
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      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 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	

	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 4
3.000e+000 Solution 2 Inter 3

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

Elements	Molality	Moles
Al	1.201e-003	4.804e-003
As	1.681e-005	6.725e-005
Ca	6.975e-003	2.790e-002
Cl	1.160e-003	4.639e-003
Cu	1.399e-004	5.595e-004
Fe	9.268e-004	3.707e-003
K	6.098e-004	2.439e-003
Mg	1.121e-003	4.484e-003
Mn	2.849e-004	1.140e-003
Na	2.494e-003	9.976e-003

S	1.155e-002	4.619e-002
Zn	6.687e-005	2.675e-004

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

pH	=	2.418	Charge balance
pe	=	12.514	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	3.708e-002	
Mass of water (kg)	=	4.000e+000	
Total alkalinity (eq/kg)	=	-6.663e-003	
Total carbon (mol/kg)	=	0.000e+000	
Total CO2 (mol/kg)	=	0.000e+000	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	3.067e-002	
Percent error, 100*(Cat- An)/(Cat+ An)	=	18.48	
Iterations	=	7	
Total H	=	4.442294e+002	
Total O	=	2.222882e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	4.399e-003	3.820e-003	-2.357	-2.418	-0.061
OH-	3.024e-012	2.521e-012	-11.519	-11.598	-0.079
H2O	5.553e+001	9.995e-001	1.744	-0.000	0.000
Al	1.201e-003				
AlSO4+	5.596e-004	4.686e-004	-3.252	-3.329	-0.077
Al+3	4.930e-004	1.348e-004	-3.307	-3.870	-0.563
Al(SO4)2-	1.476e-004	1.236e-004	-3.831	-3.908	-0.077
AlOH+2	7.977e-007	3.952e-007	-6.098	-6.403	-0.305
Al2(OH)2+4	3.731e-010	2.539e-011	-9.428	-10.595	-1.167
Al(OH)2+	2.867e-010	2.401e-010	-9.543	-9.620	-0.077
HA1O2	9.145e-014	9.145e-014	-13.039	-13.039	0.000
Al3(OH)4+5	9.171e-015	1.513e-016	-14.038	-15.820	-1.783
AlO2-	9.792e-018	8.200e-018	-17.009	-17.086	-0.077
NaAlO2	3.195e-021	3.195e-021	-20.496	-20.496	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-68.181	-71.676	-3.496
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-110.132	-110.132	0.000
As(3)	4.811e-016				
HAsO2	2.567e-016	2.567e-016	-15.591	-15.591	0.000
As(OH)3	2.244e-016	2.244e-016	-15.649	-15.649	0.000
H2AsO3-	4.289e-023	3.592e-023	-22.368	-22.445	-0.077
AsO2-	4.102e-023	3.435e-023	-22.387	-22.464	-0.077
AsO2OH-2	1.887e-031	9.185e-032	-30.724	-31.037	-0.313
HAsS2	0.000e+000	0.000e+000	-180.492	-180.492	0.000
As(5)	1.681e-005				
H2AsO4-	1.075e-005	9.005e-006	-4.968	-5.046	-0.077
H3AsO4	6.060e-006	6.060e-006	-5.218	-5.218	0.000
HAsO4-2	8.040e-010	3.913e-010	-9.095	-9.408	-0.313
AsO4-3	1.334e-018	2.627e-019	-17.875	-18.581	-0.706
Ca	6.975e-003				
Ca+2	5.544e-003	2.883e-003	-2.256	-2.540	-0.284
CaSO4	1.431e-003	1.431e-003	-2.844	-2.844	0.000
CaCl+	7.002e-007	5.864e-007	-6.155	-6.232	-0.077
CaCl2	6.618e-010	6.618e-010	-9.179	-9.179	0.000
CaOH+	1.272e-013	1.066e-013	-12.895	-12.972	-0.077
Cl(-1)	1.160e-003				
Cl-	1.157e-003	9.595e-004	-2.937	-3.018	-0.081
HCl	8.233e-007	8.233e-007	-6.084	-6.084	0.000
CaCl+	7.002e-007	5.864e-007	-6.155	-6.232	-0.077
MgCl+	3.677e-007	3.079e-007	-6.435	-6.512	-0.077
NaCl	3.444e-007	3.444e-007	-6.463	-6.463	0.000
MnCl+	2.516e-007	2.107e-007	-6.599	-6.676	-0.077

CuCl+	1.621e-007	1.357e-007	-6.790	-6.867	-0.077
FeCl+	1.577e-007	1.321e-007	-6.802	-6.879	-0.077
ZnCl+	4.879e-008	4.086e-008	-7.312	-7.389	-0.077
FeCl+2	1.912e-008	9.471e-009	-7.719	-8.024	-0.305
KCl	1.586e-008	1.586e-008	-7.800	-7.800	0.000
FeCl2+	8.785e-009	7.357e-009	-8.056	-8.133	-0.077
CaCl2	6.618e-010	6.618e-010	-9.179	-9.179	0.000
CuCl2	6.859e-011	6.859e-011	-10.164	-10.164	0.000
ZnCl2	4.579e-011	4.579e-011	-10.339	-10.339	0.000
FeCl2	6.801e-013	6.801e-013	-12.167	-12.167	0.000
Zn(OH)Cl	1.828e-013	1.828e-013	-12.738	-12.738	0.000
MnCl3-	5.059e-014	4.237e-014	-13.296	-13.373	-0.077
ZnCl3-	2.898e-014	2.427e-014	-13.538	-13.615	-0.077
CuCl2-	6.308e-016	5.282e-016	-15.200	-15.277	-0.077
ZnCl4-2	3.627e-016	1.765e-016	-15.440	-15.753	-0.313
FeCl4-	9.724e-018	8.143e-018	-17.012	-17.089	-0.077
CuCl3-2	6.689e-018	3.255e-018	-17.175	-17.487	-0.313
FeCl4-2	3.718e-018	1.809e-018	-17.430	-17.742	-0.313
CuCl4-2	2.435e-021	1.185e-021	-20.613	-20.926	-0.313
Cl(1)	7.752e-027				
HClO	7.752e-027	7.752e-027	-26.111	-26.111	0.000
ClO-	6.534e-032	5.471e-032	-31.185	-31.262	-0.077
Cl(3)	0.000e+000				
HClO2	0.000e+000	0.000e+000	-51.649	-51.649	0.000
ClO2-	0.000e+000	0.000e+000	-52.323	-52.400	-0.077
Cl(5)	0.000e+000				
ClO3-	0.000e+000	0.000e+000	-59.608	-59.687	-0.079
Cl(7)	0.000e+000				
ClO4-	0.000e+000	0.000e+000	-71.196	-71.275	-0.079
ZnClO4+	0.000e+000	0.000e+000	-74.517	-74.594	-0.077
Cu(1)	1.098e-014				
Cu+	1.034e-014	8.660e-015	-13.985	-14.062	-0.077
CuCl2-	6.308e-016	5.282e-016	-15.200	-15.277	-0.077
CuCl3-2	6.689e-018	3.255e-018	-17.175	-17.487	-0.313
Cu(2)	1.399e-004				
Cu+2	9.945e-005	5.172e-005	-4.002	-4.286	-0.284
CuSO4	4.025e-005	4.025e-005	-4.395	-4.395	0.000
CuCl+	1.621e-007	1.357e-007	-6.790	-6.867	-0.077
CuOH+	8.335e-010	6.980e-010	-9.079	-9.156	-0.077
CuCl2	6.859e-011	6.859e-011	-10.164	-10.164	0.000
CuCl4-2	2.435e-021	1.185e-021	-20.613	-20.926	-0.313
CuO2-2	1.770e-034	8.612e-035	-33.752	-34.065	-0.313
Fe(2)	4.652e-004				
Fe+2	3.634e-004	1.890e-004	-3.440	-3.724	-0.284
FeSO4	1.017e-004	1.017e-004	-3.993	-3.993	0.000
FeCl+	1.577e-007	1.321e-007	-6.802	-6.879	-0.077
FeOH+	1.867e-011	1.563e-011	-10.729	-10.806	-0.077
FeCl2	6.801e-013	6.801e-013	-12.167	-12.167	0.000
FeCl4-2	3.718e-018	1.809e-018	-17.430	-17.742	-0.313
Fe(OH)2	3.249e-020	3.249e-020	-19.488	-19.488	0.000
Fe(OH)3-	4.041e-028	3.384e-028	-27.394	-27.471	-0.077
Fe(OH)4-2	1.819e-040	0.000e+000	-39.740	-40.053	-0.313
Fe(3)	4.616e-004				
Fe+3	2.166e-004	5.924e-005	-3.664	-4.227	-0.563
FeOH+2	2.020e-004	1.001e-004	-3.695	-4.000	-0.305
FeSO4+	2.325e-005	1.947e-005	-4.634	-4.711	-0.077
Fe(OH)2+	1.035e-005	8.669e-006	-4.985	-5.062	-0.077
Fe2(OH)2+4	3.960e-006	2.695e-007	-5.402	-6.569	-1.167
Fe(SO4)2-	1.335e-006	1.118e-006	-5.875	-5.952	-0.077
Fe3(OH)4+5	2.959e-008	4.881e-010	-7.529	-9.312	-1.783
FeCl+2	1.912e-008	9.471e-009	-7.719	-8.024	-0.305
FeCl2+	8.785e-009	7.357e-009	-8.056	-8.133	-0.077
Fe(OH)3	1.061e-009	1.061e-009	-8.974	-8.974	0.000
Fe(OH)4-	8.325e-017	6.971e-017	-16.080	-16.157	-0.077
FeCl4-	9.724e-018	8.143e-018	-17.012	-17.089	-0.077
H(0)	2.147e-033				
H2	1.074e-033	1.083e-033	-32.969	-32.965	0.004

K	6.098e-004					
K+	5.936e-004	4.924e-004	-3.226	-3.308	-0.081	
KSO4-	1.612e-005	1.350e-005	-4.793	-4.870	-0.077	
KHSO4	4.550e-008	4.550e-008	-7.342	-7.342	0.000	
KCl	1.586e-008	1.586e-008	-7.800	-7.800	0.000	
KOH	4.467e-016	4.467e-016	-15.350	-15.350	0.000	
Mg	1.121e-003					
Mg+2	7.479e-004	4.110e-004	-3.126	-3.386	-0.260	
MgSO4	3.728e-004	3.728e-004	-3.428	-3.428	0.000	
MgCl+	3.677e-007	3.079e-007	-6.435	-6.512	-0.077	
Mg4(OH)4+4	0.000e+000	0.000e+000	-42.457	-43.624	-1.167	
Mn(2)	2.849e-004					
Mn+2	1.983e-004	1.031e-004	-3.703	-3.987	-0.284	
MnSO4	8.641e-005	8.641e-005	-4.063	-4.063	0.000	
MnCl+	2.516e-007	2.107e-007	-6.599	-6.676	-0.077	
MnOH+	8.280e-013	6.934e-013	-12.082	-12.159	-0.077	
MnCl3-	5.059e-014	4.237e-014	-13.296	-13.373	-0.077	
Mn2OH+3	3.597e-016	7.661e-017	-15.444	-16.116	-0.672	
Mn(OH)2	4.453e-022	4.453e-022	-21.351	-21.351	0.000	
Mn2(OH)3+	2.862e-025	2.397e-025	-24.543	-24.620	-0.077	
Mn(OH)3-	1.305e-031	1.093e-031	-30.884	-30.961	-0.077	
Mn(OH)4-2	0.000e+000	0.000e+000	-42.303	-42.616	-0.313	
Mn(3)	4.222e-017					
Mn+3	4.222e-017	8.992e-018	-16.374	-17.046	-0.672	
Mn(6)	0.000e+000					
MnO4-2	0.000e+000	0.000e+000	-52.721	-53.033	-0.313	
Mn(7)	0.000e+000					
MnO4-	0.000e+000	0.000e+000	-49.796	-49.875	-0.079	
Na	2.494e-003					
Na+	2.439e-003	2.042e-003	-2.613	-2.690	-0.077	
NaSO4-	5.474e-005	4.584e-005	-4.262	-4.339	-0.077	
NaCl	3.444e-007	3.444e-007	-6.463	-6.463	0.000	
NaOH	8.882e-016	8.882e-016	-15.051	-15.051	0.000	
NaAlO2	3.195e-021	3.195e-021	-20.496	-20.496	0.000	
O(0)	1.074e-026					
O2	5.372e-027	5.420e-027	-26.270	-26.266	0.004	
S(-2)	0.000e+000					
H2S	0.000e+000	0.000e+000	-86.046	-86.046	0.000	
HS-	0.000e+000	0.000e+000	-90.558	-90.637	-0.079	
S-2	0.000e+000	0.000e+000	-100.848	-101.146	-0.298	
S2-2	0.000e+000	0.000e+000	-160.837	-161.150	-0.313	
HAsS2	0.000e+000	0.000e+000	-180.492	-180.492	0.000	
S3-2	0.000e+000	0.000e+000	-220.883	-221.196	-0.313	
S4-2	0.000e+000	0.000e+000	-281.156	-281.469	-0.313	
S5-2	0.000e+000	0.000e+000	-341.646	-341.959	-0.313	
S(2)	0.000e+000					
S2O3-2	0.000e+000	0.000e+000	-90.402	-90.715	-0.313	
HS2O3-	0.000e+000	0.000e+000	-92.042	-92.119	-0.077	
S(3)	0.000e+000					
S2O4-2	0.000e+000	0.000e+000	-88.479	-88.776	-0.298	
S(4)	1.341e-031					
HSO3-	8.649e-032	7.243e-032	-31.063	-31.140	-0.077	
H2SO3	2.652e-032	2.652e-032	-31.576	-31.576	0.000	
SO2	2.107e-032	2.107e-032	-31.676	-31.676	0.000	
SO3-2	2.245e-036	1.112e-036	-35.649	-35.954	-0.305	
S2O6-2	0.000e+000	0.000e+000	-47.696	-48.009	-0.313	
S3O6-2	0.000e+000	0.000e+000	-110.225	-110.538	-0.313	
S4O6-2	0.000e+000	0.000e+000	-156.848	-157.161	-0.313	
S5O6-2	0.000e+000	0.000e+000	-232.350	-232.663	-0.313	
S(5)	0.000e+000					
S2O5-2	0.000e+000	0.000e+000	-66.797	-67.110	-0.313	
S(6)	1.155e-002					
SO4-2	6.980e-003	3.397e-003	-2.156	-2.469	-0.313	
HSO4-	1.565e-003	1.311e-003	-2.805	-2.882	-0.077	
CaSO4	1.431e-003	1.431e-003	-2.844	-2.844	0.000	
AlSO4+	5.596e-004	4.686e-004	-3.252	-3.329	-0.077	
MgSO4	3.728e-004	3.728e-004	-3.428	-3.428	0.000	

Al(SO4)2-	1.476e-004	1.236e-004	-3.831	-3.908	-0.077
FeSO4	1.017e-004	1.017e-004	-3.993	-3.993	0.000
MnSO4	8.641e-005	8.641e-005	-4.063	-4.063	0.000
NaSO4-	5.474e-005	4.584e-005	-4.262	-4.339	-0.077
CuSO4	4.025e-005	4.025e-005	-4.395	-4.395	0.000
FeSO4+	2.325e-005	1.947e-005	-4.634	-4.711	-0.077
ZnSO4	1.809e-005	1.809e-005	-4.743	-4.743	0.000
KSO4-	1.612e-005	1.350e-005	-4.793	-4.870	-0.077
Fe(SO4)2-	1.335e-006	1.118e-006	-5.875	-5.952	-0.077
KHSO4	4.550e-008	4.550e-008	-7.342	-7.342	0.000
H2SO4	4.725e-009	4.725e-009	-8.326	-8.326	0.000
S(7)	0.000e+000				
S2O8-2	0.000e+000	0.000e+000	-45.049	-45.362	-0.313
S(8)	6.260e-036				
HSO5-	6.260e-036	5.242e-036	-35.203	-35.280	-0.077
Zn	6.687e-005				
Zn+2	4.873e-005	2.534e-005	-4.312	-4.596	-0.284
ZnSO4	1.809e-005	1.809e-005	-4.743	-4.743	0.000
ZnCl+	4.879e-008	4.086e-008	-7.312	-7.389	-0.077
ZnCl2	4.579e-011	4.579e-011	-10.339	-10.339	0.000
ZnOH+	8.683e-012	7.271e-012	-11.061	-11.138	-0.077
Zn(OH)Cl	1.828e-013	1.828e-013	-12.738	-12.738	0.000
ZnCl3-	2.898e-014	2.427e-014	-13.538	-13.615	-0.077
ZnCl4-2	3.627e-016	1.765e-016	-15.440	-15.753	-0.313
Zn(OH)2	8.148e-018	8.148e-018	-17.089	-17.089	0.000
Zn(OH)3-	7.890e-027	6.607e-027	-26.103	-26.180	-0.077
Zn(OH)4-2	6.056e-037	2.947e-037	-36.218	-36.531	-0.313
ZnClO4+	0.000e+000	0.000e+000	-74.517	-74.594	-0.077

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

Phase	SI	log IAP	log KT	
Al	-126.83	23.08	149.91	Al
Al(g)	-177.54	23.08	200.62	Al
Al2(SO4)3	-34.05	-15.15	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-16.70	-15.15	1.56	Al2(SO4)3:6H2O
Alabandite	-91.79	-92.21	-0.42	MnS
Alum-K	-7.15	-12.12	-4.97	KAl(SO4)2:12H2O
Alunite	-4.88	-5.35	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.66	-5.01	-4.35	CaSO4
Antarcticite	-12.67	-8.58	4.09	CaCl2:6H2O
Antlerite	-14.39	-5.66	8.73	Cu3(SO4)(OH)4
Aphthitalite	-13.66	-17.55	-3.89	NaK3(SO4)2
Arcanite	-7.24	-9.08	-1.84	K2SO4
Arsenolite	-29.88	-49.72	-19.84	As2O3
Arsenopyrite	-144.99	-159.44	-14.45	FeAsS
As	-47.85	-5.16	42.68	As
As2O5	-17.06	-14.93	2.14	As2O5
As4O6(cubi)	-59.63	-99.45	-39.82	As4O6
As4O6(mono)	-59.40	-99.45	-40.05	As4O6
Atacamite	-22.94	-8.68	14.26	Cu4Cl2(OH)6
Bassanite	-1.30	-5.01	-3.71	CaSO4:0.5H2O
Birnessite	-83.82	-169.36	-85.55	Mn8O14:5H2O
Bischofite	-13.82	-9.42	4.39	MgCl2:6H2O
Bixbyite	-18.62	-19.59	-0.96	Mn2O3
Bloedite	-11.23	-13.70	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-4.17	3.38	7.55	AlO2H
Bornite	-314.61	-417.14	-102.53	Cu5FeS4
Brochantite	-20.53	-5.11	15.42	Cu4(SO4)(OH)6
Brucite	-14.83	1.45	16.28	Mg(OH)2
Ca	-124.40	15.43	139.83	Ca
Ca(g)	-149.64	15.43	165.07	Ca
Ca2Al2O5:8H2O	-48.21	11.36	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-32.57	-6.28	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-25.84	-8.04	17.80	Ca3(AsO4)2
Ca3Al2O6	-99.38	13.65	113.03	Ca3Al2O6

Ca4Al2Fe2O10	-118.48	22.00	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-91.31	15.95	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-87.74	15.94	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-70.02	-1.69	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-37.85	9.06	46.91	CaAl2O4
CaAl2O4:10H2O	-28.93	9.06	37.99	CaAl2O4:10H2O
CaAl4O7	-52.76	15.83	68.59	CaAl4O7
Carnallite	-20.02	-15.75	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.47	-5.01	-3.54	CaSO4:0.5H2O
Chalcanthite	-4.13	-6.76	-2.63	CuSO4:5H2O
Chalcocite	-81.60	-116.34	-34.74	Cu2S
Chalcocyanite	-9.67	-6.76	2.91	CuSO4
Chalcopyrite	-151.84	-184.45	-32.60	CuFeS2
Chloromagnesite	-31.24	-9.42	21.82	MgCl2
Cl2(g)	-27.00	-24.00	2.99	Cl2
Claudetite	-29.93	-49.72	-19.80	As2O3
Corundum	-11.52	6.77	18.29	Al2O3
Covellite	-69.65	-92.51	-22.86	CuS
Cu	-17.81	13.68	31.50	Cu
Cu(g)	-69.97	13.68	83.66	Cu
CuCl2	-14.04	-10.32	3.72	CuCl2
Cuprite	-21.38	-23.29	-1.91	Cu2O
Delafossite	-2.18	-8.62	-6.44	CuFeO2
Diaspore	-3.76	3.38	7.15	AlHO2
Epsomite	-3.89	-5.86	-1.96	MgSO4:7H2O
Ettringite	-63.84	-1.38	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-44.77	14.24	59.02	Fe
Fe(OH)2	-12.78	1.11	13.89	Fe(OH)2
Fe(OH)3	-2.61	3.03	5.64	Fe(OH)3
Fe2(SO4)3	-18.91	-15.86	3.05	Fe2(SO4)3
FeO	-12.41	1.11	13.52	FeO
Ferrite-Ca	-13.15	8.35	21.50	CaFe2O4
Ferrite-Cu	-3.68	6.60	10.28	CuFe2O4
Ferrite-Dicalcium	-46.16	10.64	56.80	Ca2Fe2O5
Ferrite-Mg	-13.52	7.50	21.02	MgFe2O4
Ferrite-Zn	-5.41	6.29	11.70	ZnFe2O4
FeSO4	-8.80	-6.19	2.61	FeSO4
Gibbsite	-4.36	3.38	7.74	Al(OH)3
Glauberite	-7.39	-12.86	-5.47	Na2Ca(SO4)2
Goethite	2.50	3.03	0.53	FeOOH
Gypsum	-0.48	-5.01	-4.53	CaSO4:2H2O
H2(g)	-29.86	-32.97	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-85.06	-93.06	-7.99	H2S
Halite	-7.27	-5.71	1.56	NaCl
Hausmannite	-28.88	-18.74	10.14	Mn3O4
HCl(g)	-11.74	-5.44	6.30	HCl
Hematite	5.98	6.05	0.08	Fe2O3
Hercynite	-20.92	7.88	28.80	FeAl2O4
Hexahydrite	-4.13	-5.86	-1.73	MgSO4:6H2O
Hydrophilite	-20.32	-8.58	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	2.99	-6.42	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	-0.36	-5.80	-5.45	NaFe3(SO4)2(OH)6
K	-65.30	5.68	70.98	K
K(g)	-75.90	5.68	81.58	K
K2O	-85.82	-1.78	84.04	K2O
K3H(SO4)2	-13.66	-17.28	-3.62	K3H(SO4)2
Kainite	-11.87	-12.18	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-15.39	-12.12	3.27	KAl(SO4)2
Katoite	-65.29	13.65	78.94	Ca3Al2H12O12
Kieserite	-5.59	-5.86	-0.27	MgSO4:H2O
KMgCl3	-36.99	-15.75	21.25	KMgCl3
KMgCl3:2H2O	-29.71	-15.75	13.96	KMgCl3:2H2O
Lammerite	-14.83	-13.28	1.55	Cu3(AsO4)2
Lawrencite	-18.81	-9.76	9.05	FeCl2
Leonite	-10.83	-14.94	-4.11	K2Mg(SO4)2:4H2O

Lime	-30.27	2.30	32.57	CaO
Magnetite	-3.25	7.16	10.42	Fe ₃ O ₄
Manganite	-9.63	-9.79	-0.16	MnO(OH)
Manganosite	-17.07	0.85	17.92	MnO
Mayenite	-419.24	74.91	494.15	Ca ₁₂ Al ₁₄ O ₃₃
Melanterite	-3.80	-6.19	-2.40	FeSO ₄ ·7H ₂ O
Mercallite	-6.76	-8.19	-1.44	KHSO ₄
Mg	-107.94	14.58	122.52	Mg
Mg(g)	-127.66	14.58	142.25	Mg
Mg1.25SO ₄ (OH)0.5:0.5H ₂ O	-10.69	-5.49	5.20	Mg1.25SO ₄ (OH)0.5:0.5H ₂ O
Mg1.5SO ₄ (OH)	-14.34	-5.13	9.21	Mg1.5SO ₄ (OH)
MgCl ₂ :2H ₂ O	-22.15	-9.42	12.73	MgCl ₂ :2H ₂ O
MgCl ₂ :4H ₂ O	-16.72	-9.42	7.30	MgCl ₂ :4H ₂ O
MgCl ₂ :H ₂ O	-25.49	-9.42	16.07	MgCl ₂ :H ₂ O
MgOHCl	-19.88	-3.99	15.89	MgOHCl
MgSO ₄	-10.68	-5.86	4.83	MgSO ₄
Mirabilite	-6.70	-7.85	-1.15	Na ₂ SO ₄ :10H ₂ O
Misenite	-47.18	-58.25	-11.08	K ₈ H ₆ (SO ₄) ₇
Mn	-68.95	13.98	82.93	Mn
Mn(OH)2(am)	-14.46	0.85	15.31	Mn(OH) ₂
Mn(OH)3	-16.13	-9.79	6.34	Mn(OH) ₃
MnCl ₂ :2H ₂ O	-14.02	-10.02	4.00	MnCl ₂ :2H ₂ O
MnCl ₂ :4H ₂ O	-12.78	-10.02	2.75	MnCl ₂ :4H ₂ O
MnCl ₂ :H ₂ O	-15.56	-10.02	5.54	MnCl ₂ :H ₂ O
MnO ₂ (gamma)	-12.38	-28.51	-16.13	MnO ₂
MnSO ₄	-9.06	-6.46	2.61	MnSO ₄
Molysite	-26.75	-13.28	13.47	FeCl ₃
Na	-61.08	6.29	67.37	Na
Na(g)	-74.56	6.29	80.86	Na
Na ₂ O	-67.96	-0.54	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-14.53	-15.43	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-14.81	-20.71	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
NaFeO ₂	-17.13	2.75	19.88	NaFeO ₂
Nantokite	-10.31	-17.08	-6.77	CuCl
O ₂ (g)	-23.37	-26.27	-2.89	O ₂
Orpiment	-249.40	-328.89	-79.49	As ₂ S ₃
Oxychloride-Mg	-28.37	-2.54	25.83	Mg ₂ Cl(OH) ₃ :4H ₂ O
Pentahydrite	-4.47	-5.86	-1.39	MgSO ₄ :5H ₂ O
Periclase	-19.88	1.45	21.33	MgO
Picromerite	-10.50	-14.94	-4.44	K ₂ Mg(SO ₄) ₂ :6H ₂ O
Polyhalite	-10.65	-24.96	-14.31	K ₂ MgCa ₂ (SO ₄) ₄ :2H ₂ O
Portlandite	-20.25	2.30	22.55	Ca(OH) ₂
Pyrite	-138.86	-163.56	-24.70	FeS ₂
Pyrolusite	-10.85	-28.51	-17.66	MnO ₂
Pyrrhotite	-88.20	-91.94	-3.74	FeS
Realgar	-96.66	-156.94	-60.28	AsS
S	-61.08	-106.19	-45.11	S
S ₂ (g)	-136.05	-143.23	-7.19	S ₂
Scacchite	-18.76	-10.02	8.74	MnCl ₂
SO ₂ (g)	-31.85	-31.68	0.18	SO ₂
Sphalerite	-81.35	-92.82	-11.47	ZnS
Spinel	-29.39	8.22	37.61	Al ₂ MgO ₄
Starkeyite	-4.86	-5.86	-1.00	MgSO ₄ :4H ₂ O
Sylvite	-7.15	-6.33	0.83	KCl
Syngenite	-6.49	-14.09	-7.60	K ₂ Ca(SO ₄) ₂ :H ₂ O
Tachyhydrite	-44.57	-27.42	17.14	Mg ₂ CaCl ₆ :12H ₂ O
Tenorite	-7.10	0.55	7.65	CuO
Thenardite	-7.49	-7.85	-0.36	Na ₂ SO ₄
Todorokite	-70.80	-116.63	-45.82	Mn ₇ O ₁₂ :3H ₂ O
Troilite	-88.10	-91.94	-3.84	FeS
Wurtzite	-83.65	-92.82	-9.17	ZnS
Wustite	-11.15	1.26	12.40	Fe ₉₄ 7O
Zincite	-10.96	0.24	11.20	ZnO
Zn	-55.42	13.37	68.79	Zn
Zn(ClO ₄) ₂ :6H ₂ O	-152.78	-147.15	5.63	Zn(ClO ₄) ₂ :6H ₂ O
Zn(g)	-72.04	13.37	85.41	Zn
Zn(OH)2(beta)	-11.69	0.24	11.93	Zn(OH) ₂

Zn(OH)2(epsilon)	-11.42	0.24	11.66	Zn(OH)2
Zn(OH)2(gamma)	-11.64	0.24	11.88	Zn(OH)2
Zn2(OH)3Cl	-20.25	-4.96	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-14.41	-6.83	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-23.52	-14.21	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-32.98	-13.89	19.09	Zn3O(SO4)2
ZnCl2	-17.71	-10.63	7.08	ZnCl2
ZnSO4	-10.60	-7.07	3.53	ZnSO4
ZnSO4:6H2O	-5.37	-7.07	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.19	-7.07	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.51	-7.07	-0.55	ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
