
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 3
temp 25
pH 3.07
pe 17
redox pe
units mg/l
density 1
Cl 40.91
S(6) 1264
Al 21.6
As 3.82
Ca 124.8
Cu 40.91
Fe 41.51
K 35.01
Mg 13.42
Mn 24.26
Na 20.89
Zn 9.71
C(4) 0
water 1 # kg
SOLUTION 3 AS2
temp 25
units mg/l
pe 10
pH 6.98
Cl 678.5
S(6) 427.00
Al 0.00
As 0.1526
Ca 238.3
Cu 0.00
Fe 0.00
K 40.73
Mg 13.69
Mn 0.114
Na 392.9
Zn 2.44
C(4) 153.72
MIX 2
1 1

```

3      3
SELECTED_OUTPUT
file      DAM_AS2
ph        true
percent_error true
totals    Al As Cu Fe Mg Mn Zn
          S(6)

```

Beginning of initial solution calculations.

Initial solution 1. Flujo 3

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

Elements	Molality	Moles
Al	8.019e-004	8.019e-004
As	5.107e-005	5.107e-005
Ca	3.119e-003	3.119e-003
Cl	1.156e-003	1.156e-003
Cu	6.448e-004	6.448e-004
Fe	7.445e-004	7.445e-004
K	8.969e-004	8.969e-004
Mg	5.531e-004	5.531e-004
Mn	4.423e-004	4.423e-004
Na	9.102e-004	9.102e-004
S(6)	1.318e-002	1.318e-002
Zn	1.487e-004	1.487e-004

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

```

pH = 3.070
pe = 17.000
Activity of water = 1.000
Ionic strength = 3.218e-002
Mass of water (kg) = 1.000e+000
Total alkalinity (eq/kg) = -2.266e-003
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = -1.053e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -30.80
Iterations = 8
Total H = 1.110530e+002
Total O = 5.557899e+001

```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	9.741e-004	8.511e-004	-3.011	-3.070	-0.059
OH-	1.344e-011	1.132e-011	-10.872	-10.946	-0.075
H2O	5.553e+001	9.996e-001	1.744	-0.000	0.000
Al	8.019e-004				
AlSO4+	4.097e-004	3.464e-004	-3.388	-3.460	-0.073
Al+3	2.262e-004	6.552e-005	-3.646	-4.184	-0.538
Al(SO4)2-	1.643e-004	1.389e-004	-3.784	-3.857	-0.073
AlOH+2	1.676e-006	8.621e-007	-5.776	-6.064	-0.289
Al(OH)2+	2.781e-009	2.351e-009	-8.556	-8.629	-0.073
Al2(OH)2+4	1.546e-009	1.208e-010	-8.811	-9.918	-1.107
HALO2	4.020e-012	4.020e-012	-11.396	-11.396	0.000
Al3(OH)4+5	3.475e-013	7.050e-015	-12.459	-14.152	-1.693
AlO2-	1.914e-015	1.618e-015	-14.718	-14.791	-0.073
NaAlO2	2.296e-019	2.296e-019	-18.639	-18.639	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-51.563	-54.881	-3.319

As(-3)	0.000e+000					
AsH3	0.000e+000	0.000e+000	-151.256	-151.256	0.000	
As(3)	2.419e-026					
HAsO2	1.291e-026	1.291e-026	-25.889	-25.889	0.000	
As(OH)3	1.128e-026	1.128e-026	-25.948	-25.948	0.000	
H2AsO3-	9.588e-033	8.107e-033	-32.018	-32.091	-0.073	
AsO2-	9.170e-033	7.753e-033	-32.038	-32.111	-0.073	
AsO2OH-2	1.838e-040	0.000e+000	-39.736	-40.031	-0.296	
As(5)	5.107e-005					
H2AsO4-	4.531e-005	3.831e-005	-4.344	-4.417	-0.073	
H3AsO4	5.743e-006	5.743e-006	-5.241	-5.241	0.000	
HAsO4-2	1.476e-008	7.471e-009	-7.831	-8.127	-0.296	
AsO4-3	1.045e-016	2.252e-017	-15.981	-16.647	-0.667	
Ca	3.119e-003					
Ca+2	2.219e-003	1.192e-003	-2.654	-2.924	-0.270	
CaSO4	8.999e-004	8.999e-004	-3.046	-3.046	0.000	
CaCl+	2.891e-007	2.445e-007	-6.539	-6.612	-0.073	
CaCl2	2.781e-010	2.781e-010	-9.556	-9.556	0.000	
CaOH+	2.340e-013	1.978e-013	-12.631	-12.704	-0.073	
Cl(-1)	1.156e-003					
Cl-	1.154e-003	9.673e-004	-2.938	-3.014	-0.077	
CuCl+	6.621e-007	5.598e-007	-6.179	-6.252	-0.073	
MnCl+	3.434e-007	2.903e-007	-6.464	-6.537	-0.073	
CaCl+	2.891e-007	2.445e-007	-6.539	-6.612	-0.073	
HCl	1.849e-007	1.849e-007	-6.733	-6.733	0.000	
MgCl+	1.568e-007	1.326e-007	-6.805	-6.878	-0.073	
NaCl	1.265e-007	1.265e-007	-6.898	-6.898	0.000	
ZnCl+	9.697e-008	8.198e-008	-7.013	-7.086	-0.073	
KCl	2.345e-008	2.345e-008	-7.630	-7.630	0.000	
FeCl+2	9.839e-009	5.061e-009	-8.007	-8.296	-0.289	
FeCl2+	4.688e-009	3.963e-009	-8.329	-8.402	-0.073	
CuCl2	2.852e-010	2.852e-010	-9.545	-9.545	0.000	
CaCl2	2.781e-010	2.781e-010	-9.556	-9.556	0.000	
ZnCl2	9.263e-011	9.263e-011	-10.033	-10.033	0.000	
FeCl+	2.730e-012	2.308e-012	-11.564	-11.637	-0.073	
Zn(OH)Cl	1.646e-012	1.646e-012	-11.783	-11.783	0.000	
MnCl3-	7.018e-014	5.934e-014	-13.154	-13.227	-0.073	
ZnCl3-	5.853e-014	4.948e-014	-13.233	-13.306	-0.073	
ZnCl4-2	7.166e-016	3.628e-016	-15.145	-15.440	-0.296	
FeCl2	1.198e-017	1.198e-017	-16.922	-16.922	0.000	
FeCl4-	5.273e-018	4.458e-018	-17.278	-17.351	-0.073	
CuCl2-	8.492e-020	7.180e-020	-19.071	-19.144	-0.073	
CuCl4-2	9.890e-021	5.007e-021	-20.005	-20.300	-0.296	
CuCl3-2	8.809e-022	4.460e-022	-21.055	-21.351	-0.296	
FeCl4-2	6.397e-023	3.239e-023	-22.194	-22.490	-0.296	
Cl(1)	3.282e-017					
HClO	3.282e-017	3.282e-017	-16.484	-16.484	0.000	
ClO-	1.230e-021	1.040e-021	-20.910	-20.983	-0.073	
Cl(3)	3.477e-032					
HClO2	1.792e-032	1.792e-032	-31.747	-31.747	0.000	
ClO2-	1.685e-032	1.424e-032	-31.773	-31.846	-0.073	
Cl(5)	1.650e-029					
ClO3-	1.650e-029	1.389e-029	-28.783	-28.857	-0.075	
Cl(7)	8.035e-031					
ClO4-	8.027e-031	6.758e-031	-30.095	-30.170	-0.075	
ZnClO4+	7.628e-034	6.449e-034	-33.118	-33.191	-0.073	
Cu(1)	1.456e-018					
Cu+	1.370e-018	1.158e-018	-17.863	-17.936	-0.073	
CuCl2-	8.492e-020	7.180e-020	-19.071	-19.144	-0.073	
CuCl3-2	8.809e-022	4.460e-022	-21.055	-21.351	-0.296	
Cu(2)	6.448e-004					
Cu+2	3.937e-004	2.116e-004	-3.405	-3.675	-0.270	
CuSO4	2.504e-004	2.504e-004	-3.601	-3.601	0.000	
CuCl+	6.621e-007	5.598e-007	-6.179	-6.252	-0.073	
CuOH+	1.516e-008	1.282e-008	-7.819	-7.892	-0.073	
CuCl2	2.852e-010	2.852e-010	-9.545	-9.545	0.000	
CuCl4-2	9.890e-021	5.007e-021	-20.005	-20.300	-0.296	

CuO2-2	2.825e-031	1.430e-031	-30.549	-30.845	-0.296
Fe(2)	8.779e-009				
Fe+2	6.095e-009	3.275e-009	-8.215	-8.485	-0.270
FeSO4	2.682e-009	2.682e-009	-8.572	-8.572	0.000
FeCl+	2.730e-012	2.308e-012	-11.564	-11.637	-0.073
FeOH+	1.439e-015	1.216e-015	-14.842	-14.915	-0.073
FeCl2	1.198e-017	1.198e-017	-16.922	-16.922	0.000
FeCl4-2	6.397e-023	3.239e-023	-22.194	-22.490	-0.296
Fe(OH)2	1.135e-023	1.135e-023	-22.945	-22.945	0.000
Fe(OH)3-	6.276e-031	5.306e-031	-30.202	-30.275	-0.073
Fe(OH)4-2	0.000e+000	0.000e+000	-41.910	-42.205	-0.296
Fe(3)	7.445e-004				
FeOH+2	4.629e-004	2.381e-004	-3.335	-3.623	-0.289
Fe(OH)2+	1.095e-004	9.261e-005	-3.960	-4.033	-0.073
Fe+3	1.084e-004	3.140e-005	-3.965	-4.503	-0.538
Fe2(OH)2+4	1.953e-005	1.526e-006	-4.709	-5.816	-1.107
FeSO4+	1.857e-005	1.570e-005	-4.731	-4.804	-0.073
Fe(SO4)2-	1.622e-006	1.371e-006	-5.790	-5.863	-0.073
Fe3(OH)4+5	1.455e-006	2.953e-008	-5.837	-7.530	-1.693
Fe(OH)3	5.087e-008	5.087e-008	-7.294	-7.294	0.000
FeCl+2	9.839e-009	5.061e-009	-8.007	-8.296	-0.289
FeCl2+	4.688e-009	3.963e-009	-8.329	-8.402	-0.073
Fe(OH)4-	1.775e-014	1.501e-014	-13.751	-13.824	-0.073
FeCl4-	5.273e-018	4.458e-018	-17.278	-17.351	-0.073
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-43.244	-43.240	0.003
K	8.969e-004				
K+	8.613e-004	7.219e-004	-3.065	-3.141	-0.077
KSO4-	3.561e-005	3.011e-005	-4.448	-4.521	-0.073
KCl	2.345e-008	2.345e-008	-7.630	-7.630	0.000
KHSO4	2.261e-008	2.261e-008	-7.646	-7.646	0.000
KOH	2.940e-015	2.940e-015	-14.532	-14.532	0.000
Mg	5.531e-004				
Mg+2	3.107e-004	1.755e-004	-3.508	-3.756	-0.248
MgSO4	2.422e-004	2.422e-004	-3.616	-3.616	0.000
MgCl+	1.568e-007	1.326e-007	-6.805	-6.878	-0.073
Mg4(OH)4+4	0.000e+000	0.000e+000	-41.386	-42.493	-1.107
Mn(2)	4.423e-004				
Mn+2	2.623e-004	1.410e-004	-3.581	-3.851	-0.270
MnSO4	1.797e-004	1.797e-004	-3.746	-3.746	0.000
MnCl+	3.434e-007	2.903e-007	-6.464	-6.537	-0.073
MnOH+	5.033e-012	4.255e-012	-11.298	-11.371	-0.073
MnCl3-	7.018e-014	5.934e-014	-13.154	-13.227	-0.073
Mn2OH+3	2.782e-015	6.427e-016	-14.556	-15.192	-0.636
Mn(OH)2	1.227e-020	1.227e-020	-19.911	-19.911	0.000
Mn2(OH)3+	4.793e-023	4.052e-023	-22.319	-22.392	-0.073
Mn(OH)3-	1.598e-029	1.351e-029	-28.796	-28.869	-0.073
Mn(OH)4-2	2.655e-040	1.344e-040	-39.576	-39.872	-0.296
Mn(3)	1.627e-012				
Mn+3	1.627e-012	3.760e-013	-11.789	-12.425	-0.636
Mn(6)	3.607e-030				
MnO4-2	3.607e-030	1.826e-030	-29.443	-29.738	-0.296
Mn(7)	9.551e-023				
MnO4-	9.551e-023	8.041e-023	-22.020	-22.095	-0.075
Na	9.102e-004				
Na+	8.800e-004	7.440e-004	-3.056	-3.128	-0.073
NaSO4-	3.004e-005	2.540e-005	-4.522	-4.595	-0.073
NaCl	1.265e-007	1.265e-007	-6.898	-6.898	0.000
NaOH	1.452e-015	1.452e-015	-14.838	-14.838	0.000
NaAlO2	2.296e-019	2.296e-019	-18.639	-18.639	0.000
O(0)	3.822e-006				
O2	1.911e-006	1.926e-006	-5.719	-5.715	0.003
S(6)	1.318e-002				
SO4-2	1.020e-002	5.166e-003	-1.991	-2.287	-0.296
CaSO4	8.999e-004	8.999e-004	-3.046	-3.046	0.000
HSO4-	5.254e-004	4.442e-004	-3.280	-3.352	-0.073
AlSO4+	4.097e-004	3.464e-004	-3.388	-3.460	-0.073

CuSO4	2.504e-004	2.504e-004	-3.601	-3.601	0.000
MgSO4	2.422e-004	2.422e-004	-3.616	-3.616	0.000
MnSO4	1.797e-004	1.797e-004	-3.746	-3.746	0.000
Al(SO4)2-	1.643e-004	1.389e-004	-3.784	-3.857	-0.073
ZnSO4	5.476e-005	5.476e-005	-4.262	-4.262	0.000
KSO4-	3.561e-005	3.011e-005	-4.448	-4.521	-0.073
NaSO4-	3.004e-005	2.540e-005	-4.522	-4.595	-0.073
FeSO4+	1.857e-005	1.570e-005	-4.731	-4.804	-0.073
Fe(SO4)2-	1.622e-006	1.371e-006	-5.790	-5.863	-0.073
KHSO4	2.261e-008	2.261e-008	-7.646	-7.646	0.000
FeSO4	2.682e-009	2.682e-009	-8.572	-8.572	0.000
H2SO4	3.567e-010	3.567e-010	-9.448	-9.448	0.000
Zn	1.487e-004				
Zn+2	9.388e-005	5.045e-005	-4.027	-4.297	-0.270
ZnSO4	5.476e-005	5.476e-005	-4.262	-4.262	0.000
ZnCl+	9.697e-008	8.198e-008	-7.013	-7.086	-0.073
ZnCl2	9.263e-011	9.263e-011	-10.033	-10.033	0.000
ZnOH+	7.685e-011	6.498e-011	-10.114	-10.187	-0.073
Zn(OH)Cl	1.646e-012	1.646e-012	-11.783	-11.783	0.000
ZnCl3-	5.853e-014	4.948e-014	-13.233	-13.306	-0.073
ZnCl4-2	7.166e-016	3.628e-016	-15.145	-15.440	-0.296
Zn(OH)2	3.268e-016	3.268e-016	-15.486	-15.486	0.000
Zn(OH)3-	1.407e-024	1.190e-024	-23.852	-23.925	-0.073
ZnClO4+	7.628e-034	6.449e-034	-33.118	-33.191	-0.073
Zn(OH)4-2	4.705e-034	2.382e-034	-33.327	-33.623	-0.296

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

Phase	SI	log IAP	log KT	
Al	-140.60	9.31	149.91	Al
Al(g)	-191.31	9.31	200.62	Al
Al2(SO4)3	-34.13	-15.23	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-16.78	-15.23	1.56	Al2(SO4)3:6H2O
Alum-K	-6.93	-11.90	-4.97	KAl(SO4)2:12H2O
Alunite	-1.38	-1.85	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.86	-5.21	-4.35	CaSO4
Antarcticite	-13.05	-8.95	4.09	CaCl2:6H2O
Antlerite	-9.76	-1.03	8.73	Cu3(SO4)(OH)4
Aphthitalite	-13.24	-17.13	-3.89	NaK3(SO4)2
Arcanite	-6.73	-8.57	-1.84	K2SO4
Arsenolite	-50.48	-70.32	-19.84	As2O3
As	-73.56	-30.87	42.68	As
As2O5	-17.11	-14.97	2.14	As2O5
As4O6(cubi)	-100.82	-140.64	-39.82	As4O6
As4O6(mono)	-100.59	-140.64	-40.05	As4O6
Atacamite	-16.57	-2.31	14.26	Cu4Cl2(OH)6
Bassanite	-1.50	-5.21	-3.71	CaSO4:0.5H2O
Birnessite	-10.64	-96.19	-85.55	Mn8O14:5H2O
Bischofite	-14.18	-9.79	4.39	MgCl2:6H2O
Bixbyite	-5.47	-6.43	-0.96	Mn2O3
Bloedite	-12.11	-14.59	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-2.52	5.03	7.55	AlO2H
Brochantite	-13.99	1.43	15.42	Cu4(SO4)(OH)6
Brucite	-13.90	2.38	16.28	Mg(OH)2
Ca	-133.76	6.07	139.83	Ca
Ca(g)	-159.00	6.07	165.07	Ca
Ca2Al2O5:8H2O	-43.09	16.48	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-32.03	-5.74	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-23.13	-5.32	17.80	Ca3(AsO4)2
Ca3Al2O6	-93.33	19.70	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-108.15	32.33	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-84.34	22.92	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-80.77	22.91	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-67.63	0.69	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-33.64	13.27	46.91	CaAl2O4
CaAl2O4:10H2O	-24.73	13.27	37.99	CaAl2O4:10H2O

CaAl4O7	-45.27	23.32	68.59	CaAl4O7
Carnallite	-20.21	-15.94	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.68	-5.21	-3.54	CaSO4:0.5H2O
Chalcanthite	-3.33	-5.96	-2.63	CuSO4:5H2O
Chalcocyanite	-8.87	-5.96	2.91	CuSO4
Chloromagnesite	-31.60	-9.78	21.82	MgCl2
Cl2(g)	-18.02	-15.03	2.99	Cl2
Claudetite	-50.53	-70.32	-19.80	As2O3
Corundum	-8.24	10.05	18.29	Al2O3
Cu	-26.17	5.32	31.50	Cu
Cu(g)	-78.33	5.32	83.66	Cu
CuCl2	-13.42	-9.70	3.72	CuCl2
Cuprite	-27.83	-29.73	-1.91	Cu2O
Delafossite	-3.72	-10.16	-6.44	CuFeO2
Diaspore	-2.12	5.03	7.15	AlHO2
Epsomite	-4.08	-6.04	-1.96	MgSO4:7H2O
Ettringite	-58.40	4.06	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-58.50	0.51	59.02	Fe
Fe(OH)2	-16.24	-2.35	13.89	Fe(OH)2
Fe(OH)3	-0.93	4.71	5.64	Fe(OH)3
Fe2(SO4)3	-18.91	-15.87	3.05	Fe2(SO4)3
FeO	-15.87	-2.34	13.52	FeO
Ferrite-Ca	-8.87	12.63	21.50	CaFe2O4
Ferrite-Cu	1.60	11.88	10.28	CuFe2O4
Ferrite-Dicalcium	-40.95	15.85	56.80	Ca2Fe2O5
Ferrite-Mg	-9.22	11.80	21.02	MgFe2O4
Ferrite-Zn	-0.44	11.26	11.70	ZnFe2O4
FeSO4	-13.38	-10.77	2.61	FeSO4
Gibbsite	-2.71	5.03	7.74	Al(OH)3
Glauberite	-8.29	-13.75	-5.47	Na2Ca(SO4)2
Goethite	4.18	4.71	0.53	FeOOH
Gypsum	-0.68	-5.21	-4.53	CaSO4:2H2O
H2(g)	-40.14	-43.24	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.71	-6.14	1.56	NaCl
Hausmannite	-14.29	-4.14	10.14	Mn3O4
HCl(g)	-12.39	-6.08	6.30	HCl
Hematite	9.34	9.41	0.08	Fe2O3
Hercynite	-21.10	7.71	28.80	FeAl2O4
Hexahydrite	-4.32	-6.04	-1.73	MgSO4:6H2O
Hydrophilite	-20.70	-8.95	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	6.61	-2.81	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	2.66	-2.79	-5.45	NaFe3(SO4)2(OH)6
K	-69.62	1.36	70.98	K
K(g)	-80.22	1.36	81.58	K
K2O	-84.18	-0.14	84.04	K2O
K3H(SO4)2	-13.44	-17.07	-3.62	K3H(SO4)2
Kainite	-11.89	-12.20	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-15.17	-11.90	3.27	KAl(SO4)2
Katoite	-59.24	19.70	78.94	Ca3Al2H12O12
Kieserite	-5.78	-6.04	-0.27	MgSO4:H2O
KMgCl3	-37.19	-15.94	21.25	KMgCl3
KMgCl3:2H2O	-29.90	-15.94	13.96	KMgCl3:2H2O
Lammerite	-9.13	-7.58	1.55	Cu3(AsO4)2
Lawrencite	-23.57	-14.51	9.05	FeCl2
Leonite	-10.50	-14.61	-4.11	K2Mg(SO4)2:4H2O
Lime	-29.35	3.22	32.57	CaO
Magnetite	-3.35	7.07	10.42	Fe3O4
Manganite	-3.05	-3.22	-0.16	MnO(OH)
Manganosite	-15.63	2.29	17.92	MnO
Mayenite	-385.19	108.96	494.15	Ca12Al14O33
Melanterite	-8.37	-10.77	-2.40	FeSO4:7H2O
Mercallite	-7.06	-8.50	-1.44	KHSO4
Mg	-117.28	5.24	122.52	Mg
Mg(g)	-137.00	5.24	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.64	-5.45	5.20	Mg1.25SO4(OH)0.5:0.5H2O

Mg1.5SO4(OH)	-14.06	-4.85	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.52	-9.78	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.09	-9.79	7.30	MgCl2:4H2O
MgCl2:H2O	-25.86	-9.78	16.07	MgCl2:H2O
MgOHCl	-19.59	-3.70	15.89	MgOHCl
MgSO4	-10.87	-6.04	4.83	MgSO4
Mirabilite	-7.39	-8.55	-1.15	Na2SO4:10H2O
Misenite	-48.48	-59.56	-11.08	K8H6(SO4)7
Mn	-77.79	5.15	82.93	Mn
Mn(OH)2(am)	-13.02	2.29	15.31	Mn(OH)2
Mn(OH)3	-9.56	-3.22	6.34	Mn(OH)3
MnCl2:2H2O	-13.88	-9.88	4.00	MnCl2:2H2O
MnCl2:4H2O	-12.63	-9.88	2.75	MnCl2:4H2O
MnCl2:H2O	-15.42	-9.88	5.54	MnCl2:H2O
MnO2(gamma)	-0.67	-16.79	-16.13	MnO2
MnSO4	-8.75	-6.14	2.61	MnSO4
Molysite	-27.02	-13.55	13.47	FeCl3
Na	-66.00	1.37	67.37	Na
Na(g)	-79.49	1.37	80.86	Na
Na2O	-67.53	-0.12	67.42	Na2O
Na3H(SO4)2	-16.14	-17.03	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.40	-22.30	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-15.24	4.65	19.88	NaFeO2
Nantokite	-14.18	-20.95	-6.77	CuCl
O2(g)	-2.82	-5.72	-2.89	O2
Oxychloride-Mg	-27.15	-1.32	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.66	-6.04	-1.39	MgSO4:5H2O
Periclase	-18.94	2.38	21.33	MgO
Picromerite	-10.17	-14.61	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-10.72	-25.03	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-19.33	3.22	22.55	Ca(OH)2
Pyrolusite	0.87	-16.79	-17.66	MnO2
Scacchite	-18.62	-9.88	8.74	MnCl2
Spinel	-25.17	12.44	37.61	Al2MgO4
Starkeyite	-5.04	-6.04	-1.00	MgSO4:4H2O
Sylvite	-6.98	-6.16	0.83	KCl
Syngenite	-6.18	-13.78	-7.60	K2Ca(SO4)2:H2O
Tachyhydrate	-45.67	-28.52	17.14	Mg2CaCl6:12H2O
Tenorite	-5.18	2.47	7.65	CuO
Thenardite	-8.19	-8.54	-0.36	Na2SO4
Todorokite	-9.35	-55.17	-45.82	Mn7O12:3H2O
Wustite	-13.88	-1.47	12.40	Fe.947O
Zincite	-9.36	1.84	11.20	ZnO
Zn	-64.09	4.70	68.79	Zn
Zn(ClO4)2:6H2O	-70.27	-64.64	5.63	Zn(ClO4)2:6H2O
Zn(g)	-80.71	4.70	85.41	Zn
Zn(OH)2(beta)	-10.09	1.84	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-9.82	1.84	11.66	Zn(OH)2
Zn(OH)2(gamma)	-10.04	1.84	11.88	Zn(OH)2
Zn2(OH)3Cl	-17.69	-2.40	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-12.32	-4.74	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-18.76	-9.44	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-30.42	-11.33	19.09	Zn3O(SO4)2
ZnCl2	-17.40	-10.33	7.08	ZnCl2
ZnSO4	-10.12	-6.58	3.53	ZnSO4
ZnSO4:6H2O	-4.89	-6.58	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-4.71	-6.59	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.03	-6.58	-0.55	ZnSO4:H2O

Initial solution 3. AS2

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

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

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

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

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

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

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

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

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

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

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

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

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

Beginning of batch-reaction calculations.

Reaction step 1.

Using mix 2.

Mixture 2.

1.000e+000 Solution 1 Flujo 3
3.000e+000 Solution 3 AS2

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

Elements	Molality	Moles
Al	2.005e-004	8.019e-004
As	1.430e-005	5.719e-005
C	1.894e-003	7.575e-003
Ca	5.248e-003	2.099e-002
Cl	1.467e-002	5.868e-002
Cu	1.612e-004	6.448e-004
Fe	1.861e-004	7.445e-004
K	1.007e-003	4.028e-003
Mg	5.615e-004	2.246e-003
Mn	1.121e-004	4.486e-004
Na	1.307e-002	5.228e-002
S	6.637e-003	2.655e-002
Zn	6.522e-005	2.609e-004

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

pH	=	5.808	Charge balance
pe	=	14.111	Adjusted to redox equilibrium
Activity of water	=	0.999	
Ionic strength	=	3.565e-002	
Mass of water (kg)	=	4.000e+000	
Total alkalinity (eq/kg)	=	1.030e-003	
Total CO2 (mol/kg)	=	1.894e-003	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	-7.308e-003	
Percent error, 100*(Cat- An)/(Cat+ An)	=	-3.65	
Iterations	=	15	
Total H	=	4.442113e+002	
Total O	=	2.222300e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	1.787e-006	1.555e-006	-5.748	-5.808	-0.060
OH-	7.407e-009	6.192e-009	-8.130	-8.208	-0.078
H2O	5.553e+001	9.993e-001	1.744	-0.000	0.000
Al	2.005e-004				
Al13O4(OH)24+7	1.525e-005	5.464e-009	-4.817	-8.263	-3.446
AlOH+2	6.609e-007	3.309e-007	-6.180	-6.480	-0.300
Al(OH)2+	5.881e-007	4.938e-007	-6.231	-6.306	-0.076
HAlo2	4.621e-007	4.621e-007	-6.335	-6.335	0.000
Al+3	1.654e-007	4.596e-008	-6.782	-7.338	-0.556
AlSO4+	1.459e-007	1.225e-007	-6.836	-6.912	-0.076
AlO2-	1.212e-007	1.018e-007	-6.916	-6.992	-0.076
Al(SO4)2-	2.949e-008	2.476e-008	-7.530	-7.606	-0.076
Al2(OH)2+4	2.517e-010	1.781e-011	-9.599	-10.749	-1.150
NaAlO2	2.091e-010	2.091e-010	-9.680	-9.680	0.000
Al3(OH)4+5	1.248e-011	2.182e-013	-10.904	-12.661	-1.757
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-153.367	-153.367	0.000
As(3)	2.345e-029				
HAsO2	1.251e-029	1.251e-029	-28.903	-28.903	0.000
As(OH)3	1.093e-029	1.093e-029	-28.961	-28.961	0.000
H2AsO3-	5.119e-033	4.298e-033	-32.291	-32.367	-0.076
AsO2-	4.897e-033	4.112e-033	-32.310	-32.386	-0.076
AsO2OH-2	5.487e-038	2.700e-038	-37.261	-37.569	-0.308
HAsS2	0.000e+000	0.000e+000	-287.390	-287.390	0.000
As(5)	1.430e-005				
H2AsO4-	1.209e-005	1.015e-005	-4.917	-4.993	-0.076
HAsO4-2	2.203e-006	1.084e-006	-5.657	-5.965	-0.308
H3AsO4	2.781e-009	2.781e-009	-8.556	-8.556	0.000
AsO4-3	8.854e-012	1.788e-012	-11.053	-11.748	-0.695
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-253.896	-253.896	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-224.848	-224.848	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-140.672	-140.672	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-47.730	-47.730	0.000
C(4)	1.894e-003				
CO2	1.401e-003	1.413e-003	-2.854	-2.850	0.004
HCO3-	4.662e-004	3.914e-004	-3.331	-3.407	-0.076
CaHCO3+	1.264e-005	1.061e-005	-4.898	-4.974	-0.076
CuCO3	6.389e-006	6.389e-006	-5.195	-5.195	0.000
NaHCO3	6.027e-006	6.027e-006	-5.220	-5.220	0.000
MgHCO3+	1.208e-006	1.014e-006	-5.918	-5.994	-0.076
ZnHCO3+	3.147e-007	2.643e-007	-6.502	-6.578	-0.076

MnHCO3+	1.541e-007	1.294e-007	-6.812	-6.888	-0.076
CaCO3	5.920e-008	5.920e-008	-7.228	-7.228	0.000
CO3-2	2.230e-008	1.117e-008	-7.652	-7.952	-0.300
MnCO3	1.697e-008	1.697e-008	-7.770	-7.770	0.000
FeCO3+	1.079e-008	9.058e-009	-7.967	-8.043	-0.076
MgCO3	2.635e-009	2.635e-009	-8.579	-8.579	0.000
ZnCO3	2.456e-009	2.456e-009	-8.610	-8.610	0.000
NaCO3-	5.009e-010	4.206e-010	-9.300	-9.376	-0.076
Cu(CO3)2-2	2.583e-010	1.271e-010	-9.588	-9.896	-0.308
FeHCO3+	2.774e-012	2.329e-012	-11.557	-11.633	-0.076
CuCO3(OH)2-2	4.558e-014	2.243e-014	-13.341	-13.649	-0.308
FeCO3	7.188e-015	7.188e-015	-14.143	-14.143	0.000
Ca	5.248e-003				
Ca+2	4.358e-003	2.287e-003	-2.361	-2.641	-0.280
CaSO4	8.701e-004	8.701e-004	-3.060	-3.060	0.000
CaHCO3+	1.264e-005	1.061e-005	-4.898	-4.974	-0.076
CaCl+	7.028e-006	5.902e-006	-5.153	-5.229	-0.076
CaCl2	8.450e-008	8.450e-008	-7.073	-7.073	0.000
CaCO3	5.920e-008	5.920e-008	-7.228	-7.228	0.000
CaOH+	2.473e-010	2.076e-010	-9.607	-9.683	-0.076
Cl(-1)	1.467e-002				
Cl-	1.463e-002	1.217e-002	-1.835	-1.915	-0.080
NaCl	2.303e-005	2.303e-005	-4.638	-4.638	0.000
CaCl+	7.028e-006	5.902e-006	-5.153	-5.229	-0.076
MgCl+	2.524e-006	2.120e-006	-5.598	-5.674	-0.076
CuCl+	2.378e-006	1.997e-006	-5.624	-5.700	-0.076
MnCl+	1.340e-006	1.125e-006	-5.873	-5.949	-0.076
ZnCl+	6.379e-007	5.357e-007	-6.195	-6.271	-0.076
KCl	3.354e-007	3.354e-007	-6.474	-6.474	0.000
CaCl2	8.450e-008	8.450e-008	-7.073	-7.073	0.000
CuCl2	1.280e-008	1.280e-008	-7.893	-7.893	0.000
ZnCl2	7.617e-009	7.617e-009	-8.118	-8.118	0.000
Zn(OH)Cl	5.886e-009	5.886e-009	-8.230	-8.230	0.000
HCl	4.251e-009	4.251e-009	-8.371	-8.371	0.000
ZnCl3-	6.098e-011	5.121e-011	-10.215	-10.291	-0.076
MnCl3-	4.339e-011	3.643e-011	-10.363	-10.439	-0.076
ZnCl4-2	9.601e-012	4.725e-012	-11.018	-11.326	-0.308
FeCl2+	3.343e-012	2.807e-012	-11.476	-11.552	-0.076
FeCl+2	5.689e-013	2.849e-013	-12.245	-12.545	-0.300
FeCl+	1.197e-013	1.005e-013	-12.922	-12.998	-0.076
CuCl2-	2.971e-015	2.495e-015	-14.527	-14.603	-0.076
CuCl3-2	3.964e-016	1.951e-016	-15.402	-15.710	-0.308
CuCl4-2	7.235e-017	3.560e-017	-16.141	-16.449	-0.308
FeCl2	6.567e-018	6.567e-018	-17.183	-17.183	0.000
FeCl4-	5.956e-019	5.001e-019	-18.225	-18.301	-0.076
FeCl4-2	5.715e-021	2.812e-021	-20.243	-20.551	-0.308
Cl(1)	3.850e-019				
HClO	3.772e-019	3.772e-019	-18.423	-18.423	0.000
ClO-	7.790e-021	6.541e-021	-20.108	-20.184	-0.076
Cl(3)	5.346e-032				
ClO2-	5.336e-032	4.480e-032	-31.273	-31.349	-0.076
HClO2	1.030e-034	1.030e-034	-33.987	-33.987	0.000
Cl(5)	2.612e-029				
ClO3-	2.612e-029	2.184e-029	-28.583	-28.661	-0.078
Cl(7)	6.359e-031				
ClO4-	6.356e-031	5.313e-031	-30.197	-30.275	-0.078
ZnClO4+	3.134e-034	2.632e-034	-33.504	-33.580	-0.076
Cu(1)	3.670e-015				
CuCl2-	2.971e-015	2.495e-015	-14.527	-14.603	-0.076
CuCl3-2	3.964e-016	1.951e-016	-15.402	-15.710	-0.308
Cu+	3.027e-016	2.541e-016	-15.519	-15.595	-0.076
Cu(2)	1.612e-004				
Cu+2	1.143e-004	5.998e-005	-3.942	-4.222	-0.280
CuSO4	3.578e-005	3.578e-005	-4.446	-4.446	0.000
CuCO3	6.389e-006	6.389e-006	-5.195	-5.195	0.000
CuCl+	2.378e-006	1.997e-006	-5.624	-5.700	-0.076
CuOH+	2.368e-006	1.988e-006	-5.626	-5.702	-0.076

CuCl2	1.280e-008	1.280e-008	-7.893	-7.893	0.000
Cu(CO3)2-2	2.583e-010	1.271e-010	-9.588	-9.896	-0.308
CuCO3(OH)2-2	4.558e-014	2.243e-014	-13.341	-13.649	-0.308
CuCl4-2	7.235e-017	3.560e-017	-16.141	-16.449	-0.308
CuO2-2	7.391e-021	3.637e-021	-20.131	-20.439	-0.308
Fe(2)	2.918e-011				
Fe+2	2.160e-011	1.134e-011	-10.666	-10.945	-0.280
FeSO4	4.679e-012	4.679e-012	-11.330	-11.330	0.000
FeHCO3+	2.774e-012	2.329e-012	-11.557	-11.633	-0.076
FeCl+	1.197e-013	1.005e-013	-12.922	-12.998	-0.076
FeCO3	7.188e-015	7.188e-015	-14.143	-14.143	0.000
FeOH+	2.744e-015	2.304e-015	-14.562	-14.638	-0.076
FeCl2	6.567e-018	6.567e-018	-17.183	-17.183	0.000
Fe(OH)2	1.176e-020	1.176e-020	-19.930	-19.930	0.000
FeCl4-2	5.715e-021	2.812e-021	-20.243	-20.551	-0.308
Fe(OH)3-	3.583e-025	3.009e-025	-24.446	-24.522	-0.076
Fe(OH)4-2	3.929e-034	1.933e-034	-33.406	-33.714	-0.308
Fe(3)	1.861e-004				
Fe(OH)2+	1.477e-004	1.240e-004	-3.831	-3.907	-0.076
Fe(OH)3	3.727e-005	3.727e-005	-4.429	-4.429	0.000
FeOH+2	1.164e-006	5.827e-007	-5.934	-6.235	-0.300
FeCO3+	1.079e-008	9.058e-009	-7.967	-8.043	-0.076
Fe(OH)4-	7.165e-009	6.016e-009	-8.145	-8.221	-0.076
Fe+3	5.053e-010	1.404e-010	-9.296	-9.853	-0.556
Fe2(OH)2+4	1.292e-010	9.139e-012	-9.889	-11.039	-1.150
FeSO4+	4.214e-011	3.538e-011	-10.375	-10.451	-0.076
Fe3(OH)4+5	1.354e-011	2.368e-013	-10.868	-12.626	-1.757
FeCl2+	3.343e-012	2.807e-012	-11.476	-11.552	-0.076
Fe(SO4)2-	1.855e-012	1.558e-012	-11.732	-11.808	-0.076
FeCl+2	5.689e-013	2.849e-013	-12.245	-12.545	-0.300
FeCl4-	5.956e-019	5.001e-019	-18.225	-18.301	-0.076
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-42.943	-42.940	0.004
K	1.007e-003				
K+	9.862e-004	8.204e-004	-3.006	-3.086	-0.080
KSO4-	2.054e-005	1.724e-005	-4.687	-4.763	-0.076
KCl	3.354e-007	3.354e-007	-6.474	-6.474	0.000
KHSO4	2.366e-011	2.366e-011	-10.626	-10.626	0.000
KOH	1.828e-012	1.828e-012	-11.738	-11.738	0.000
Mg	5.615e-004				
Mg+2	4.027e-004	2.230e-004	-3.395	-3.652	-0.257
MgSO4	1.551e-004	1.551e-004	-3.809	-3.809	0.000
MgCl+	2.524e-006	2.120e-006	-5.598	-5.674	-0.076
MgHCO3+	1.208e-006	1.014e-006	-5.918	-5.994	-0.076
MgCO3	2.635e-009	2.635e-009	-8.579	-8.579	0.000
Mg4(OH)4+4	1.061e-030	7.505e-032	-29.974	-31.125	-1.150
Mn(2)	1.121e-004				
Mn+2	8.273e-005	4.342e-005	-4.082	-4.362	-0.280
MnSO4	2.790e-005	2.790e-005	-4.554	-4.554	0.000
MnCl+	1.340e-006	1.125e-006	-5.873	-5.949	-0.076
MnHCO3+	1.541e-007	1.294e-007	-6.812	-6.888	-0.076
MnCO3	1.697e-008	1.697e-008	-7.770	-7.770	0.000
MnOH+	8.542e-010	7.172e-010	-9.068	-9.144	-0.076
MnCl3-	4.339e-011	3.643e-011	-10.363	-10.439	-0.076
Mn2OH+3	1.531e-013	3.337e-014	-12.815	-13.477	-0.662
Mn(OH)2	1.131e-015	1.131e-015	-14.946	-14.946	0.000
Mn2(OH)3+	7.502e-016	6.299e-016	-15.125	-15.201	-0.076
Mn(OH)3-	8.122e-022	6.820e-022	-21.090	-21.166	-0.076
Mn(OH)4-2	7.542e-030	3.711e-030	-29.123	-29.430	-0.308
Mn(3)	6.867e-016				
Mn+3	6.867e-016	1.496e-016	-15.163	-15.825	-0.662
Mn(6)	2.563e-020				
MnO4-2	2.563e-020	1.261e-020	-19.591	-19.899	-0.308
Mn(7)	8.583e-016				
MnO4-	8.583e-016	7.175e-016	-15.066	-15.144	-0.078
Na	1.307e-002				
Na+	1.282e-002	1.076e-002	-1.892	-1.968	-0.076

NaSO4-	2.206e-004	1.852e-004	-3.656	-3.732	-0.076
NaCl	2.303e-005	2.303e-005	-4.638	-4.638	0.000
NaHCO3	6.027e-006	6.027e-006	-5.220	-5.220	0.000
NaCO3-	5.009e-010	4.206e-010	-9.300	-9.376	-0.076
NaAlO2	2.091e-010	2.091e-010	-9.680	-9.680	0.000
NaOH	1.150e-011	1.150e-011	-10.939	-10.939	0.000
O(0)	9.543e-007				
O2	4.772e-007	4.813e-007	-6.321	-6.318	0.004
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-132.839	-132.839	0.000
HS-	0.000e+000	0.000e+000	-133.962	-134.040	-0.078
S-2	0.000e+000	0.000e+000	-140.864	-141.158	-0.293
S2-2	0.000e+000	0.000e+000	-237.673	-237.981	-0.308
HAsS2	0.000e+000	0.000e+000	-287.390	-287.390	0.000
S3-2	0.000e+000	0.000e+000	-334.538	-334.846	-0.308
S4-2	0.000e+000	0.000e+000	-431.629	-431.937	-0.308
S5-2	0.000e+000	0.000e+000	-528.938	-529.246	-0.308
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-137.316	-137.624	-0.308
HS2O3-	0.000e+000	0.000e+000	-142.342	-142.418	-0.076
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-125.417	-125.711	-0.293
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-44.544	-44.620	-0.076
SO3-2	0.000e+000	0.000e+000	-45.743	-46.043	-0.300
H2SO3	0.000e+000	0.000e+000	-48.447	-48.447	0.000
SO2	0.000e+000	0.000e+000	-48.547	-48.547	0.000
S2O6-2	0.000e+000	0.000e+000	-64.687	-64.995	-0.308
S3O6-2	0.000e+000	0.000e+000	-164.034	-164.342	-0.308
S4O6-2	0.000e+000	0.000e+000	-247.476	-247.784	-0.308
S5O6-2	0.000e+000	0.000e+000	-359.797	-360.105	-0.308
S(5)	0.000e+000				
S2O5-2	0.000e+000	0.000e+000	-93.762	-94.070	-0.308
S(6)	6.637e-003				
SO4-2	5.292e-003	2.604e-003	-2.276	-2.584	-0.308
CaSO4	8.701e-004	8.701e-004	-3.060	-3.060	0.000
NaSO4-	2.206e-004	1.852e-004	-3.656	-3.732	-0.076
MgSO4	1.551e-004	1.551e-004	-3.809	-3.809	0.000
CuSO4	3.578e-005	3.578e-005	-4.446	-4.446	0.000
MnSO4	2.790e-005	2.790e-005	-4.554	-4.554	0.000
KSO4-	2.054e-005	1.724e-005	-4.687	-4.763	-0.076
ZnSO4	1.433e-005	1.433e-005	-4.844	-4.844	0.000
HSO4-	4.871e-007	4.090e-007	-6.312	-6.388	-0.076
AlSO4+	1.459e-007	1.225e-007	-6.836	-6.912	-0.076
Al(SO4)2-	2.949e-008	2.476e-008	-7.530	-7.606	-0.076
FeSO4+	4.214e-011	3.538e-011	-10.375	-10.451	-0.076
KHSO4	2.366e-011	2.366e-011	-10.626	-10.626	0.000
FeSO4	4.679e-012	4.679e-012	-11.330	-11.330	0.000
Fe(SO4)2-	1.855e-012	1.558e-012	-11.732	-11.808	-0.076
H2SO4	6.001e-016	6.001e-016	-15.222	-15.222	0.000
S(7)	0.000e+000				
S2O8-2	0.000e+000	0.000e+000	-42.091	-42.399	-0.308
S(8)	1.836e-029				
HSO5-	1.836e-029	1.541e-029	-28.736	-28.812	-0.076
Zn	6.522e-005				
Zn+2	4.990e-005	2.619e-005	-4.302	-4.582	-0.280
ZnSO4	1.433e-005	1.433e-005	-4.844	-4.844	0.000
ZnCl+	6.379e-007	5.357e-007	-6.195	-6.271	-0.076
ZnHCO3+	3.147e-007	2.643e-007	-6.502	-6.578	-0.076
ZnOH+	2.198e-008	1.846e-008	-7.658	-7.734	-0.076
ZnCl2	7.617e-009	7.617e-009	-8.118	-8.118	0.000
Zn(OH)Cl	5.886e-009	5.886e-009	-8.230	-8.230	0.000
ZnCO3	2.456e-009	2.456e-009	-8.610	-8.610	0.000
ZnCl3-	6.098e-011	5.121e-011	-10.215	-10.291	-0.076
Zn(OH)2	5.080e-011	5.080e-011	-10.294	-10.294	0.000
ZnCl4-2	9.601e-012	4.725e-012	-11.018	-11.326	-0.308
Zn(OH)3-	1.205e-016	1.012e-016	-15.919	-15.995	-0.076

Zn(OH)4-2	2.253e-023	1.109e-023	-22.647	-22.955	-0.308
ZnClO4+	3.134e-034	2.632e-034	-33.504	-33.580	-0.076

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

Phase	SI	log IAP	log KT	
Al	-135.09	14.82	149.91	Al
Al(g)	-185.79	14.82	200.62	Al
Al2(SO4)3	-41.33	-22.43	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-23.99	-22.43	1.56	Al2(SO4)3:6H2O
Alabandite	-132.17	-132.59	-0.42	MnS
Alum-K	-10.63	-15.60	-4.97	KAl(SO4)2:12H2O
Alunite	5.05	4.58	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.88	-5.23	-4.35	CaSO4
Antarcticite	-10.57	-6.47	4.09	CaCl2:6H2O
Antlerite	-0.75	7.98	8.73	Cu3(SO4)(OH)4
Aphthitalite	-12.51	-16.39	-3.89	NaK3(SO4)2
Aragonite	-2.21	-0.24	1.97	CaCO3
Arcanite	-6.91	-8.76	-1.84	K2SO4
Arsenolite	-56.51	-76.35	-19.84	As2O3
Arsenopyrite	-220.50	-234.95	-14.45	FeAsS
Artinite	-12.91	6.71	19.63	Mg2CO3(OH)2:3H2O
As	-76.12	-33.44	42.68	As
As2O5	-23.74	-21.60	2.14	As2O5
As4O6(cubi)	-112.87	-152.70	-39.82	As4O6
As4O6(mono)	-112.65	-152.70	-40.05	As4O6
Atacamite	-0.13	14.13	14.26	Cu4Cl2(OH)6
Azurite	-5.36	3.75	9.12	Cu3(CO3)2(OH)2
Bassanite	-1.52	-5.23	-3.71	CaSO4:0.5H2O
Birnessite	27.27	-58.28	-85.55	Mn8O14:5H2O
Bischofite	-11.88	-7.48	4.39	MgCl2:6H2O
Bixbyite	4.16	3.20	-0.96	Mn2O3
Bloedite	-10.28	-12.76	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	2.54	10.09	7.55	AlO2H
Bornite	-487.94	-590.47	-102.53	Cu5FeS4
Brochantite	-0.05	15.38	15.42	Cu4(SO4)(OH)6
Brucite	-8.32	7.96	16.28	Mg(OH)2
Burkeite	-24.06	-14.58	9.49	Na6CO3(SO4)2
C	-67.04	-2.90	64.15	C
C(g)	-184.66	-2.90	181.77	C
Ca	-127.70	12.13	139.83	Ca
Ca(g)	-152.94	12.13	165.07	Ca
Ca2Al2O5:8H2O	-21.45	38.12	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-23.79	2.51	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-12.48	5.32	17.80	Ca3(AsO4)2
Ca3Al2O6	-65.93	47.10	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-69.26	71.22	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-51.18	56.07	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-47.61	56.07	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-47.88	20.45	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-17.76	29.15	46.91	CaAl2O4
CaAl2O4:10H2O	-8.85	29.15	37.99	CaAl2O4:10H2O
CaAl4O7	-19.27	49.32	68.59	CaAl4O7
Calcite	-2.06	-0.24	1.82	CaCO3
Carnallite	-16.76	-12.48	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.69	-5.23	-3.54	CaSO4:0.5H2O
CH4(g)	-137.83	-140.67	-2.84	CH4
Chalcanthite	-4.18	-6.81	-2.63	CuSO4:5H2O
Chalcocite	-124.68	-159.42	-34.74	Cu2S
Chalcocyanite	-9.72	-6.81	2.91	CuSO4
Chalcopyrite	-239.03	-271.63	-32.60	CuFeS2
Chloromagnesite	-29.30	-7.48	21.82	MgCl2
Cl2(g)	-21.60	-18.60	2.99	Cl2
Claudetite	-56.55	-76.35	-19.80	As2O3
CO(g)	-44.73	-47.73	-3.00	CO
CO2(g)	-1.39	-9.22	-7.83	CO2

Corundum	1.88	20.17	18.29	Al ₂ O ₃
Covellite	-109.59	-132.45	-22.86	CuS
Cu	-20.94	10.55	31.50	Cu
Cu(g)	-73.10	10.55	83.66	Cu
CuCl ₂	-11.77	-8.05	3.72	CuCl ₂
Cuprite	-17.67	-19.57	-1.91	Cu ₂ O
Dawsonite	0.37	4.71	4.34	NaAlCO ₃ (OH) ₂
Delafossite	4.22	-2.21	-6.44	CuFeO ₂
Diaspore	2.94	10.09	7.15	AlHO ₂
Dolomite	-3.96	-1.49	2.47	CaMg(CO ₃) ₂
Dolomite-dis	-5.50	-1.49	4.01	CaMg(CO ₃) ₂
Dolomite-ord	-3.96	-1.49	2.46	CaMg(CO ₃) ₂
Epsomite	-4.28	-6.24	-1.96	MgSO ₄ ·7H ₂ O
Ettringite	-31.05	31.42	62.46	Ca ₆ Al ₂ (SO ₄) ₃ (OH) ₁₂ ·26H ₂ O
Fe	-55.19	3.83	59.02	Fe
Fe(OH) ₂	-13.22	0.67	13.89	Fe(OH) ₂
Fe(OH) ₃	1.93	7.57	5.64	Fe(OH) ₃
Fe ₂ (SO ₄) ₃	-30.51	-27.46	3.05	Fe ₂ (SO ₄) ₃
FeO	-12.85	0.67	13.52	FeO
Ferrite-Ca	2.62	24.12	21.50	CaFe ₂ O ₄
Ferrite-Cu	12.25	22.54	10.28	CuFe ₂ O ₄
Ferrite-Dicalcium	-23.70	33.09	56.80	Ca ₂ Fe ₂ O ₅
Ferrite-Mg	2.09	23.11	21.02	MgFe ₂ O ₄
Ferrite-Zn	10.48	22.18	11.70	ZnFe ₂ O ₄
FeSO ₄	-16.14	-13.53	2.61	FeSO ₄
Gaylussite	-12.94	-1.78	11.16	CaNa ₂ (CO ₃) ₂ ·5H ₂ O
Gibbsite	2.35	10.09	7.74	Al(OH) ₃
Glauberite	-6.28	-11.75	-5.47	Na ₂ Ca(SO ₄) ₂
Goethite	7.04	7.57	0.53	FeOOH
Gypsum	-0.69	-5.23	-4.53	CaSO ₄ ·2H ₂ O
H ₂ (g)	-39.84	-42.94	-3.10	H ₂
H ₂ O(g)	-1.59	-0.00	1.59	H ₂ O
H ₂ S(g)	-131.86	-139.85	-7.99	H ₂ S
Halite	-5.45	-3.88	1.56	NaCl
Hausmannite	0.31	10.45	10.14	Mn ₃ O ₄
HCl(g)	-14.02	-7.72	6.30	HCl
Hematite	15.07	15.14	0.08	Fe ₂ O ₃
Hercynite	-7.96	20.84	28.80	FeAl ₂ O ₄
Hexahydrite	-4.51	-6.24	-1.73	MgSO ₄ ·6H ₂ O
Huntite	-14.21	-3.99	10.22	CaMg ₃ (CO ₃) ₄
Hydromagnesite	-27.78	2.96	30.74	Mg ₅ (CO ₃) ₄ (OH) ₂ ·4H ₂ O
Hydrophilite	-18.22	-6.47	11.75	CaCl ₂
Hydrozincite	-13.57	16.74	30.31	Zn ₅ (OH) ₆ (CO ₃) ₂
Ice	-0.14	-0.00	0.14	H ₂ O
Jarosite	6.45	-2.96	-9.41	KFe ₃ (SO ₄) ₂ (OH) ₆
Jarosite-Na	3.60	-1.85	-5.45	NaFe ₃ (SO ₄) ₂ (OH) ₆
K	-66.67	4.30	70.98	K
K(g)	-77.28	4.30	81.58	K
K ₂ CO ₃ ·1.5H ₂ O	-17.15	-3.77	13.38	K ₂ CO ₃ ·1.5H ₂ O
K ₂ O	-78.59	5.44	84.04	K ₂ O
K ₃ H(SO ₄) ₂	-16.61	-20.23	-3.62	K ₃ H(SO ₄) ₂
K ₈ H ₄ (CO ₃) ₆ ·3H ₂ O	-61.23	-33.52	27.71	K ₈ H ₄ (CO ₃) ₆ ·3H ₂ O
Kainite	-10.93	-11.24	-0.31	KMgClSO ₄ ·3H ₂ O
KAl(SO ₄) ₂	-18.87	-15.59	3.27	KAl(SO ₄) ₂
Kalinite	-6.78	-6.49	0.28	KHCO ₃
Katoite	-31.85	47.10	78.94	Ca ₃ Al ₂ H ₁₂ O ₁₂
Kieserite	-5.97	-6.24	-0.27	MgSO ₄ ·H ₂ O
KMgCl ₃	-33.73	-12.48	21.25	KMgCl ₃
KMgCl ₃ ·2H ₂ O	-26.44	-12.48	13.96	KMgCl ₃ ·2H ₂ O
KNaCO ₃ ·6H ₂ O	-12.91	-2.65	10.26	KNaCO ₃ ·6H ₂ O
Lammerite	-0.97	0.58	1.55	Cu ₃ (AsO ₄) ₂
Lansfordite	-6.09	-1.25	4.84	MgCO ₃ ·5H ₂ O
Lawrencite	-23.83	-14.77	9.05	FeCl ₂
Leonite	-10.88	-14.99	-4.11	K ₂ Mg(SO ₄) ₂ ·4H ₂ O
Lime	-23.59	8.98	32.57	CaO
Magnesite	-3.52	-1.25	2.27	MgCO ₃
Magnetite	5.40	15.81	10.42	Fe ₃ O ₄

Malachite	-0.33	5.57	5.90	Cu ₂ CO ₃ (OH) ₂
Manganite	1.76	1.60	-0.16	MnO(OH)
Manganosite	-10.66	7.25	17.92	MnO
Mayenite	-245.23	248.92	494.15	Ca ₁₂ Al ₁₄ O ₃₃
Melanterite	-11.13	-13.53	-2.40	FeSO ₄ ·7H ₂ O
Mercallite	-10.04	-11.48	-1.44	KHSO ₄
Mg	-111.40	11.12	122.52	Mg
Mg(g)	-131.12	11.12	142.25	Mg
Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O	-9.44	-4.25	5.20	Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O
Mg _{1.5} SO ₄ (OH)	-11.46	-2.25	9.21	Mg _{1.5} SO ₄ (OH)
MgCl ₂ :2H ₂ O	-20.21	-7.48	12.73	MgCl ₂ :2H ₂ O
MgCl ₂ :4H ₂ O	-14.78	-7.48	7.30	MgCl ₂ :4H ₂ O
MgCl ₂ :H ₂ O	-23.55	-7.48	16.07	MgCl ₂ :H ₂ O
MgOHCl	-15.65	0.24	15.89	MgOHCl
MgSO ₄	-11.06	-6.24	4.83	MgSO ₄
Mirabilite	-5.37	-6.52	-1.15	Na ₂ SO ₄ :10H ₂ O
Misenite	-66.55	-77.63	-11.08	K ₈ H ₆ (SO ₄) ₇
Mn	-72.52	10.41	82.93	Mn
Mn(OH) ₂ (am)	-8.05	7.25	15.31	Mn(OH) ₂
Mn(OH) ₃	-4.74	1.60	6.34	Mn(OH) ₃
MnCl ₂ :2H ₂ O	-12.19	-8.19	4.00	MnCl ₂ :2H ₂ O
MnCl ₂ :4H ₂ O	-10.94	-8.19	2.75	MnCl ₂ :4H ₂ O
MnCl ₂ :H ₂ O	-13.73	-8.19	5.54	MnCl ₂ :H ₂ O
MnO ₂ (gamma)	4.00	-12.13	-16.13	MnO ₂
MnSO ₄	-9.56	-6.95	2.61	MnSO ₄
Molysite	-29.07	-15.60	13.47	FeCl ₃
Monohydrocalcite	-2.92	-0.24	2.68	CaCO ₃ :H ₂ O
Na	-61.95	5.42	67.37	Na
Na(g)	-75.44	5.42	80.86	Na
Na ₂ CO ₃	-12.70	-1.54	11.16	Na ₂ CO ₃
Na ₂ CO ₃ :7H ₂ O	-11.48	-1.54	9.94	Na ₂ CO ₃ :7H ₂ O
Na ₂ O	-59.74	7.68	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-15.99	-16.88	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-12.37	-18.27	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
NaFeO ₂	-8.47	11.41	19.88	NaFeO ₂
Nahcolite	-5.23	-5.38	-0.14	NaHCO ₃
Nantokite	-10.74	-17.51	-6.77	CuCl
Natron	-11.13	-1.54	9.59	Na ₂ CO ₃ :10H ₂ O
Nesquehonite	-6.54	-1.25	5.29	MgCO ₃ :3H ₂ O
O ₂ (g)	-3.43	-6.32	-2.89	O ₂
Orpiment	-416.41	-495.89	-79.49	As ₂ S ₃
Oxychloride-Mg	-17.63	8.20	25.83	Mg ₂ Cl(OH) ₃ :4H ₂ O
Pentahydrite	-4.85	-6.24	-1.39	MgSO ₄ :5H ₂ O
Periclase	-13.36	7.96	21.33	MgO
Picromerite	-10.55	-14.99	-4.44	K ₂ Mg(SO ₄) ₂ :6H ₂ O
Pirssonite	-13.10	-1.78	11.32	Na ₂ Ca(CO ₃) ₂ :2H ₂ O
Polyhalite	-11.13	-25.44	-14.31	K ₂ MgCa ₂ (SO ₄) ₄ :2H ₂ O
Portlandite	-13.57	8.98	22.55	Ca(OH) ₂
Pyrite	-222.91	-247.61	-24.70	FeS ₂
Pyrolusite	5.53	-12.13	-17.66	MnO ₂
Pyrrhotite	-135.44	-139.18	-3.74	FeS
Realgar	-161.75	-222.03	-60.28	AsS
Rhodochrosite	-1.74	-1.96	-0.22	MnCO ₃
S	-97.90	-143.01	-45.11	S
S ₂ (g)	-209.69	-216.87	-7.19	S ₂
Scacchite	-16.93	-8.19	8.74	MnCl ₂
Siderite	-8.33	-8.54	-0.22	FeCO ₃
Smithsonite	-2.63	-2.18	0.44	ZnCO ₃
SO ₂ (g)	-48.72	-48.55	0.18	SO ₂
Sphalerite	-121.34	-132.81	-11.47	ZnS
Spinel	-9.47	28.14	37.61	Al ₂ MgO ₄
Starkeyite	-5.24	-6.24	-1.00	MgSO ₄ :4H ₂ O
Sylvite	-5.83	-5.00	0.83	KCl
Syngenite	-6.38	-13.98	-7.60	K ₂ Ca(SO ₄) ₂ :H ₂ O
Tachyhydrite	-38.58	-21.44	17.14	Mg ₂ CaCl ₆ :12H ₂ O
Tenorite	-0.25	7.39	7.65	CuO
Thenardite	-6.16	-6.52	-0.36	Na ₂ SO ₄

Thermonatrite	-12.47	-1.54	10.94	Na2CO3:H2O
Todorokite	23.90	-21.92	-45.82	Mn7O12:3H2O
Troilite	-135.33	-139.18	-3.84	FeS
Trona-K	-20.74	-9.15	11.59	K2NaH(CO3)2:2H2O
Wurtzite	-123.65	-132.81	-9.17	ZnS
Wustite	-11.04	1.37	12.40	Fe.9470
Zincite	-4.16	7.03	11.20	ZnO
Zn	-58.59	10.19	68.79	Zn
Zn(ClO4)2:6H2O	-70.77	-65.13	5.63	Zn(ClO4)2:6H2O
Zn(g)	-75.21	10.19	85.41	Zn
Zn(OH)2(beta)	-4.90	7.03	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-4.63	7.03	11.66	Zn(OH)2
Zn(OH)2(gamma)	-4.85	7.03	11.88	Zn(OH)2
Zn2(OH)3Cl	-8.95	6.35	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-7.71	-0.13	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-9.81	-0.50	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-26.39	-7.30	19.09	Zn3O(SO4)2
ZnCl2	-15.49	-8.41	7.08	ZnCl2
ZnCO3:H2O	-2.32	-2.18	0.14	ZnCO3:H2O
ZnSO4	-10.70	-7.17	3.53	ZnSO4
ZnSO4:6H2O	-5.47	-7.17	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.29	-7.17	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.62	-7.17	-0.55	ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
