO ₄₋	0.000e+000	0.000e+000	-53.434	-53.513	-0.079
Na		2.843e-003				
	Na+	2.783e-003	2.332e-003	-2.555	-2.632	-0.077
	NaSO ₄₋	5.953e-005	4.988e-005	-4.225	-4.302	-0.077
	NaCl	3.748e-007	3.748e-007	-6.426	-6.426	0.000
	NaOH	7.555e-016	7.555e-016	-15.122	-15.122	0.000
	NaAlO ₂	1.245e-021	1.245e-021	-20.905	-20.905	0.000
O(0)		2.895e-029				
	O ₂	1.448e-029	1.460e-029	-28.839	-28.836	0.004
S(6)		1.161e-002				
	SO ₄₋₂	6.638e-003	3.237e-003	-2.178	-2.490	-0.312
	HSO ₄₋	2.002e-003	1.677e-003	-2.699	-2.775	-0.077
	CaSO ₄	1.507e-003	1.507e-003	-2.822	-2.822	0.000
	AlSO ₄₊	5.907e-004	4.949e-004	-3.229	-3.305	-0.077
	MgSO ₄	3.941e-004	3.941e-004	-3.404	-3.404	0.000
	Al(SO ₄) ₂₋	1.484e-004	1.244e-004	-3.828	-3.905	-0.077
	MnSO ₄	7.478e-005	7.478e-005	-4.126	-4.126	0.000
	NaSO ₄₋	5.953e-005	4.988e-005	-4.225	-4.302	-0.077
	FeSO ₄	3.640e-005	3.640e-005	-4.439	-4.439	0.000
	KSO ₄₋	5.603e-006	4.694e-006	-5.252	-5.328	-0.077
	FeSO ₄₊	2.543e-006	2.131e-006	-5.595	-5.671	-0.077
	CuSO ₄	5.704e-007	5.704e-007	-6.244	-6.244	0.000
	Fe(SO ₄) ₂₋	1.392e-007	1.166e-007	-6.856	-6.933	-0.077
	ZnSO ₄	8.010e-008	8.010e-008	-7.096	-7.096	0.000
	KHSO ₄	2.124e-008	2.124e-008	-7.673	-7.673	0.000
	H ₂ SO ₄	8.115e-009	8.115e-009	-8.091	-8.091	0.000
Zn		3.064e-007				
	Zn+2	2.260e-007	1.178e-007	-6.646	-6.929	-0.283
	ZnSO ₄	8.010e-008	8.010e-008	-7.096	-7.096	0.000
	ZnCl+	2.159e-010	1.809e-010	-9.666	-9.743	-0.077
	ZnCl ₂	1.932e-013	1.932e-013	-12.714	-12.714	0.000
	ZnOH+	3.004e-014	2.517e-014	-13.522	-13.599	-0.077
	Zn(OH)Cl	6.029e-016	6.029e-016	-15.220	-15.220	0.000

ZnCl3-	1.165e-016	9.758e-017	-15.934	-16.011	-0.077
ZnCl4-2	1.387e-018	6.763e-019	-17.858	-18.170	-0.312
Zn(OH)2	2.101e-020	2.101e-020	-19.678	-19.678	0.000
Zn(OH)3-	1.515e-029	1.269e-029	-28.820	-28.897	-0.077
Zn(OH)4-2	8.646e-040	4.216e-040	-39.063	-39.375	-0.312
ZnClO4+	0.000e+000	0.000e+000	-82.010	-82.087	-0.077

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

Phase	SI	log IAP	log KT	
Al	-125.24	24.67	149.91	Al
Al(g)	-175.95	24.67	200.62	Al
Al2(SO4)3	-34.02	-15.12	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-16.68	-15.12	1.56	Al2(SO4)3:6H2O
Alum-K	-7.58	-12.55	-4.97	KAl(SO4)2:12H2O
Alunite	-5.99	-6.46	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.64	-4.99	-4.35	CaSO4
Antarcticite	-12.67	-8.58	4.09	CaCl2:6H2O
Antlerite	-20.40	-11.67	8.73	Cu3(SO4)(OH)4
Aphthitalite	-14.96	-18.85	-3.89	NaK3(SO4)2
Arcanite	-8.14	-9.98	-1.84	K2SO4
Arsenolite	-31.36	-51.20	-19.84	As2O3
As	-46.66	-3.97	42.68	As
As2O5	-21.11	-18.97	2.14	As2O5
As4O6(cubi)	-62.57	-102.40	-39.82	As4O6
As4O6(mono)	-62.35	-102.40	-40.05	As4O6
Atacamite	-31.06	-16.79	14.26	Cu4Cl2(OH)6
Bassanite	-1.28	-4.99	-3.71	CaSO4:0.5H2O
Birnessite	-93.91	-179.45	-85.55	Mn8O14:5H2O
Bischofite	-13.81	-9.42	4.39	MgCl2:6H2O
Bixbyite	-20.50	-21.47	-0.96	Mn2O3
Bloedite	-11.11	-13.59	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-4.51	3.04	7.55	AlO2H
Brochantite	-28.63	-13.21	15.42	Cu4(SO4)(OH)6
Brucite	-15.04	1.24	16.28	Mg(OH)2
Ca	-123.33	16.50	139.83	Ca
Ca(g)	-148.57	16.50	165.07	Ca
Ca2Al2O5:8H2O	-49.32	10.25	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-32.78	-6.49	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-30.52	-12.72	17.80	Ca3(AsO4)2
Ca3Al2O6	-100.69	12.34	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-122.66	17.82	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-92.84	14.42	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-89.27	14.42	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-70.66	-2.33	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-38.74	8.17	46.91	CaAl2O4
CaAl2O4:10H2O	-29.83	8.17	37.99	CaAl2O4:10H2O
CaAl4O7	-54.33	14.26	68.59	CaAl4O7
Carnallite	-20.48	-16.20	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.45	-4.99	-3.54	CaSO4:0.5H2O
Chalcanthite	-5.98	-8.60	-2.63	CuSO4:5H2O
Chalcocyanite	-11.52	-8.60	2.91	CuSO4
Chloromagnesite	-31.23	-9.42	21.82	MgCl2
Cl2(g)	-28.07	-25.08	2.99	Cl2
Claudetite	-31.40	-51.20	-19.80	As2O3
Corundum	-12.20	6.09	18.29	Al2O3
Cu	-18.61	12.88	31.50	Cu
Cu(g)	-70.77	12.88	83.66	Cu
CuCl2	-15.91	-12.19	3.72	CuCl2
Cuprite	-24.26	-26.17	-1.91	Cu2O
Delafossite	-4.95	-11.38	-6.44	CuFeO2
Diaspore	-4.10	3.04	7.15	AlHO2
Epsomite	-3.87	-5.83	-1.96	MgSO4:7H2O
Ettringite	-65.09	-2.63	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-44.17	14.85	59.02	Fe
Fe(OH)2	-13.46	0.43	13.89	Fe(OH)2

Fe(OH)3	-3.94	1.70	5.64	Fe(OH)3
Fe2(SO4)3	-20.85	-17.80	3.05	Fe2(SO4)3
FeO	-13.09	0.43	13.52	FeO
Ferrite-Ca	-16.01	5.49	21.50	CaFe2O4
Ferrite-Cu	-8.41	1.87	10.28	CuFe2O4
Ferrite-Dicalcium	-49.23	7.57	56.80	Ca2Fe2O5
Ferrite-Mg	-16.38	4.64	21.02	MgFe2O4
Ferrite-Zn	-10.64	1.06	11.70	ZnFe2O4
FeSO4	-9.25	-6.64	2.61	FeSO4
Gibbsite	-4.70	3.04	7.74	Al(OH)3
Glauberite	-7.27	-12.74	-5.47	Na2Ca(SO4)2
Goethite	1.17	1.70	0.53	FeOOH
Gypsum	-0.46	-4.99	-4.53	CaSO4:2H2O
H2(g)	-28.58	-31.68	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.23	-5.67	1.56	NaCl
Hausmannite	-31.06	-20.91	10.14	Mn3O4
HCl(g)	-11.63	-5.33	6.30	HCl
Hematite	3.33	3.40	0.08	Fe2O3
Hercynite	-22.28	6.52	28.80	FeAl2O4
Hexahydrite	-4.11	-5.83	-1.73	MgSO4:6H2O
Hydrophilite	-20.32	-8.57	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	-1.08	-10.49	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	-3.93	-9.38	-5.45	NaFe3(SO4)2(OH)6
K	-65.22	5.75	70.98	K
K(g)	-75.83	5.75	81.58	K
K2O	-86.95	-2.91	84.04	K2O
K3H(SO4)2	-14.88	-18.51	-3.62	K3H(SO4)2
Kainite	-12.30	-12.62	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-15.82	-12.55	3.27	KAl(SO4)2
Katoite	-66.61	12.34	78.94	Ca3Al2H12O12
Kieserite	-5.56	-5.83	-0.27	MgSO4:H2O
KMgCl3	-37.45	-16.20	21.25	KMgCl3
KMgCl3:2H2O	-30.17	-16.20	13.96	KMgCl3:2H2O
Lammerite	-25.13	-23.57	1.55	Cu3(AsO4)2
Lawrencite	-19.28	-10.23	9.05	FeCl2
Leonite	-11.70	-15.81	-4.11	K2Mg(SO4)2:4H2O
Lime	-30.49	2.08	32.57	CaO
Magnetite	-6.58	3.84	10.42	Fe3O4
Manganite	-10.57	-10.73	-0.16	MnO(OH)
Manganosite	-17.36	0.55	17.92	MnO
Mayenite	-426.54	67.61	494.15	Ca12Al14O33
Melanterite	-4.24	-6.64	-2.40	FeSO4:7H2O
Mercallite	-7.09	-8.53	-1.44	KHSO4
Mg	-106.86	15.66	122.52	Mg
Mg(g)	-126.59	15.66	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.72	-5.52	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-14.42	-5.21	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.15	-9.42	12.73	MgCl2:2H2O
MgCl2:4H2O	-16.72	-9.42	7.30	MgCl2:4H2O
MgCl2:H2O	-25.49	-9.42	16.07	MgCl2:H2O
MgOHCl	-19.98	-4.09	15.89	MgOHCl
MgSO4	-10.66	-5.83	4.83	MgSO4
Mirabilite	-6.60	-7.76	-1.15	Na2SO4:10H2O
Misenite	-50.06	-61.13	-11.08	K8H6(SO4)7
Mn	-67.96	14.97	82.93	Mn
Mn(OH)2(am)	-14.76	0.55	15.31	Mn(OH)2
Mn(OH)3	-17.07	-10.73	6.34	Mn(OH)3
MnCl2:2H2O	-14.10	-10.11	4.00	MnCl2:2H2O
MnCl2:4H2O	-12.86	-10.11	2.75	MnCl2:4H2O
MnCl2:H2O	-15.65	-10.11	5.54	MnCl2:H2O
MnO2(gamma)	-13.97	-30.09	-16.13	MnO2
MnSO4	-9.13	-6.52	2.61	MnSO4
Molysite	-27.75	-14.28	13.47	FeCl3
Na	-60.50	6.87	67.37	Na
Na(g)	-73.99	6.87	80.86	Na

Na2O	-68.10	-0.68	67.42	Na2O
Na3H(SO4)2	-14.28	-15.17	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-14.60	-20.50	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-18.52	1.36	19.88	NaFeO2
Nantokite	-11.65	-18.41	-6.77	CuCl
O2(g)	-25.94	-28.84	-2.89	O2
Oxychloride-Mg	-28.68	-2.85	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.44	-5.83	-1.39	MgSO4:5H2O
Periclase	-20.09	1.24	21.33	MgO
Picromerite	-11.37	-15.81	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-11.47	-25.79	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-20.46	2.08	22.55	Ca(OH)2
Pyrolusite	-12.43	-30.09	-17.66	MnO2
Scacchite	-18.85	-10.11	8.74	MnCl2
Spinel	-30.28	7.33	37.61	Al2MgO4
Starkeyite	-4.83	-5.83	-1.00	MgSO4:4H2O
Sylvite	-7.61	-6.78	0.83	KCl
Syngenite	-7.37	-14.97	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-44.56	-27.41	17.14	Mg2CaCl6:12H2O
Tenorite	-9.18	-1.53	7.65	CuO
Thenardite	-7.40	-7.75	-0.36	Na2SO4
Todorokite	-79.31	-125.13	-45.82	Mn7O12:3H2O
Wustite	-11.86	0.54	12.40	Fe.9470
Zincite	-13.55	-2.35	11.20	ZnO
Zn	-56.72	12.07	68.79	Zn
Zn(ClO4)2:6H2O	-165.43	-159.80	5.63	Zn(ClO4)2:6H2O
Zn(g)	-73.34	12.07	85.41	Zn
Zn(OH)2(beta)	-14.28	-2.35	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-14.01	-2.35	11.66	Zn(OH)2
Zn(OH)2(gamma)	-14.23	-2.35	11.88	Zn(OH)2
Zn2(OH)3Cl	-25.32	-10.03	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-19.35	-11.77	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-35.33	-26.02	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-40.28	-21.19	19.09	Zn3O(SO4)2
ZnCl2	-20.09	-13.01	7.08	ZnCl2
ZnSO4	-12.95	-9.42	3.53	ZnSO4
ZnSO4:6H2O	-7.72	-9.42	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-7.54	-9.42	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-8.87	-9.42	-0.55	ZnSO4:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using mix 1.

Mixture 1.

1.000e+000 Solution 1 Flujo 2
3.000e+000 Solution 2 Inter 3

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

Elements	Molality	Moles
Al	1.041e-003	4.165e-003
As	1.102e-006	4.410e-006
Ca	5.935e-003	2.374e-002
Cl	1.148e-003	4.593e-003
Cu	1.931e-006	7.723e-006
Fe	3.581e-004	1.432e-003
K	2.677e-004	1.071e-003
Mg	1.035e-003	4.142e-003
Mn	2.184e-004	8.734e-004
Na	2.287e-003	9.148e-003

S	1.117e-002	4.470e-002
Zn	5.971e-006	2.388e-005

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

pH	=	2.379	Charge balance
pe	=	12.797	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	3.299e-002	
Mass of water (kg)	=	4.000e+000	
Total alkalinity (eq/kg)	=	-6.875e-003	
Total carbon (mol/kg)	=	0.000e+000	
Total CO2 (mol/kg)	=	0.000e+000	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	1.575e-002	
Percent error, 100*(Cat- An)/(Cat+ An)	=	10.46	
Iterations	=	6	
Total H	=	4.442296e+002	
Total O	=	2.222808e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	4.791e-003	4.182e-003	-2.320	-2.379	-0.059
OH-	2.740e-012	2.303e-012	-11.562	-11.638	-0.075
H2O	5.553e+001	9.996e-001	1.744	-0.000	0.000
Al	1.041e-003				
AlSO4+	4.958e-004	4.185e-004	-3.305	-3.378	-0.074
Al+3	4.116e-004	1.181e-004	-3.386	-3.928	-0.542
Al(SO4)2-	1.333e-004	1.125e-004	-3.875	-3.949	-0.074
AlOH+2	6.184e-007	3.161e-007	-6.209	-6.500	-0.291
Al2(OH)2+4	2.129e-010	1.625e-011	-9.672	-10.789	-1.117
Al(OH)2+	2.078e-010	1.754e-010	-9.682	-9.756	-0.074
HA1O2	6.105e-014	6.105e-014	-13.214	-13.214	0.000
Al3(OH)4+5	3.612e-015	7.073e-017	-14.442	-16.150	-1.708
AlO2-	5.924e-018	5.000e-018	-17.227	-17.301	-0.074
NaAlO2	1.800e-021	1.800e-021	-20.745	-20.745	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-70.334	-73.683	-3.349
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-113.235	-113.235	0.000
As(3)	1.094e-017				
HAsO2	5.838e-018	5.838e-018	-17.234	-17.234	0.000
As(OH)3	5.102e-018	5.102e-018	-17.292	-17.292	0.000
H2AsO3-	8.839e-025	7.461e-025	-24.054	-24.127	-0.074
AsO2-	8.453e-025	7.135e-025	-24.073	-24.147	-0.074
AsO2OH-2	3.466e-033	1.743e-033	-32.460	-32.759	-0.299
HAsS2	0.000e+000	0.000e+000	-185.856	-185.856	0.000
As(5)	1.102e-006				
H2AsO4-	6.797e-007	5.738e-007	-6.168	-6.241	-0.074
H3AsO4	4.227e-007	4.227e-007	-6.374	-6.374	0.000
HAsO4-2	4.529e-011	2.277e-011	-10.344	-10.643	-0.299
AsO4-3	6.585e-020	1.397e-020	-19.181	-19.855	-0.673
Ca	5.935e-003				
Ca+2	4.671e-003	2.496e-003	-2.331	-2.603	-0.272
CaSO4	1.263e-003	1.263e-003	-2.899	-2.899	0.000
CaCl+	6.010e-007	5.072e-007	-6.221	-6.295	-0.074
CaCl2	5.720e-010	5.720e-010	-9.243	-9.243	0.000
CaOH+	9.984e-014	8.427e-014	-13.001	-13.074	-0.074
Cl(-1)	1.148e-003				
Cl-	1.146e-003	9.588e-004	-2.941	-3.018	-0.077
HCl	9.006e-007	9.006e-007	-6.045	-6.045	0.000
CaCl+	6.010e-007	5.072e-007	-6.221	-6.295	-0.074
MgCl+	3.395e-007	2.866e-007	-6.469	-6.543	-0.074
NaCl	3.180e-007	3.180e-007	-6.498	-6.498	0.000
MnCl+	1.936e-007	1.634e-007	-6.713	-6.787	-0.074

FeCl+	4.420e-008	3.731e-008	-7.355	-7.428	-0.074
FeCl+2	1.003e-008	5.129e-009	-7.999	-8.290	-0.291
KCl	7.017e-009	7.017e-009	-8.154	-8.154	0.000
FeCl2+	4.716e-009	3.981e-009	-8.326	-8.400	-0.074
ZnCl+	4.381e-009	3.698e-009	-8.358	-8.432	-0.074
CuCl+	2.248e-009	1.898e-009	-8.648	-8.722	-0.074
CaCl2	5.720e-010	5.720e-010	-9.243	-9.243	0.000
ZnCl2	4.141e-012	4.141e-012	-11.383	-11.383	0.000
CuCl2	9.582e-013	9.582e-013	-12.019	-12.019	0.000
FeCl2	1.920e-013	1.920e-013	-12.717	-12.717	0.000
MnCl3-	3.887e-014	3.281e-014	-13.410	-13.484	-0.074
Zn(OH)Cl	1.511e-014	1.511e-014	-13.821	-13.821	0.000
ZnCl3-	2.598e-015	2.193e-015	-14.585	-14.659	-0.074
ZnCl4-2	3.169e-017	1.594e-017	-16.499	-16.798	-0.299
FeCl4-	5.212e-018	4.400e-018	-17.283	-17.357	-0.074
CuCl2-	4.560e-018	3.849e-018	-17.341	-17.415	-0.074
FeCl4-2	1.014e-018	5.099e-019	-17.994	-18.293	-0.299
CuCl3-2	4.713e-020	2.370e-020	-19.327	-19.625	-0.299
CuCl4-2	3.287e-023	1.653e-023	-22.483	-22.782	-0.299
Cl(1)	2.601e-026				
HClO	2.601e-026	2.601e-026	-25.585	-25.585	0.000
ClO-	1.987e-031	1.677e-031	-30.702	-30.775	-0.074
Cl(3)	0.000e+000				
HClO2	0.000e+000	0.000e+000	-50.636	-50.636	0.000
ClO2-	0.000e+000	0.000e+000	-51.354	-51.427	-0.074
Cl(5)	0.000e+000				
ClO3-	0.000e+000	0.000e+000	-58.151	-58.227	-0.075
Cl(7)	0.000e+000				
ClO4-	0.000e+000	0.000e+000	-69.253	-69.328	-0.075
ZnClO4+	0.000e+000	0.000e+000	-73.617	-73.690	-0.074
Cu(1)	7.947e-017				
Cu+	7.487e-017	6.319e-017	-16.126	-16.199	-0.074
CuCl2-	4.560e-018	3.849e-018	-17.341	-17.415	-0.074
CuCl3-2	4.713e-020	2.370e-020	-19.327	-19.625	-0.299
Cu(2)	1.931e-006				
Cu+2	1.354e-006	7.236e-007	-5.868	-6.140	-0.272
CuSO4	5.742e-007	5.742e-007	-6.241	-6.241	0.000
CuCl+	2.248e-009	1.898e-009	-8.648	-8.722	-0.074
CuOH+	1.057e-011	8.921e-012	-10.976	-11.050	-0.074
CuCl2	9.582e-013	9.582e-013	-12.019	-12.019	0.000
CuCl4-2	3.287e-023	1.653e-023	-22.483	-22.782	-0.299
CuO2-2	1.669e-036	8.391e-037	-35.778	-36.076	-0.299
Fe(2)	1.293e-004				
Fe+2	9.996e-005	5.342e-005	-4.000	-4.272	-0.272
FeSO4	2.933e-005	2.933e-005	-4.533	-4.533	0.000
FeCl+	4.420e-008	3.731e-008	-7.355	-7.428	-0.074
FeOH+	4.783e-012	4.037e-012	-11.320	-11.394	-0.074
FeCl2	1.920e-013	1.920e-013	-12.717	-12.717	0.000
FeCl4-2	1.014e-018	5.099e-019	-17.994	-18.293	-0.299
Fe(OH)2	7.665e-021	7.665e-021	-20.116	-20.116	0.000
Fe(OH)3-	8.640e-029	7.293e-029	-28.063	-28.137	-0.074
Fe(OH)4-2	0.000e+000	0.000e+000	-40.460	-40.759	-0.299
Fe(3)	2.287e-004				
Fe+3	1.119e-004	3.210e-005	-3.951	-4.493	-0.542
FeOH+2	9.693e-005	4.954e-005	-4.014	-4.305	-0.291
FeSO4+	1.275e-005	1.076e-005	-4.895	-4.968	-0.074
Fe(OH)2+	4.645e-006	3.921e-006	-5.333	-5.407	-0.074
Fe2(OH)2+4	8.655e-007	6.606e-008	-6.063	-7.180	-1.117
Fe(SO4)2-	7.465e-007	6.301e-007	-6.127	-6.201	-0.074
FeCl+2	1.003e-008	5.129e-009	-7.999	-8.290	-0.291
FeCl2+	4.716e-009	3.981e-009	-8.326	-8.400	-0.074
Fe3(OH)4+5	2.763e-009	5.411e-011	-8.559	-10.267	-1.708
Fe(OH)3	4.383e-010	4.383e-010	-9.358	-9.358	0.000
Fe(OH)4-	3.118e-017	2.631e-017	-16.506	-16.580	-0.074
FeCl4-	5.212e-018	4.400e-018	-17.283	-17.357	-0.074
H(0)	7.008e-034				
H2	3.504e-034	3.532e-034	-33.455	-33.452	0.003

K	2.677e-004					
K+	2.605e-004	2.179e-004	-3.584	-3.662	-0.077	
KSO4-	7.219e-006	6.094e-006	-5.141	-5.215	-0.074	
KHSO4	2.249e-008	2.249e-008	-7.648	-7.648	0.000	
KCl	7.017e-009	7.017e-009	-8.154	-8.154	0.000	
KOH	1.806e-016	1.806e-016	-15.743	-15.743	0.000	
Mg	1.035e-003					
Mg+2	6.810e-004	3.829e-004	-3.167	-3.417	-0.250	
MgSO4	3.542e-004	3.542e-004	-3.451	-3.451	0.000	
MgCl+	3.395e-007	2.866e-007	-6.469	-6.543	-0.074	
Mg4(OH)4+4	0.000e+000	0.000e+000	-42.787	-43.904	-1.117	
Mn(2)	2.184e-004					
Mn+2	1.498e-004	8.003e-005	-3.825	-4.097	-0.272	
MnSO4	6.840e-005	6.840e-005	-4.165	-4.165	0.000	
MnCl+	1.936e-007	1.634e-007	-6.713	-6.787	-0.074	
MnOH+	5.825e-013	4.917e-013	-12.235	-12.308	-0.074	
MnCl3-	3.887e-014	3.281e-014	-13.410	-13.484	-0.074	
Mn2OH+3	1.850e-016	4.216e-017	-15.733	-16.375	-0.642	
Mn(OH)2	2.884e-022	2.884e-022	-21.540	-21.540	0.000	
Mn2(OH)3+	1.304e-025	1.101e-025	-24.885	-24.958	-0.074	
Mn(OH)3-	7.661e-032	6.467e-032	-31.116	-31.189	-0.074	
Mn(OH)4-2	0.000e+000	0.000e+000	-42.585	-42.883	-0.299	
Mn(3)	5.873e-017					
Mn+3	5.873e-017	1.338e-017	-16.231	-16.874	-0.642	
Mn(6)	0.000e+000					
MnO4-2	0.000e+000	0.000e+000	-52.028	-52.327	-0.299	
Mn(7)	0.000e+000					
MnO4-	0.000e+000	0.000e+000	-48.811	-48.886	-0.075	
Na	2.287e-003					
Na+	2.236e-003	1.887e-003	-2.651	-2.724	-0.074	
NaSO4-	5.116e-005	4.319e-005	-4.291	-4.365	-0.074	
NaCl	3.180e-007	3.180e-007	-6.498	-6.498	0.000	
NaOH	7.497e-016	7.497e-016	-15.125	-15.125	0.000	
NaAlO2	1.800e-021	1.800e-021	-20.745	-20.745	0.000	
O(0)	1.012e-025					
O2	5.060e-026	5.100e-026	-25.296	-25.292	0.003	
S(-2)	0.000e+000					
H2S	0.000e+000	0.000e+000	-87.906	-87.906	0.000	
HS-	0.000e+000	0.000e+000	-92.461	-92.537	-0.075	
S-2	0.000e+000	0.000e+000	-102.799	-103.084	-0.285	
S2-2	0.000e+000	0.000e+000	-164.164	-164.462	-0.299	
HAsS2	0.000e+000	0.000e+000	-185.856	-185.856	0.000	
S3-2	0.000e+000	0.000e+000	-225.583	-225.881	-0.299	
S4-2	0.000e+000	0.000e+000	-287.229	-287.527	-0.299	
S5-2	0.000e+000	0.000e+000	-349.092	-349.390	-0.299	
S(2)	0.000e+000					
S2O3-2	0.000e+000	0.000e+000	-92.268	-92.567	-0.299	
HS2O3-	0.000e+000	0.000e+000	-93.858	-93.931	-0.074	
S(3)	0.000e+000					
S2O4-2	0.000e+000	0.000e+000	-89.856	-90.141	-0.285	
S(4)	5.019e-032					
HSO3-	3.123e-032	2.636e-032	-31.505	-31.579	-0.074	
H2SO3	1.057e-032	1.057e-032	-31.976	-31.976	0.000	
SO2	8.392e-033	8.392e-033	-32.076	-32.076	0.000	
SO3-2	7.235e-037	3.698e-037	-36.141	-36.432	-0.291	
S2O6-2	0.000e+000	0.000e+000	-48.102	-48.400	-0.299	
S3O6-2	0.000e+000	0.000e+000	-112.004	-112.302	-0.299	
S4O6-2	0.000e+000	0.000e+000	-160.000	-160.299	-0.299	
S5O6-2	0.000e+000	0.000e+000	-236.876	-237.174	-0.299	
S(5)	0.000e+000					
S2O5-2	0.000e+000	0.000e+000	-67.690	-67.988	-0.299	
S(6)	1.117e-002					
SO4-2	6.888e-003	3.464e-003	-2.162	-2.460	-0.299	
HSO4-	1.734e-003	1.463e-003	-2.761	-2.835	-0.074	
CaSO4	1.263e-003	1.263e-003	-2.899	-2.899	0.000	
AlSO4+	4.958e-004	4.185e-004	-3.305	-3.378	-0.074	
MgSO4	3.542e-004	3.542e-004	-3.451	-3.451	0.000	

Al(SO4)2-	1.333e-004	1.125e-004	-3.875	-3.949	-0.074
MnSO4	6.840e-005	6.840e-005	-4.165	-4.165	0.000
NaSO4-	5.116e-005	4.319e-005	-4.291	-4.365	-0.074
FeSO4	2.933e-005	2.933e-005	-4.533	-4.533	0.000
FeSO4+	1.275e-005	1.076e-005	-4.895	-4.968	-0.074
KSO4-	7.219e-006	6.094e-006	-5.141	-5.215	-0.074
ZnSO4	1.671e-006	1.671e-006	-5.777	-5.777	0.000
Fe(SO4)2-	7.465e-007	6.301e-007	-6.127	-6.201	-0.074
CuSO4	5.742e-007	5.742e-007	-6.241	-6.241	0.000
KHSO4	2.249e-008	2.249e-008	-7.648	-7.648	0.000
H2SO4	5.774e-009	5.774e-009	-8.239	-8.239	0.000
S(7)	0.000e+000				
S2O8-2	0.000e+000	0.000e+000	-44.481	-44.779	-0.299
S(8)	2.127e-035				
HSO5-	2.127e-035	1.795e-035	-34.672	-34.746	-0.074
Zn	5.971e-006				
Zn+2	4.296e-006	2.296e-006	-5.367	-5.639	-0.272
ZnSO4	1.671e-006	1.671e-006	-5.777	-5.777	0.000
ZnCl+	4.381e-009	3.698e-009	-8.358	-8.432	-0.074
ZnCl2	4.141e-012	4.141e-012	-11.383	-11.383	0.000
ZnOH+	7.128e-013	6.017e-013	-12.147	-12.221	-0.074
Zn(OH)Cl	1.511e-014	1.511e-014	-13.821	-13.821	0.000
ZnCl3-	2.598e-015	2.193e-015	-14.585	-14.659	-0.074
ZnCl4-2	3.169e-017	1.594e-017	-16.499	-16.798	-0.299
Zn(OH)2	6.159e-019	6.159e-019	-18.210	-18.210	0.000
Zn(OH)3-	5.405e-028	4.563e-028	-27.267	-27.341	-0.074
Zn(OH)4-2	3.697e-038	1.859e-038	-37.432	-37.731	-0.299
ZnClO4+	0.000e+000	0.000e+000	-73.617	-73.690	-0.074

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

Phase	SI	log IAP	log KT	
Al	-127.74	22.18	149.91	Al
Al(g)	-178.44	22.18	200.62	Al
Al2(SO4)3	-34.14	-15.24	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-16.79	-15.24	1.56	Al2(SO4)3:6H2O
Alabandite	-93.83	-94.25	-0.42	MnS
Alum-K	-7.54	-12.51	-4.97	KAl(SO4)2:12H2O
Alunite	-5.63	-6.10	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.71	-5.06	-4.35	CaSO4
Antarcticite	-12.73	-8.64	4.09	CaCl2:6H2O
Antlerite	-20.10	-11.37	8.73	Cu3(SO4)(OH)4
Aphthitalite	-14.74	-18.63	-3.89	NaK3(SO4)2
Arcanite	-7.94	-9.78	-1.84	K2SO4
Arsenolite	-33.17	-53.01	-19.84	As2O3
Arsenopyrite	-149.86	-164.30	-14.45	FeAsS
As	-50.22	-7.54	42.68	As
As2O5	-19.37	-17.24	2.14	As2O5
As4O6(cubi)	-66.20	-106.02	-39.82	As4O6
As4O6(mono)	-65.97	-106.02	-40.05	As4O6
Atacamite	-30.59	-16.33	14.26	Cu4Cl2(OH)6
Bassanite	-1.36	-5.06	-3.71	CaSO4:0.5H2O
Birnessite	-82.41	-167.95	-85.55	Mn8O14:5H2O
Bischofite	-13.85	-9.45	4.39	MgCl2:6H2O
Bixbyite	-18.51	-19.48	-0.96	Mn2O3
Bloedite	-11.31	-13.79	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-4.34	3.21	7.55	AlO2H
Bornite	-333.31	-435.84	-102.53	Cu5FeS4
Brochantite	-28.17	-12.75	15.42	Cu4(SO4)(OH)6
Brucite	-14.94	1.34	16.28	Mg(OH)2
Ca	-125.03	14.80	139.83	Ca
Ca(g)	-150.27	14.80	165.07	Ca
Ca2Al2O5:8H2O	-48.85	10.72	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-32.78	-6.49	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-28.58	-10.78	17.80	Ca3(AsO4)2
Ca3Al2O6	-100.15	12.88	113.03	Ca3Al2O6

Ca4Al2Fe2O10	-120.17	20.32	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-92.22	15.03	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-88.65	15.03	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-70.51	-2.18	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-38.34	8.57	46.91	CaAl2O4
CaAl2O4:10H2O	-29.43	8.57	37.99	CaAl2O4:10H2O
CaAl4O7	-53.61	14.98	68.59	CaAl4O7
Carnallite	-20.41	-16.13	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.53	-5.06	-3.54	CaSO4:0.5H2O
Chalcanthite	-5.97	-8.60	-2.63	CuSO4:5H2O
Chalcocite	-87.81	-122.56	-34.74	Cu2S
Chalcocyanite	-11.51	-8.60	2.91	CuSO4
Chalcopyrite	-158.12	-190.73	-32.60	CuFeS2
Chloromagnesite	-31.27	-9.45	21.82	MgCl2
Cl2(g)	-26.43	-23.44	2.99	Cl2
Claudetite	-33.22	-53.01	-19.80	As2O3
Corundum	-11.88	6.42	18.29	Al2O3
Covellite	-73.44	-96.30	-22.86	CuS
Cu	-20.23	11.26	31.50	Cu
Cu(g)	-72.39	11.26	83.66	Cu
CuCl2	-15.90	-12.18	3.72	CuCl2
Cuprite	-25.73	-27.64	-1.91	Cu2O
Delafossite	-4.74	-11.18	-6.44	CuFeO2
Diaspore	-3.94	3.21	7.15	AlHO2
Epsomite	-3.92	-5.88	-1.96	MgSO4:7H2O
Ettringite	-64.78	-2.32	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-45.89	13.13	59.02	Fe
Fe(OH)2	-13.41	0.48	13.89	Fe(OH)2
Fe(OH)3	-3.00	2.64	5.64	Fe(OH)3
Fe2(SO4)3	-19.42	-16.37	3.05	Fe2(SO4)3
FeO	-13.04	0.48	13.52	FeO
Ferrite-Ca	-14.06	7.44	21.50	CaFe2O4
Ferrite-Cu	-6.38	3.90	10.28	CuFe2O4
Ferrite-Dicalcium	-47.21	9.59	56.80	Ca2Fe2O5
Ferrite-Mg	-14.40	6.62	21.02	MgFe2O4
Ferrite-Zn	-7.30	4.40	11.70	ZnFe2O4
FeSO4	-9.34	-6.73	2.61	FeSO4
Gibbsite	-4.53	3.21	7.74	Al(OH)3
Glauberite	-7.50	-12.97	-5.47	Na2Ca(SO4)2
Goethite	2.11	2.64	0.53	FeOOH
Gypsum	-0.53	-5.06	-4.53	CaSO4:2H2O
H2(g)	-30.35	-33.45	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-86.92	-94.92	-7.99	H2S
Halite	-7.31	-5.74	1.56	NaCl
Hausmannite	-28.96	-18.82	10.14	Mn3O4
HCl(g)	-11.70	-5.40	6.30	HCl
Hematite	5.21	5.28	0.08	Fe2O3
Hercynite	-21.90	6.90	28.80	FeAl2O4
Hexahydrite	-4.15	-5.88	-1.73	MgSO4:6H2O
Hydrophilite	-20.38	-8.64	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	1.62	-7.79	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	-1.41	-6.85	-5.45	NaFe3(SO4)2(OH)6
K	-65.94	5.04	70.98	K
K(g)	-76.54	5.04	81.58	K
K2O	-86.60	-2.57	84.04	K2O
K3H(SO4)2	-14.66	-18.28	-3.62	K3H(SO4)2
Kainite	-12.25	-12.56	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-15.78	-12.51	3.27	KAl(SO4)2
Katoite	-66.07	12.88	78.94	Ca3Al2H12O12
Kieserite	-5.61	-5.88	-0.27	MgSO4:H2O
KMgCl3	-37.38	-16.13	21.25	KMgCl3
KMgCl3:2H2O	-30.10	-16.13	13.96	KMgCl3:2H2O
Lammerite	-22.94	-21.39	1.55	Cu3(AsO4)2
Lawrencite	-19.36	-10.31	9.05	FeCl2
Leonite	-11.55	-15.66	-4.11	K2Mg(SO4)2:4H2O

Lime	-30.41	2.15	32.57	CaO
Magnetite	-4.65	5.77	10.42	Fe ₃ O ₄
Manganite	-9.57	-9.74	-0.16	MnO(OH)
Manganosite	-17.26	0.66	17.92	MnO
Mayenite	-423.39	70.76	494.15	Ca ₁₂ Al ₁₄ O ₃₃
Melanterite	-4.34	-6.73	-2.40	FeSO ₄ ·7H ₂ O
Mercallite	-7.06	-8.50	-1.44	KHSO ₄
Mg	-108.53	13.99	122.52	Mg
Mg(g)	-128.26	13.99	142.25	Mg
Mg1.25SO ₄ (OH)0.5:0.5H ₂ O	-10.74	-5.54	5.20	Mg1.25SO ₄ (OH)0.5:0.5H ₂ O
Mg1.5SO ₄ (OH)	-14.42	-5.21	9.21	Mg1.5SO ₄ (OH)
MgCl ₂ :2H ₂ O	-22.19	-9.45	12.73	MgCl ₂ :2H ₂ O
MgCl ₂ :4H ₂ O	-16.76	-9.45	7.30	MgCl ₂ :4H ₂ O
MgCl ₂ :H ₂ O	-25.53	-9.45	16.07	MgCl ₂ :H ₂ O
MgOHCl	-19.95	-4.06	15.89	MgOHCl
MgSO ₄	-10.71	-5.88	4.83	MgSO ₄
Mirabilite	-6.76	-7.91	-1.15	Na ₂ SO ₄ ·10H ₂ O
Misenite	-49.71	-60.79	-11.08	K ₈ H ₆ (SO ₄) ₇
Mn	-69.63	13.31	82.93	Mn
Mn(OH)2(am)	-14.65	0.66	15.31	Mn(OH) ₂
Mn(OH)3	-16.08	-9.74	6.34	Mn(OH) ₃
MnCl ₂ :2H ₂ O	-14.13	-10.13	4.00	MnCl ₂ :2H ₂ O
MnCl ₂ :4H ₂ O	-12.89	-10.13	2.75	MnCl ₂ :4H ₂ O
MnCl ₂ :H ₂ O	-15.68	-10.13	5.54	MnCl ₂ :H ₂ O
MnO ₂ (gamma)	-12.09	-28.21	-16.13	MnO ₂
MnSO ₄	-9.17	-6.56	2.61	MnSO ₄
Molysite	-27.02	-13.55	13.47	FeCl ₃
Na	-61.39	5.98	67.37	Na
Na(g)	-74.88	5.98	80.86	Na
Na ₂ O	-68.11	-0.69	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-14.58	-15.47	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-14.99	-20.88	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
NaFeO ₂	-17.59	2.30	19.88	NaFeO ₂
Nantokite	-12.45	-19.22	-6.77	CuCl
O ₂ (g)	-22.40	-25.29	-2.89	O ₂
Orpiment	-258.27	-337.76	-79.49	As ₂ S ₃
Oxychloride-Mg	-28.55	-2.72	25.83	Mg ₂ Cl(OH) ₃ :4H ₂ O
Pentahydrite	-4.49	-5.88	-1.39	MgSO ₄ ·5H ₂ O
Periclase	-19.98	1.34	21.33	MgO
Picromerite	-11.22	-15.66	-4.44	K ₂ Mg(SO ₄) ₂ :6H ₂ O
Polyhalite	-11.48	-25.79	-14.31	K ₂ MgCa ₂ (SO ₄) ₄ :2H ₂ O
Portlandite	-20.39	2.15	22.55	Ca(OH) ₂
Pyrite	-142.72	-167.42	-24.70	FeS ₂
Pyrolusite	-10.55	-28.21	-17.66	MnO ₂
Pyrrhotite	-90.69	-94.43	-3.74	FeS
Realgar	-100.41	-160.68	-60.28	AsS
S	-62.45	-107.56	-45.11	S
S ₂ (g)	-138.79	-145.98	-7.19	S ₂
Scacchite	-18.87	-10.13	8.74	MnCl ₂
SO ₂ (g)	-32.25	-32.08	0.18	SO ₂
Sphalerite	-84.33	-95.80	-11.47	ZnS
Spinel	-29.85	7.76	37.61	Al ₂ MgO ₄
Starkeyite	-4.88	-5.88	-1.00	MgSO ₄ ·4H ₂ O
Sylvite	-7.51	-6.68	0.83	KCl
Syngenite	-7.25	-14.85	-7.60	K ₂ Ca(SO ₄) ₂ :H ₂ O
Tachyhydrite	-44.69	-27.55	17.14	Mg ₂ CaCl ₆ :12H ₂ O
Tenorite	-9.03	-1.38	7.65	CuO
Thenardite	-7.55	-7.91	-0.36	Na ₂ SO ₄
Todorokite	-69.69	-115.51	-45.82	Mn ₇ O ₁₂ :3H ₂ O
Troilite	-90.59	-94.43	-3.84	FeS
Wurtzite	-86.63	-95.80	-9.17	ZnS
Wustite	-11.72	0.69	12.40	Fe ₉₄ 7O
Zincite	-12.08	-0.88	11.20	ZnO
Zn	-57.02	11.76	68.79	Zn
Zn(ClO ₄) ₂ :6H ₂ O	-149.93	-144.30	5.63	Zn(ClO ₄) ₂ :6H ₂ O
Zn(g)	-73.64	11.76	85.41	Zn
Zn(OH)2(beta)	-12.81	-0.88	11.93	Zn(OH) ₂

Zn(OH)2(epsilon)	-12.54	-0.88	11.66	Zn(OH)2
Zn(OH)2(gamma)	-12.77	-0.88	11.88	Zn(OH)2
Zn2(OH)3Cl	-22.45	-7.16	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-16.56	-8.98	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-29.20	-19.89	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-36.17	-17.08	19.09	Zn3O(SO4)2
ZnCl2	-18.75	-11.68	7.08	ZnCl2
ZnSO4	-11.63	-8.10	3.53	ZnSO4
ZnSO4:6H2O	-6.40	-8.10	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-6.22	-8.10	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-7.55	-8.10	-0.55	ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
