
Reading data base.

LLNL_AQUEOUS_MODEL_PARAMETERS
NAMED_EXPRESSIONS
SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\llnl.dat
SOLUTION 1 Flujo 4
temp 25
pH 3.17
pe 12
redox pe
units mg/l
density 1
Cl 46.9
S(6) 1089.6
Al 25.6
As 5.0
Ca 201.4
Cu 35.1
Fe 170.2
K 69.2
Mg 19.8
Mn 20.6
Na 33.2
Zn 17.4
C(4) 0
water 1 # kg
SOLUTION 2 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      1
SELECTED_OUTPUT
file          DAM_AGUASUP
ph            true
percent_error true
totals        Al  As  Cu  Fe  Mg  Mn  Zn
              S(6)

```

Beginning of initial solution calculations.

Initial solution 1. Flujo 4

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

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

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

```

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

```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	7.785e-004	6.761e-004	-3.109	-3.170	-0.061
OH-	1.709e-011	1.424e-011	-10.767	-10.846	-0.079
H2O	5.553e+001	9.996e-001	1.744	-0.000	0.000
Al	9.504e-004				
AlSO4+	4.577e-004	3.832e-004	-3.339	-3.417	-0.077
Al+3	3.507e-004	9.580e-005	-3.455	-4.019	-0.564
Al(SO4)2-	1.389e-004	1.163e-004	-3.857	-3.935	-0.077
AlOH+2	3.206e-006	1.587e-006	-5.494	-5.799	-0.305
Al(OH)2+	6.507e-009	5.448e-009	-8.187	-8.264	-0.077
Al2(OH)2+4	6.033e-009	4.095e-010	-8.219	-9.388	-1.168
HALO2	1.173e-011	1.173e-011	-10.931	-10.931	0.000
Al3(OH)4+5	3.369e-012	5.535e-014	-11.472	-13.257	-1.784
AlO2-	7.097e-015	5.942e-015	-14.149	-14.226	-0.077
NaAlO2	1.338e-018	1.338e-018	-17.874	-17.874	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-46.038	-49.537	-3.499

As(-3)	0.000e+000					
AsH3	0.000e+000	0.000e+000	-112.033	-112.033	0.000	
As(3)	1.610e-016					
HAsO2	8.593e-017	8.593e-017	-16.066	-16.066	0.000	
As(OH)3	7.510e-017	7.510e-017	-16.124	-16.124	0.000	
H2AsO3-	8.114e-023	6.793e-023	-22.091	-22.168	-0.077	
AsO2-	7.760e-023	6.497e-023	-22.110	-22.187	-0.077	
AsO2OH-2	2.019e-030	9.817e-031	-29.695	-30.008	-0.313	
As(5)	6.685e-005					
H2AsO4-	6.077e-005	5.088e-005	-4.216	-4.293	-0.077	
H3AsO4	6.059e-006	6.059e-006	-5.218	-5.218	0.000	
HAsO4-2	2.569e-008	1.249e-008	-7.590	-7.903	-0.313	
AsO4-3	2.411e-016	4.740e-017	-15.618	-16.324	-0.706	
Ca	5.034e-003					
Ca+2	3.882e-003	2.017e-003	-2.411	-2.695	-0.284	
CaSO4	1.152e-003	1.152e-003	-2.939	-2.939	0.000	
CaCl+	5.599e-007	4.688e-007	-6.252	-6.329	-0.077	
CaCl2	6.044e-010	6.044e-010	-9.219	-9.219	0.000	
CaOH+	5.032e-013	4.213e-013	-12.298	-12.375	-0.077	
Cl(-1)	1.325e-003					
Cl-	1.322e-003	1.096e-003	-2.879	-2.960	-0.081	
CuCl+	7.019e-007	5.877e-007	-6.154	-6.231	-0.077	
CaCl+	5.599e-007	4.688e-007	-6.252	-6.329	-0.077	
FeCl+	5.035e-007	4.215e-007	-6.298	-6.375	-0.077	
MnCl+	3.622e-007	3.033e-007	-6.441	-6.518	-0.077	
MgCl+	2.911e-007	2.438e-007	-6.536	-6.613	-0.077	
NaCl	2.275e-007	2.275e-007	-6.643	-6.643	0.000	
ZnCl+	2.134e-007	1.787e-007	-6.671	-6.748	-0.077	
HCl	1.665e-007	1.665e-007	-6.779	-6.779	0.000	
KCl	5.248e-008	5.248e-008	-7.280	-7.280	0.000	
FeCl+2	1.867e-008	9.244e-009	-7.729	-8.034	-0.305	
FeCl2+	9.799e-009	8.204e-009	-8.009	-8.086	-0.077	
CaCl2	6.044e-010	6.044e-010	-9.219	-9.219	0.000	
CuCl2	3.393e-010	3.393e-010	-9.469	-9.469	0.000	
ZnCl2	2.288e-010	2.288e-010	-9.640	-9.640	0.000	
Zn(OH)Cl	4.517e-012	4.517e-012	-11.345	-11.345	0.000	
FeCl2	2.480e-012	2.480e-012	-11.606	-11.606	0.000	
ZnCl3-	1.655e-013	1.385e-013	-12.781	-12.858	-0.077	
MnCl3-	9.510e-014	7.962e-014	-13.022	-13.099	-0.077	
CuCl2-	1.020e-014	8.543e-015	-13.991	-14.068	-0.077	
ZnCl4-2	2.368e-015	1.151e-015	-14.626	-14.939	-0.313	
CuCl3-2	1.237e-016	6.015e-017	-15.908	-16.221	-0.313	
FeCl4-2	1.771e-017	8.612e-018	-16.752	-17.065	-0.313	
FeCl4-	1.416e-017	1.185e-017	-16.849	-16.926	-0.077	
CuCl4-2	1.574e-020	7.653e-021	-19.803	-20.116	-0.313	
Cl(1)	4.682e-027					
HClO	4.682e-027	4.682e-027	-26.330	-26.330	0.000	
ClO-	2.230e-031	1.867e-031	-30.652	-30.729	-0.077	
Cl(3)	0.000e+000					
ClO2-	0.000e+000	0.000e+000	-51.315	-51.392	-0.077	
HClO2	0.000e+000	0.000e+000	-51.392	-51.392	0.000	
Cl(5)	0.000e+000					
ClO3-	0.000e+000	0.000e+000	-58.124	-58.203	-0.079	
Cl(7)	0.000e+000					
ClO4-	0.000e+000	0.000e+000	-69.237	-69.316	-0.079	
ZnClO4+	0.000e+000	0.000e+000	-71.975	-72.052	-0.077	
Cu(1)	1.385e-013					
Cu+	1.281e-013	1.073e-013	-12.892	-12.969	-0.077	
CuCl2-	1.020e-014	8.543e-015	-13.991	-14.068	-0.077	
CuCl3-2	1.237e-016	6.015e-017	-15.908	-16.221	-0.313	
Cu(2)	5.533e-004					
Cu+2	3.771e-004	1.960e-004	-3.424	-3.708	-0.284	
CuSO4	1.755e-004	1.755e-004	-3.756	-3.756	0.000	
CuCl+	7.019e-007	5.877e-007	-6.154	-6.231	-0.077	
CuOH+	1.785e-008	1.495e-008	-7.748	-7.825	-0.077	
CuCl2	3.393e-010	3.393e-010	-9.469	-9.469	0.000	
CuCl4-2	1.574e-020	7.653e-021	-19.803	-20.116	-0.313	

CuO2-2	6.844e-031	3.328e-031	-30.165	-30.478	-0.313
Fe(2)	1.343e-003				
Fe+2	1.016e-003	5.278e-004	-2.993	-3.278	-0.284
FeSO4	3.270e-004	3.270e-004	-3.486	-3.486	0.000
FeCl+	5.035e-007	4.215e-007	-6.298	-6.375	-0.077
FeOH+	2.947e-010	2.468e-010	-9.531	-9.608	-0.077
FeCl2	2.480e-012	2.480e-012	-11.606	-11.606	0.000
FeCl4-2	1.771e-017	8.612e-018	-16.752	-17.065	-0.313
Fe(OH)2	2.898e-018	2.898e-018	-17.538	-17.538	0.000
Fe(OH)3-	2.037e-025	1.706e-025	-24.691	-24.768	-0.077
Fe(OH)4-2	5.187e-037	2.522e-037	-36.285	-36.598	-0.313
Fe(3)	1.710e-003				
FeOH+2	9.759e-004	4.831e-004	-3.011	-3.316	-0.305
Fe(OH)2+	2.825e-004	2.365e-004	-3.549	-3.626	-0.077
Fe+3	1.852e-004	5.061e-005	-3.732	-4.296	-0.564
Fe2(OH)2+4	9.255e-005	6.281e-006	-4.034	-5.202	-1.168
FeSO4+	2.286e-005	1.914e-005	-4.641	-4.718	-0.077
Fe3(OH)4+5	1.889e-005	3.104e-007	-4.724	-6.508	-1.784
Fe(SO4)2-	1.510e-006	1.265e-006	-5.821	-5.898	-0.077
Fe(OH)3	1.635e-007	1.635e-007	-6.786	-6.786	0.000
FeCl+2	1.867e-008	9.244e-009	-7.729	-8.034	-0.305
FeCl2+	9.799e-009	8.204e-009	-8.009	-8.086	-0.077
Fe(OH)4-	7.254e-014	6.074e-014	-13.139	-13.217	-0.077
FeCl4-	1.416e-017	1.185e-017	-16.849	-16.926	-0.077
H(0)	7.189e-034				
H2	3.595e-034	3.627e-034	-33.444	-33.440	0.004
K	1.773e-003				
K+	1.719e-003	1.426e-003	-2.765	-2.846	-0.081
KSO4-	5.372e-005	4.497e-005	-4.270	-4.347	-0.077
KCl	5.248e-008	5.248e-008	-7.280	-7.280	0.000
KHSO4	2.683e-008	2.683e-008	-7.571	-7.571	0.000
KOH	7.308e-015	7.308e-015	-14.136	-14.136	0.000
Mg	8.161e-004				
Mg+2	5.185e-004	2.848e-004	-3.285	-3.545	-0.260
MgSO4	2.973e-004	2.973e-004	-3.527	-3.527	0.000
MgCl+	2.911e-007	2.438e-007	-6.536	-6.613	-0.077
Mg4(OH)4+4	0.000e+000	0.000e+000	-40.084	-41.252	-1.168
Mn(2)	3.756e-004				
Mn+2	2.500e-004	1.299e-004	-3.602	-3.886	-0.284
MnSO4	1.253e-004	1.253e-004	-3.902	-3.902	0.000
MnCl+	3.622e-007	3.033e-007	-6.441	-6.518	-0.077
MnOH+	5.897e-012	4.937e-012	-11.229	-11.307	-0.077
MnCl3-	9.510e-014	7.962e-014	-13.022	-13.099	-0.077
Mn2OH+3	3.232e-015	6.873e-016	-14.490	-15.163	-0.672
Mn(OH)2	1.792e-020	1.792e-020	-19.747	-19.747	0.000
Mn2(OH)3+	8.202e-023	6.867e-023	-22.086	-22.163	-0.077
Mn(OH)3-	2.968e-029	2.485e-029	-28.528	-28.605	-0.077
Mn(OH)4-2	6.398e-040	3.111e-040	-39.194	-39.507	-0.313
Mn(3)	1.630e-017				
Mn+3	1.630e-017	3.465e-018	-16.788	-17.460	-0.672
Mn(6)	0.000e+000				
MnO4-2	0.000e+000	0.000e+000	-48.661	-48.974	-0.313
Mn(7)	0.000e+000				
MnO4-	0.000e+000	0.000e+000	-46.251	-46.330	-0.079
Na	1.447e-003				
Na+	1.410e-003	1.181e-003	-2.851	-2.928	-0.077
NaSO4-	3.641e-005	3.049e-005	-4.439	-4.516	-0.077
NaCl	2.275e-007	2.275e-007	-6.643	-6.643	0.000
NaOH	2.901e-015	2.901e-015	-14.537	-14.537	0.000
NaAlO2	1.338e-018	1.338e-018	-17.874	-17.874	0.000
O(0)	9.587e-026				
O2	4.793e-026	4.837e-026	-25.319	-25.315	0.004
S(6)	1.136e-002				
SO4-2	8.038e-003	3.909e-003	-2.095	-2.408	-0.313
CaSO4	1.152e-003	1.152e-003	-2.939	-2.939	0.000
AlSO4+	4.577e-004	3.832e-004	-3.339	-3.417	-0.077
FeSO4	3.270e-004	3.270e-004	-3.486	-3.486	0.000

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

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

Phase	SI	log IAP	log KT	
Al	-125.44	24.48	149.91	Al
Al(g)	-176.14	24.48	200.62	Al
Al2(SO4)3	-34.16	-15.26	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-16.82	-15.26	1.56	Al2(SO4)3:6H2O
Alum-K	-6.71	-11.68	-4.97	KAl(SO4)2:12H2O
Alunite	-0.23	-0.70	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.75	-5.10	-4.35	CaSO4
Antarcticite	-12.71	-8.62	4.09	CaCl2:6H2O
Antlerite	-9.58	-0.85	8.73	Cu3(SO4)(OH)4
Aphthitalite	-12.39	-16.28	-3.89	NaK3(SO4)2
Arcanite	-6.26	-8.10	-1.84	K2SO4
Arsenolite	-30.83	-50.68	-19.84	As2O3
As	-49.03	-6.35	42.68	As
As2O5	-17.06	-14.93	2.14	As2O5
As4O6(cubi)	-61.53	-101.35	-39.82	As4O6
As4O6(mono)	-61.30	-101.35	-40.05	As4O6
Atacamite	-16.00	-1.73	14.26	Cu4Cl2(OH)6
Bassanite	-1.40	-5.10	-3.71	CaSO4:0.5H2O
Birnessite	-68.13	-153.67	-85.55	Mn8O14:5H2O
Bischofite	-13.86	-9.47	4.39	MgCl2:6H2O
Bixbyite	-14.94	-15.90	-0.96	Mn2O3
Bloedite	-11.74	-14.22	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-2.06	5.49	7.55	AlO2H
Brochantite	-13.64	1.78	15.42	Cu4(SO4)(OH)6
Brucite	-13.49	2.79	16.28	Mg(OH)2
Ca	-123.53	16.30	139.83	Ca
Ca(g)	-148.77	16.30	165.07	Ca
Ca2Al2O5:8H2O	-41.30	18.27	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-31.26	-4.97	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-21.80	-3.99	17.80	Ca3(AsO4)2
Ca3Al2O6	-91.12	21.92	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-104.49	35.99	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-81.70	25.56	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-78.12	25.56	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-66.01	2.32	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-32.28	14.63	46.91	CaAl2O4
CaAl2O4:10H2O	-23.37	14.63	37.99	CaAl2O4:10H2O

CaAl4O7	-42.98	25.61	68.59	CaAl4O7
Carnallite	-19.54	-15.27	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.57	-5.10	-3.54	CaSO4:0.5H2O
Chalcanthite	-3.49	-6.12	-2.63	CuSO4:5H2O
Chalcocyanite	-9.03	-6.12	2.91	CuSO4
Chloromagnesite	-31.28	-9.47	21.82	MgCl2
Cl2(g)	-27.91	-24.92	2.99	Cl2
Claudetite	-30.88	-50.68	-19.80	As2O3
Corundum	-7.31	10.98	18.29	Al2O3
Cu	-16.21	15.29	31.50	Cu
Cu(g)	-68.37	15.29	83.66	Cu
CuCl2	-13.35	-9.63	3.72	CuCl2
Cuprite	-17.69	-19.60	-1.91	Cu2O
Delafossite	1.85	-4.59	-6.44	CuFeO2
Diaspore	-1.66	5.49	7.15	AlHO2
Epsomite	-3.99	-5.95	-1.96	MgSO4:7H2O
Ettringite	-55.86	6.60	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-43.30	15.72	59.02	Fe
Fe(OH)2	-10.83	3.06	13.89	Fe(OH)2
Fe(OH)3	-0.43	5.21	5.64	Fe(OH)3
Fe2(SO4)3	-18.86	-15.82	3.05	Fe2(SO4)3
FeO	-10.46	3.06	13.52	FeO
Ferrite-Ca	-7.42	14.07	21.50	CaFe2O4
Ferrite-Cu	2.78	13.06	10.28	CuFe2O4
Ferrite-Dicalcium	-39.08	17.72	56.80	Ca2Fe2O5
Ferrite-Mg	-7.80	13.22	21.02	MgFe2O4
Ferrite-Zn	1.05	12.75	11.70	ZnFe2O4
FeSO4	-8.29	-5.69	2.61	FeSO4
Gibbsite	-2.25	5.49	7.74	Al(OH)3
Glauberite	-7.90	-13.37	-5.47	Na2Ca(SO4)2
Goethite	4.68	5.21	0.53	FeOOH
Gypsum	-0.57	-5.10	-4.53	CaSO4:2H2O
H2(g)	-30.34	-33.44	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.45	-5.89	1.56	NaCl
Hausmannite	-23.59	-13.45	10.14	Mn3O4
HCl(g)	-12.43	-6.13	6.30	HCl
Hematite	10.35	10.43	0.08	Fe2O3
Hercynite	-14.76	14.04	28.80	FeAl2O4
Hexahydrite	-4.23	-5.95	-1.73	MgSO4:6H2O
Hydrophilite	-20.36	-8.62	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	7.88	-1.53	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	3.84	-1.61	-5.45	NaFe3(SO4)2(OH)6
K	-64.32	6.65	70.98	K
K(g)	-74.93	6.65	81.58	K
K2O	-83.39	0.65	84.04	K2O
K3H(SO4)2	-12.90	-16.52	-3.62	K3H(SO4)2
Kainite	-11.45	-11.76	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-14.95	-11.68	3.27	KAl(SO4)2
Katoite	-57.03	21.91	78.94	Ca3Al2H12O12
Kieserite	-5.69	-5.95	-0.27	MgSO4:H2O
KMgCl3	-36.52	-15.27	21.25	KMgCl3
KMgCl3:2H2O	-29.23	-15.27	13.96	KMgCl3:2H2O
Lammerite	-8.58	-7.03	1.55	Cu3(AsO4)2
Lawrencite	-18.25	-9.20	9.05	FeCl2
Leonite	-9.94	-14.05	-4.11	K2Mg(SO4)2:4H2O
Lime	-28.92	3.64	32.57	CaO
Magnetite	3.07	13.49	10.42	Fe3O4
Manganite	-7.79	-7.95	-0.16	MnO(OH)
Manganosite	-15.46	2.45	17.92	MnO
Mayenite	-373.54	120.61	494.15	Ca12Al14O33
Melanterite	-3.29	-5.69	-2.40	FeSO4:7H2O
Mercallite	-6.99	-8.42	-1.44	KHSO4
Mg	-107.07	15.45	122.52	Mg
Mg(g)	-126.79	15.45	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.45	-5.25	5.20	Mg1.25SO4(OH)0.5:0.5H2O

Mg1.5SO4(OH)	-13.77	-4.56	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.20	-9.47	12.73	MgCl2:2H2O
MgCl2:4H2O	-16.77	-9.47	7.30	MgCl2:4H2O
MgCl2:H2O	-25.54	-9.47	16.07	MgCl2:H2O
MgOHCl	-19.23	-3.34	15.89	MgOHCl
MgSO4	-10.78	-5.95	4.83	MgSO4
Mirabilite	-7.11	-8.27	-1.15	Na2SO4:10H2O
Misenite	-47.57	-58.64	-11.08	K8H6(SO4)7
Mn	-67.82	15.11	82.93	Mn
Mn(OH)2(am)	-12.85	2.45	15.31	Mn(OH)2
Mn(OH)3	-14.29	-7.95	6.34	Mn(OH)3
MnCl2:2H2O	-13.80	-9.81	4.00	MnCl2:2H2O
MnCl2:4H2O	-12.56	-9.81	2.75	MnCl2:4H2O
MnCl2:H2O	-15.35	-9.81	5.54	MnCl2:H2O
MnO2(gamma)	-10.30	-26.43	-16.13	MnO2
MnSO4	-8.90	-6.29	2.61	MnSO4
Molysite	-26.65	-13.18	13.47	FeCl3
Na	-60.80	6.57	67.37	Na
Na(g)	-74.29	6.57	80.86	Na
Na2O	-66.93	0.48	67.42	Na2O
Na3H(SO4)2	-15.88	-16.77	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-15.74	-21.63	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-14.43	5.46	19.88	NaFeO2
Nantokite	-9.16	-15.93	-6.77	CuCl
O2(g)	-22.42	-25.32	-2.89	O2
Oxychloride-Mg	-26.37	-0.54	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.57	-5.95	-1.39	MgSO4:5H2O
Periclase	-18.53	2.79	21.33	MgO
Picromerite	-9.61	-14.05	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-9.95	-24.26	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-18.90	3.64	22.55	Ca(OH)2
Pyrolusite	-8.77	-26.43	-17.66	MnO2
Scacchite	-18.55	-9.81	8.74	MnCl2
Spinel	-23.83	13.78	37.61	Al2MgO4
Starkeyite	-4.95	-5.95	-1.00	MgSO4:4H2O
Sylvite	-6.63	-5.81	0.83	KCl
Syngenite	-5.60	-13.20	-7.60	K2Ca(SO4)2:H2O
Tachyhydrate	-44.69	-27.55	17.14	Mg2CaCl6:12H2O
Tenorite	-5.01	2.63	7.65	CuO
Thenardite	-7.91	-8.26	-0.36	Na2SO4
Todorokite	-57.19	-103.02	-45.82	Mn7O12:3H2O
Wustite	-9.27	3.13	12.40	Fe.9470
Zincite	-8.87	2.33	11.20	ZnO
Zn	-53.80	14.98	68.79	Zn
Zn(ClO4)2:6H2O	-148.28	-142.65	5.63	Zn(ClO4)2:6H2O
Zn(g)	-70.42	14.98	85.41	Zn
Zn(OH)2(beta)	-9.61	2.33	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-9.33	2.33	11.66	Zn(OH)2
Zn(OH)2(gamma)	-9.56	2.33	11.88	Zn(OH)2
Zn2(OH)3Cl	-16.77	-1.48	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-11.68	-4.09	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-17.26	-7.95	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-29.61	-10.52	19.09	Zn3O(SO4)2
ZnCl2	-17.01	-9.93	7.08	ZnCl2
ZnSO4	-9.95	-6.42	3.53	ZnSO4
ZnSO4:6H2O	-4.72	-6.42	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-4.54	-6.42	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-5.87	-6.42	-0.55	ZnSO4:H2O

Initial solution 2. 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	

	FeCl2+	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
	Fe3(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
	FeCl4-	9.205e-019	7.713e-019	-18.036	-18.113	-0.077
H(0)		4.137e-032				
	H2	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
	KSO4-	5.603e-006	4.694e-006	-5.252	-5.328	-0.077
	KHSO4	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
	MgSO4	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
	Mg4(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
	MnSO4	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
	MnCl3-	3.974e-014	3.329e-014	-13.401	-13.478	-0.077
	Mn2OH+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
	Mn2(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				
	MnO4-2	0.000e+000	0.000e+000	-55.845	-56.156	-0.312
Mn(7)		0.000e+000				
	MnO4-	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
	NaSO4-	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
	NaAlO2	1.245e-021	1.245e-021	-20.905	-20.905	0.000
O(0)		2.895e-029				
	O2	1.448e-029	1.460e-029	-28.839	-28.836	0.004
S(6)		1.161e-002				
	SO4-2	6.638e-003	3.237e-003	-2.178	-2.490	-0.312
	HSO4-	2.002e-003	1.677e-003	-2.699	-2.775	-0.077
	CaSO4	1.507e-003	1.507e-003	-2.822	-2.822	0.000
	AlSO4+	5.907e-004	4.949e-004	-3.229	-3.305	-0.077
	MgSO4	3.941e-004	3.941e-004	-3.404	-3.404	0.000
	Al(SO4)2-	1.484e-004	1.244e-004	-3.828	-3.905	-0.077
	MnSO4	7.478e-005	7.478e-005	-4.126	-4.126	0.000
	NaSO4-	5.953e-005	4.988e-005	-4.225	-4.302	-0.077
	FeSO4	3.640e-005	3.640e-005	-4.439	-4.439	0.000
	KSO4-	5.603e-006	4.694e-006	-5.252	-5.328	-0.077
	FeSO4+	2.543e-006	2.131e-006	-5.595	-5.671	-0.077
	CuSO4	5.704e-007	5.704e-007	-6.244	-6.244	0.000
	Fe(SO4)2-	1.392e-007	1.166e-007	-6.856	-6.933	-0.077
	ZnSO4	8.010e-008	8.010e-008	-7.096	-7.096	0.000
	KHSO4	2.124e-008	2.124e-008	-7.673	-7.673	0.000
	H2SO4	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
	ZnSO4	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
	ZnCl2	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 4
1.000e+000 Solution 2 Inter 3

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

Elements	Molality	Moles
Al	1.117e-003	2.235e-003
As	3.349e-005	6.699e-005
Ca	6.328e-003	1.266e-002
Cl	1.215e-003	2.430e-003
Cu	2.777e-004	5.554e-004
Fe	1.635e-003	3.271e-003
K	9.975e-004	1.995e-003
Mg	1.019e-003	2.039e-003
Mn	3.152e-004	6.303e-004
Na	2.145e-003	4.290e-003

S	1.149e-002	2.297e-002
Zn	1.334e-004	2.669e-004

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

pH	=	2.583	Charge balance
pe	=	12.482	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	3.729e-002	
Mass of water (kg)	=	2.000e+000	
Total alkalinity (eq/kg)	=	-5.348e-003	
Total carbon (mol/kg)	=	0.000e+000	
Total CO2 (mol/kg)	=	0.000e+000	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	1.233e-002	
Percent error, 100*(Cat- An)/(Cat+ An)	=	15.15	
Iterations	=	7	
Total H	=	2.221123e+002	
Total O	=	1.111446e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	3.008e-003	2.612e-003	-2.522	-2.583	-0.061
OH-	4.425e-012	3.687e-012	-11.354	-11.433	-0.079
H2O	5.553e+001	9.995e-001	1.744	-0.000	0.000
Al	1.117e-003				
AlSO4+	5.272e-004	4.413e-004	-3.278	-3.355	-0.077
Al+3	4.433e-004	1.210e-004	-3.353	-3.917	-0.564
Al(SO4)2-	1.459e-004	1.221e-004	-3.836	-3.913	-0.077
AlOH+2	1.048e-006	5.186e-007	-5.979	-6.285	-0.306
Al2(OH)2+4	6.461e-010	4.373e-011	-9.190	-10.359	-1.170
Al(OH)2+	5.505e-010	4.608e-010	-9.259	-9.336	-0.077
HA1O2	2.568e-013	2.568e-013	-12.590	-12.590	0.000
Al3(OH)4+5	3.057e-014	5.001e-016	-13.515	-15.301	-1.786
AlO2-	4.023e-017	3.368e-017	-16.395	-16.473	-0.077
NaAlO2	1.127e-020	1.127e-020	-19.948	-19.948	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-63.501	-67.004	-3.502
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-111.007	-111.007	0.000
As(3)	4.011e-016				
HAsO2	2.140e-016	2.140e-016	-15.669	-15.669	0.000
As(OH)3	1.871e-016	1.871e-016	-15.728	-15.728	0.000
H2AsO3-	5.233e-023	4.380e-023	-22.281	-22.359	-0.077
AsO2-	5.005e-023	4.189e-023	-22.301	-22.378	-0.077
AsO2OH-2	3.372e-031	1.638e-031	-30.472	-30.786	-0.313
HAsS2	0.000e+000	0.000e+000	-183.314	-183.314	0.000
As(5)	3.349e-005				
H2AsO4-	2.418e-005	2.024e-005	-4.617	-4.694	-0.077
H3AsO4	9.312e-006	9.312e-006	-5.031	-5.031	0.000
HAsO4-2	2.647e-009	1.286e-009	-8.577	-8.891	-0.313
AsO4-3	6.438e-018	1.263e-018	-17.191	-17.898	-0.707
Ca	6.328e-003				
Ca+2	4.980e-003	2.587e-003	-2.303	-2.587	-0.285
CaSO4	1.347e-003	1.347e-003	-2.871	-2.871	0.000
CaCl+	6.581e-007	5.509e-007	-6.182	-6.259	-0.077
CaCl2	6.510e-010	6.510e-010	-9.186	-9.186	0.000
CaOH+	1.670e-013	1.398e-013	-12.777	-12.854	-0.077
Cl(-1)	1.215e-003				
Cl-	1.212e-003	1.005e-003	-2.917	-2.998	-0.081
CaCl+	6.581e-007	5.509e-007	-6.182	-6.259	-0.077
HCl	5.894e-007	5.894e-007	-6.230	-6.230	0.000
MgCl+	3.443e-007	2.882e-007	-6.463	-6.540	-0.077
CuCl+	3.321e-007	2.780e-007	-6.479	-6.556	-0.077
NaCl	3.097e-007	3.097e-007	-6.509	-6.509	0.000

MnCl+	2.869e-007	2.402e-007	-6.542	-6.620	-0.077
FeCl+	2.660e-007	2.227e-007	-6.575	-6.652	-0.077
ZnCl+	1.005e-007	8.416e-008	-6.998	-7.075	-0.077
FeCl+2	2.996e-008	1.482e-008	-7.524	-7.829	-0.306
KCl	2.713e-008	2.713e-008	-7.567	-7.567	0.000
FeCl2+	1.440e-008	1.205e-008	-7.842	-7.919	-0.077
CaCl2	6.510e-010	6.510e-010	-9.186	-9.186	0.000
CuCl2	1.471e-010	1.471e-010	-9.832	-9.832	0.000
ZnCl2	9.877e-011	9.877e-011	-10.005	-10.005	0.000
FeCl2	1.200e-012	1.200e-012	-11.921	-11.921	0.000
Zn(OH)Cl	5.507e-013	5.507e-013	-12.259	-12.259	0.000
ZnCl3-	6.547e-014	5.481e-014	-13.184	-13.261	-0.077
MnCl3-	6.327e-014	5.296e-014	-13.199	-13.276	-0.077
CuCl2-	1.458e-015	1.220e-015	-14.836	-14.914	-0.077
ZnCl4-2	8.591e-016	4.174e-016	-15.066	-15.379	-0.313
FeCl4-	1.748e-017	1.463e-017	-16.758	-16.835	-0.077
CuCl3-2	1.621e-017	7.875e-018	-16.790	-17.104	-0.313
FeCl4-2	7.208e-018	3.502e-018	-17.142	-17.456	-0.313
CuCl4-2	5.735e-021	2.787e-021	-20.241	-20.555	-0.313
Cl(1)	1.023e-026				
HClO	1.023e-026	1.023e-026	-25.990	-25.990	0.000
ClO-	1.261e-031	1.056e-031	-30.899	-30.976	-0.077
Cl(3)	0.000e+000				
HClO2	0.000e+000	0.000e+000	-51.263	-51.263	0.000
ClO2-	0.000e+000	0.000e+000	-51.772	-51.849	-0.077
Cl(5)	0.000e+000				
ClO3-	0.000e+000	0.000e+000	-58.791	-58.870	-0.079
Cl(7)	0.000e+000				
ClO4-	0.000e+000	0.000e+000	-70.113	-70.193	-0.079
ZnClO4+	0.000e+000	0.000e+000	-73.141	-73.218	-0.077
Cu(1)	2.327e-014				
Cu+	2.180e-014	1.825e-014	-13.662	-13.739	-0.077
CuCl2-	1.458e-015	1.220e-015	-14.836	-14.914	-0.077
CuCl3-2	1.621e-017	7.875e-018	-16.790	-17.104	-0.313
Cu(2)	2.777e-004				
Cu+2	1.947e-004	1.011e-004	-3.711	-3.995	-0.285
CuSO4	8.261e-005	8.261e-005	-4.083	-4.083	0.000
CuCl+	3.321e-007	2.780e-007	-6.479	-6.556	-0.077
CuOH+	2.385e-009	1.997e-009	-8.622	-8.700	-0.077
CuCl2	1.471e-010	1.471e-010	-9.832	-9.832	0.000
CuCl4-2	5.735e-021	2.787e-021	-20.241	-20.555	-0.313
CuO2-2	1.587e-033	7.709e-034	-32.800	-33.113	-0.313
Fe(2)	7.578e-004				
Fe+2	5.857e-004	3.042e-004	-3.232	-3.517	-0.285
FeSO4	1.719e-004	1.719e-004	-3.765	-3.765	0.000
FeCl+	2.660e-007	2.227e-007	-6.575	-6.652	-0.077
FeOH+	4.398e-011	3.681e-011	-10.357	-10.434	-0.077
FeCl2	1.200e-012	1.200e-012	-11.921	-11.921	0.000
FeCl4-2	7.208e-018	3.502e-018	-17.142	-17.456	-0.313
Fe(OH)2	1.119e-019	1.119e-019	-18.951	-18.951	0.000
Fe(OH)3-	2.037e-027	1.705e-027	-26.691	-26.768	-0.077
Fe(OH)4-2	1.343e-039	6.524e-040	-38.872	-39.185	-0.313
Fe(3)	8.777e-004				
FeOH+2	4.421e-004	2.187e-004	-3.354	-3.660	-0.306
Fe+3	3.244e-004	8.851e-005	-3.489	-4.053	-0.564
FeSO4+	3.647e-005	3.053e-005	-4.438	-4.515	-0.077
Fe(OH)2+	3.310e-005	2.771e-005	-4.480	-4.557	-0.077
Fe2(OH)2+4	1.902e-005	1.287e-006	-4.721	-5.890	-1.170
Fe(SO4)2-	2.198e-006	1.840e-006	-5.658	-5.735	-0.077
Fe3(OH)4+5	4.555e-007	7.452e-009	-6.342	-8.128	-1.786
FeCl+2	2.996e-008	1.482e-008	-7.524	-7.829	-0.306
FeCl2+	1.440e-008	1.205e-008	-7.842	-7.919	-0.077
Fe(OH)3	4.960e-009	4.960e-009	-8.304	-8.304	0.000
Fe(OH)4-	5.696e-016	4.768e-016	-15.244	-15.322	-0.077
FeCl4-	1.748e-017	1.463e-017	-16.758	-16.835	-0.077
H(0)	1.165e-033				
H2	5.826e-034	5.878e-034	-33.235	-33.231	0.004

K	9.975e-004					
K+	9.698e-004	8.040e-004	-3.013	-3.095	-0.081	
KSO4-	2.764e-005	2.314e-005	-4.558	-4.636	-0.077	
KHSO4	5.332e-008	5.332e-008	-7.273	-7.273	0.000	
KCl	2.713e-008	2.713e-008	-7.567	-7.567	0.000	
KOH	1.067e-015	1.067e-015	-14.972	-14.972	0.000	
Mg	1.019e-003					
Mg+2	6.692e-004	3.674e-004	-3.174	-3.435	-0.260	
MgSO4	3.498e-004	3.498e-004	-3.456	-3.456	0.000	
MgCl+	3.443e-007	2.882e-007	-6.463	-6.540	-0.077	
Mg4(OH)4+4	0.000e+000	0.000e+000	-41.988	-43.158	-1.170	
Mn(2)	3.152e-004					
Mn+2	2.161e-004	1.123e-004	-3.665	-3.950	-0.285	
MnSO4	9.875e-005	9.875e-005	-4.005	-4.005	0.000	
MnCl+	2.869e-007	2.402e-007	-6.542	-6.620	-0.077	
MnOH+	1.319e-012	1.104e-012	-11.880	-11.957	-0.077	
MnCl3-	6.327e-014	5.296e-014	-13.199	-13.276	-0.077	
Mn2OH+3	6.256e-016	1.328e-016	-15.204	-15.877	-0.673	
Mn(OH)2	1.037e-021	1.037e-021	-20.984	-20.984	0.000	
Mn2(OH)3+	1.062e-024	8.891e-025	-23.974	-24.051	-0.077	
Mn(OH)3-	4.448e-031	3.723e-031	-30.352	-30.429	-0.077	
Mn(OH)4-2	0.000e+000	0.000e+000	-41.605	-41.918	-0.313	
Mn(3)	4.280e-017					
Mn+3	4.280e-017	9.086e-018	-16.369	-17.042	-0.673	
Mn(6)	0.000e+000					
MnO4-2	0.000e+000	0.000e+000	-51.491	-51.805	-0.313	
Mn(7)	0.000e+000					
MnO4-	0.000e+000	0.000e+000	-48.600	-48.679	-0.079	
Na	2.145e-003					
Na+	2.095e-003	1.754e-003	-2.679	-2.756	-0.077	
NaSO4-	4.936e-005	4.132e-005	-4.307	-4.384	-0.077	
NaCl	3.097e-007	3.097e-007	-6.509	-6.509	0.000	
NaOH	1.116e-015	1.116e-015	-14.952	-14.952	0.000	
NaAlO2	1.127e-020	1.127e-020	-19.948	-19.948	0.000	
O(0)	3.649e-026					
O2	1.825e-026	1.841e-026	-25.739	-25.735	0.004	
S(-2)	0.000e+000					
H2S	0.000e+000	0.000e+000	-87.417	-87.417	0.000	
HS-	0.000e+000	0.000e+000	-91.764	-91.844	-0.079	
S-2	0.000e+000	0.000e+000	-101.888	-102.187	-0.298	
S2-2	0.000e+000	0.000e+000	-162.984	-163.297	-0.313	
HAsS2	0.000e+000	0.000e+000	-183.314	-183.314	0.000	
S3-2	0.000e+000	0.000e+000	-224.135	-224.449	-0.313	
S4-2	0.000e+000	0.000e+000	-285.514	-285.828	-0.313	
S5-2	0.000e+000	0.000e+000	-347.110	-347.423	-0.313	
S(2)	0.000e+000					
S2O3-2	0.000e+000	0.000e+000	-91.752	-92.066	-0.313	
HS2O3-	0.000e+000	0.000e+000	-93.558	-93.635	-0.077	
S(3)	0.000e+000					
S2O4-2	0.000e+000	0.000e+000	-89.563	-89.861	-0.298	
S(4)	4.636e-032					
HSO3-	3.369e-032	2.820e-032	-31.473	-31.550	-0.077	
H2SO3	7.060e-033	7.060e-033	-32.151	-32.151	0.000	
SO2	5.607e-033	5.607e-033	-32.251	-32.251	0.000	
SO3-2	1.281e-036	6.334e-037	-35.893	-36.198	-0.306	
S2O6-2	0.000e+000	0.000e+000	-48.249	-48.563	-0.313	
S3O6-2	0.000e+000	0.000e+000	-111.884	-112.197	-0.313	
S4O6-2	0.000e+000	0.000e+000	-159.613	-159.926	-0.313	
S5O6-2	0.000e+000	0.000e+000	-236.221	-236.535	-0.313	
S(5)	0.000e+000					
S2O5-2	0.000e+000	0.000e+000	-67.616	-67.930	-0.313	
S(6)	1.149e-002					
SO4-2	7.338e-003	3.565e-003	-2.134	-2.448	-0.313	
CaSO4	1.347e-003	1.347e-003	-2.871	-2.871	0.000	
HSO4-	1.124e-003	9.407e-004	-2.949	-3.027	-0.077	
AlSO4+	5.272e-004	4.413e-004	-3.278	-3.355	-0.077	
MgSO4	3.498e-004	3.498e-004	-3.456	-3.456	0.000	

FeSO4	1.719e-004	1.719e-004	-3.765	-3.765	0.000
Al(SO4)2-	1.459e-004	1.221e-004	-3.836	-3.913	-0.077
MnSO4	9.875e-005	9.875e-005	-4.005	-4.005	0.000
CuSO4	8.261e-005	8.261e-005	-4.083	-4.083	0.000
NaSO4-	4.936e-005	4.132e-005	-4.307	-4.384	-0.077
ZnSO4	3.735e-005	3.735e-005	-4.428	-4.428	0.000
FeSO4+	3.647e-005	3.053e-005	-4.438	-4.515	-0.077
KSO4-	2.764e-005	2.314e-005	-4.558	-4.636	-0.077
Fe(SO4)2-	2.198e-006	1.840e-006	-5.658	-5.735	-0.077
KHSO4	5.332e-008	5.332e-008	-7.273	-7.273	0.000
H2SO4	2.318e-009	2.318e-009	-8.635	-8.635	0.000
S(7)	0.000e+000				
S2O8-2	0.000e+000	0.000e+000	-45.071	-45.384	-0.313
S(8)	8.283e-036				
HSO5-	8.283e-036	6.934e-036	-35.082	-35.159	-0.077
Zn	1.334e-004				
Zn+2	9.598e-005	4.985e-005	-4.018	-4.302	-0.285
ZnSO4	3.735e-005	3.735e-005	-4.428	-4.428	0.000
ZnCl+	1.005e-007	8.416e-008	-6.998	-7.075	-0.077
ZnCl2	9.877e-011	9.877e-011	-10.005	-10.005	0.000
ZnOH+	2.499e-011	2.092e-011	-10.602	-10.679	-0.077
Zn(OH)Cl	5.507e-013	5.507e-013	-12.259	-12.259	0.000
ZnCl3-	6.547e-014	5.481e-014	-13.184	-13.261	-0.077
ZnCl4-2	8.591e-016	4.174e-016	-15.066	-15.379	-0.313
Zn(OH)2	3.429e-017	3.429e-017	-16.465	-16.465	0.000
Zn(OH)3-	4.859e-026	4.067e-026	-25.313	-25.391	-0.077
Zn(OH)4-2	5.462e-036	2.654e-036	-35.263	-35.576	-0.313
ZnClO4+	0.000e+000	0.000e+000	-73.141	-73.218	-0.077

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

Phase	SI	log IAP	log KT	
Al	-126.78	23.13	149.91	Al
Al(g)	-177.49	23.13	200.62	Al
Al2(SO4)3	-34.08	-15.18	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-16.74	-15.18	1.56	Al2(SO4)3:6H2O
Alabandite	-92.79	-93.21	-0.42	MnS
Alum-K	-6.94	-11.91	-4.97	KAl(SO4)2:12H2O
Alunite	-3.78	-4.25	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.69	-5.04	-4.35	CaSO4
Antarcticite	-12.68	-8.58	4.09	CaCl2:6H2O
Antlerite	-12.83	-4.10	8.73	Cu3(SO4)(OH)4
Aphthitalite	-13.05	-16.94	-3.89	NaK3(SO4)2
Arcanite	-6.79	-8.64	-1.84	K2SO4
Arsenolite	-30.04	-49.88	-19.84	As2O3
Arsenopyrite	-146.31	-160.75	-14.45	FeAsS
As	-48.32	-5.64	42.68	As
As2O5	-16.69	-14.55	2.14	As2O5
As4O6(cubi)	-59.94	-99.77	-39.82	As4O6
As4O6(mono)	-59.72	-99.77	-40.05	As4O6
Atacamite	-20.74	-6.48	14.26	Cu4Cl2(OH)6
Bassanite	-1.33	-5.04	-3.71	CaSO4:0.5H2O
Birnessite	-79.29	-164.83	-85.55	Mn8O14:5H2O
Bischofite	-13.82	-9.43	4.39	MgCl2:6H2O
Bixbyite	-17.62	-18.59	-0.96	Mn2O3
Bloedite	-11.37	-13.84	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-3.72	3.83	7.55	AlO2H
Bornite	-316.98	-419.51	-102.53	Cu5FeS4
Brochantite	-18.35	-2.93	15.42	Cu4(SO4)(OH)6
Brucite	-14.55	1.73	16.28	Mg(OH)2
Ca	-124.39	15.45	139.83	Ca
Ca(g)	-149.63	15.45	165.07	Ca
Ca2Al2O5:8H2O	-46.75	12.82	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-32.29	-6.00	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-24.62	-6.82	17.80	Ca3(AsO4)2
Ca3Al2O6	-97.63	15.40	113.03	Ca3Al2O6

Ca4Al2Fe2O10	-115.11	25.37	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-89.28	17.97	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-85.71	17.97	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-69.18	-0.85	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-36.67	10.24	46.91	CaAl2O4
CaAl2O4:10H2O	-27.75	10.24	37.99	CaAl2O4:10H2O
CaAl4O7	-50.69	17.90	68.59	CaAl4O7
Carnallite	-19.80	-15.52	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.50	-5.04	-3.54	CaSO4:0.5H2O
Chalcanthite	-3.81	-6.44	-2.63	CuSO4:5H2O
Chalcocite	-81.99	-116.74	-34.74	Cu2S
Chalcocyanite	-9.35	-6.44	2.91	CuSO4
Chalcopyrite	-153.43	-186.03	-32.60	CuFeS2
Chloromagnesite	-31.25	-9.43	21.82	MgCl2
Cl2(g)	-27.02	-24.03	2.99	Cl2
Claudetite	-30.09	-49.88	-19.80	As2O3
Corundum	-10.63	7.66	18.29	Al2O3
Covellite	-70.40	-93.26	-22.86	CuS
Cu	-17.46	14.04	31.50	Cu
Cu(g)	-69.62	14.04	83.66	Cu
CuCl2	-13.71	-9.99	3.72	CuCl2
Cuprite	-20.40	-22.31	-1.91	Cu2O
Delafossite	-1.02	-7.46	-6.44	CuFeO2
Diaspore	-3.31	3.83	7.15	AlHO2
Epsomite	-3.92	-5.88	-1.96	MgSO4:7H2O
Ettringite	-62.18	0.29	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-44.50	14.52	59.02	Fe
Fe(OH)2	-12.25	1.65	13.89	Fe(OH)2
Fe(OH)3	-1.94	3.70	5.64	Fe(OH)3
Fe2(SO4)3	-18.50	-15.45	3.05	Fe2(SO4)3
FeO	-11.87	1.65	13.52	FeO
Ferrite-Ca	-11.53	9.97	21.50	CaFe2O4
Ferrite-Cu	-1.72	8.56	10.28	CuFe2O4
Ferrite-Dicalcium	-44.25	12.55	56.80	Ca2Fe2O5
Ferrite-Mg	-11.90	9.12	21.02	MgFe2O4
Ferrite-Zn	-3.45	8.26	11.70	ZnFe2O4
FeSO4	-8.57	-5.96	2.61	FeSO4
Gibbsite	-3.91	3.83	7.74	Al(OH)3
Glauberite	-7.53	-13.00	-5.47	Na2Ca(SO4)2
Goethite	3.17	3.70	0.53	FeOOH
Gypsum	-0.50	-5.04	-4.53	CaSO4:2H2O
H2(g)	-30.13	-33.23	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-86.43	-94.43	-7.99	H2S
Halite	-7.32	-5.75	1.56	NaCl
Hausmannite	-27.51	-17.37	10.14	Mn3O4
HCl(g)	-11.88	-5.58	6.30	HCl
Hematite	7.32	7.39	0.08	Fe2O3
Hercynite	-19.49	9.31	28.80	FeAl2O4
Hexahydrite	-4.16	-5.88	-1.73	MgSO4:6H2O
Hydrophilite	-20.33	-8.58	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	4.76	-4.65	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	1.13	-4.31	-5.45	NaFe3(SO4)2(OH)6
K	-65.05	5.92	70.98	K
K(g)	-75.66	5.92	81.58	K
K2O	-85.06	-1.02	84.04	K2O
K3H(SO4)2	-13.14	-16.76	-3.62	K3H(SO4)2
Kainite	-11.66	-11.98	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-15.18	-11.91	3.27	KAl(SO4)2
Katoite	-63.55	15.40	78.94	Ca3Al2H12O12
Kieserite	-5.62	-5.88	-0.27	MgSO4:H2O
KMgCl3	-36.77	-15.52	21.25	KMgCl3
KMgCl3:2H2O	-29.49	-15.52	13.96	KMgCl3:2H2O
Lammerite	-12.59	-11.04	1.55	Cu3(AsO4)2
Lawrencite	-18.57	-9.51	9.05	FeCl2
Leonite	-10.41	-14.52	-4.11	K2Mg(SO4)2:4H2O

Lime	-29.99	2.58	32.57	CaO
Magnetite	-1.38	9.04	10.42	Fe ₃ O ₄
Manganite	-9.13	-9.29	-0.16	MnO(OH)
Manganosite	-16.70	1.22	17.92	MnO
Mayenite	-409.57	84.58	494.15	Ca ₁₂ Al ₁₄ O ₃₃
Melanterite	-3.57	-5.97	-2.40	FeSO ₄ ·7H ₂ O
Mercallite	-6.69	-8.13	-1.44	KHSO ₄
Mg	-107.92	14.60	122.52	Mg
Mg(g)	-127.65	14.60	142.25	Mg
Mg1.25SO ₄ (OH)0.5:0.5H ₂ O	-10.65	-5.45	5.20	Mg1.25SO ₄ (OH)0.5:0.5H ₂ O
Mg1.5SO ₄ (OH)	-14.23	-5.02	9.21	Mg1.5SO ₄ (OH)
MgCl ₂ :2H ₂ O	-22.16	-9.43	12.73	MgCl ₂ :2H ₂ O
MgCl ₂ :4H ₂ O	-16.73	-9.43	7.30	MgCl ₂ :4H ₂ O
MgCl ₂ :H ₂ O	-25.50	-9.43	16.07	MgCl ₂ :H ₂ O
MgOHCl	-19.74	-3.85	15.89	MgOHCl
MgSO ₄	-10.71	-5.88	4.83	MgSO ₄
Mirabilite	-6.81	-7.96	-1.15	Na ₂ SO ₄ :10H ₂ O
Misenite	-46.32	-57.39	-11.08	K ₈ H ₆ (SO ₄) ₇
Mn	-68.85	14.08	82.93	Mn
Mn(OH) ₂ (am)	-14.09	1.22	15.31	Mn(OH) ₂
Mn(OH) ₃	-15.63	-9.29	6.34	Mn(OH) ₃
MnCl ₂ :2H ₂ O	-13.94	-9.95	4.00	MnCl ₂ :2H ₂ O
MnCl ₂ :4H ₂ O	-12.70	-9.95	2.75	MnCl ₂ :4H ₂ O
MnCl ₂ :H ₂ O	-15.49	-9.95	5.54	MnCl ₂ :H ₂ O
MnO ₂ (gamma)	-11.75	-27.88	-16.13	MnO ₂
MnSO ₄	-9.01	-6.40	2.61	MnSO ₄
Molysite	-26.52	-13.05	13.47	FeCl ₃
Na	-61.11	6.26	67.37	Na
Na(g)	-74.60	6.26	80.86	Na
Na ₂ O	-67.76	-0.35	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-14.86	-15.75	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-15.06	-20.96	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
NaFeO ₂	-16.36	3.52	19.88	NaFeO ₂
Nantokite	-9.97	-16.74	-6.77	CuCl
O ₂ (g)	-22.84	-25.73	-2.89	O ₂
Orpiment	-253.68	-333.16	-79.49	As ₂ S ₃
Oxychloride-Mg	-27.95	-2.12	25.83	Mg ₂ Cl(OH) ₃ :4H ₂ O
Pentahydrite	-4.50	-5.88	-1.39	MgSO ₄ :5H ₂ O
Periclase	-19.59	1.73	21.33	MgO
Picromerite	-10.08	-14.52	-4.44	K ₂ Mg(SO ₄) ₂ :6H ₂ O
Polyhalite	-10.28	-24.59	-14.31	K ₂ MgCa ₂ (SO ₄) ₄ :2H ₂ O
Portlandite	-19.97	2.58	22.55	Ca(OH) ₂
Pyrite	-140.80	-165.50	-24.70	FeS ₂
Pyrolusite	-10.22	-27.88	-17.66	MnO ₂
Pyrrhotite	-89.04	-92.78	-3.74	FeS
Realgar	-98.24	-158.52	-60.28	AsS
S	-62.18	-107.29	-45.11	S
S ₂ (g)	-138.26	-145.45	-7.19	S ₂
Scacchite	-18.69	-9.95	8.74	MnCl ₂
SO ₂ (g)	-32.43	-32.25	0.18	SO ₂
Sphalerite	-82.09	-93.56	-11.47	ZnS
Spinel	-28.21	9.39	37.61	Al ₂ MgO ₄
Starkeyite	-4.88	-5.88	-1.00	MgSO ₄ :4H ₂ O
Sylvite	-6.92	-6.09	0.83	KCl
Syngenite	-6.07	-13.67	-7.60	K ₂ Ca(SO ₄) ₂ :H ₂ O
Tachyhydrite	-44.59	-27.45	17.14	Mg ₂ CaCl ₆ :12H ₂ O
Tenorite	-6.48	1.17	7.65	CuO
Thenardite	-7.60	-7.96	-0.36	Na ₂ SO ₄
Todorokite	-66.90	-112.73	-45.82	Mn ₇ O ₁₂ :3H ₂ O
Troilite	-88.93	-92.78	-3.84	FeS
Wurtzite	-84.39	-93.56	-9.17	ZnS
Wustite	-10.62	1.78	12.40	Fe ₉₄ 7O
Zincite	-10.34	0.86	11.20	ZnO
Zn	-55.06	13.73	68.79	Zn
Zn(ClO ₄) ₂ :6H ₂ O	-150.32	-144.69	5.63	Zn(ClO ₄) ₂ :6H ₂ O
Zn(g)	-71.68	13.73	85.41	Zn
Zn(OH) ₂ (beta)	-11.07	0.86	11.93	Zn(OH) ₂

Zn(OH)2(epsilon)	-10.80	0.86	11.66	Zn(OH)2
Zn(OH)2(gamma)	-11.02	0.86	11.88	Zn(OH)2
Zn2(OH)3Cl	-19.15	-3.85	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-13.47	-5.89	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-21.27	-11.96	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-31.73	-12.64	19.09	Zn3O(SO4)2
ZnCl2	-17.38	-10.30	7.08	ZnCl2
ZnSO4	-10.28	-6.75	3.53	ZnSO4
ZnSO4:6H2O	-5.05	-6.75	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-4.87	-6.75	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.20	-6.75	-0.55	ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
