
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      1
SELECTED_OUTPUT
file          DAM_AS2
ph            true
percent_error true
totals        Al  As  Cu  Fe  Mg  Mn  Zn
              S(6)

```

Beginning of initial solution calculations.

Initial solution 1. Flujo 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
Tachyhydrite	-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
1.000e+000 Solution 3 AS2

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

Elements	Molality	Moles
Al	4.009e-004	8.019e-004
As	2.656e-005	5.311e-005
C	1.262e-003	2.525e-003
Ca	4.538e-003	9.077e-003
Cl	1.017e-002	2.033e-002
Cu	3.224e-004	6.448e-004
Fe	3.722e-004	7.445e-004
K	9.703e-004	1.941e-003
Mg	5.587e-004	1.117e-003
Mn	2.222e-004	4.444e-004
Na	9.017e-003	1.803e-002
S	8.818e-003	1.764e-002
Zn	9.306e-005	1.861e-004

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

pH = 4.430 Charge balance
 pe = 15.565 Adjusted to redox equilibrium
 Activity of water = 0.999
 Ionic strength = 3.391e-002
 Mass of water (kg) = 2.000e+000
 Total alkalinity (eq/kg) = -6.875e-005
 Total CO2 (mol/kg) = 1.262e-003
 Temperature (deg C) = 25.000
 Electrical balance (eq) = -9.458e-003
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -10.73
 Iterations = 24
 Total H = 2.221058e+002
 Total O = 1.111293e+002

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	4.262e-005	3.716e-005	-4.370	-4.430	-0.060
OH-	3.089e-010	2.591e-010	-9.510	-9.587	-0.076
H2O	5.553e+001	9.994e-001	1.744	-0.000	0.000
Al	4.009e-004				
AlSO4+	1.777e-004	1.497e-004	-3.750	-3.825	-0.074
Al+3	1.485e-004	4.213e-005	-3.828	-4.375	-0.547
Al(SO4)2-	4.791e-005	4.037e-005	-4.320	-4.394	-0.074
AlOH+2	2.502e-005	1.269e-005	-4.602	-4.896	-0.295
Al(OH)2+	9.408e-007	7.927e-007	-6.026	-6.101	-0.074
Al2(OH)2+4	3.525e-007	2.620e-008	-6.453	-7.582	-1.129
HALO2	3.104e-008	3.104e-008	-7.508	-7.508	0.000
Al3(OH)4+5	2.739e-008	5.153e-010	-7.562	-9.288	-1.726
AlO2-	3.396e-010	2.862e-010	-9.469	-9.543	-0.074
Al13O4(OH)24+7	3.333e-011	1.379e-014	-10.477	-13.860	-3.383
NaAlO2	4.049e-013	4.049e-013	-12.393	-12.393	0.000
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-152.253	-152.253	0.000
As(3)	8.614e-028				
HAsO2	4.597e-028	4.597e-028	-27.338	-27.338	0.000
As(OH)3	4.017e-028	4.017e-028	-27.396	-27.396	0.000
H2AsO3-	7.846e-033	6.611e-033	-32.105	-32.180	-0.074
AsO2-	7.505e-033	6.323e-033	-32.125	-32.199	-0.074
AsO2OH-2	3.483e-039	1.738e-039	-38.458	-38.760	-0.302
HAsS2	0.000e+000	0.000e+000	-281.266	-281.266	0.000
As(5)	2.656e-005				
H2AsO4-	2.621e-005	2.209e-005	-4.581	-4.656	-0.074
HAsO4-2	1.977e-007	9.865e-008	-6.704	-7.006	-0.302
H3AsO4	1.446e-007	1.446e-007	-6.840	-6.840	0.000
AsO4-3	3.266e-014	6.810e-015	-13.486	-14.167	-0.681
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-254.902	-254.902	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-226.004	-226.004	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-141.326	-141.326	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-47.932	-47.932	0.000
C(4)	1.262e-003				
CO2	1.245e-003	1.255e-003	-2.905	-2.901	0.004
HCO3-	1.727e-005	1.455e-005	-4.763	-4.837	-0.074
CaHCO3+	3.881e-007	3.270e-007	-6.411	-6.486	-0.074
NaHCO3	1.543e-007	1.543e-007	-6.812	-6.812	0.000
MgHCO3+	4.114e-008	3.466e-008	-7.386	-7.460	-0.074
FeCO3+	2.009e-008	1.693e-008	-7.697	-7.771	-0.074
CuCO3	1.972e-008	1.972e-008	-7.705	-7.705	0.000

ZnHCO3+	1.575e-008	1.327e-008	-7.803	-7.877	-0.074
MnHCO3+	1.058e-008	8.912e-009	-7.976	-8.050	-0.074
CaCO3	7.634e-011	7.634e-011	-10.117	-10.117	0.000
MnCO3	4.892e-011	4.892e-011	-10.311	-10.311	0.000
CO3-2	3.423e-011	1.737e-011	-10.466	-10.760	-0.295
ZnCO3	5.160e-012	5.160e-012	-11.287	-11.287	0.000
FeHCO3+	4.344e-012	3.660e-012	-11.362	-11.437	-0.074
MgCO3	3.769e-012	3.769e-012	-11.424	-11.424	0.000
NaCO3-	5.350e-013	4.507e-013	-12.272	-12.346	-0.074
Cu(CO3)2-2	1.223e-015	6.102e-016	-14.913	-15.215	-0.302
FeCO3	4.727e-016	4.727e-016	-15.325	-15.325	0.000
CuCO3(OH)2-2	2.430e-019	1.213e-019	-18.614	-18.916	-0.302
Ca	4.538e-003				
Ca+2	3.572e-003	1.896e-003	-2.447	-2.722	-0.275
CaSO4	9.621e-004	9.621e-004	-3.017	-3.017	0.000
CaCl+	4.041e-006	3.404e-006	-5.394	-5.468	-0.074
CaHCO3+	3.881e-007	3.270e-007	-6.411	-6.486	-0.074
CaCl2	3.391e-008	3.391e-008	-7.470	-7.470	0.000
CaCO3	7.634e-011	7.634e-011	-10.117	-10.117	0.000
CaOH+	8.551e-012	7.204e-012	-11.068	-11.142	-0.074
Cl(-1)	1.017e-002				
Cl-	1.014e-002	8.469e-003	-1.994	-2.072	-0.078
NaCl	1.104e-005	1.104e-005	-4.957	-4.957	0.000
CaCl+	4.041e-006	3.404e-006	-5.394	-5.468	-0.074
CuCl+	3.273e-006	2.758e-006	-5.485	-5.559	-0.074
MnCl+	1.722e-006	1.451e-006	-5.764	-5.838	-0.074
MgCl+	1.610e-006	1.356e-006	-5.793	-5.868	-0.074
ZnCl+	5.975e-007	5.034e-007	-6.224	-6.298	-0.074
KCl	2.242e-007	2.242e-007	-6.649	-6.649	0.000
HCl	7.069e-008	7.069e-008	-7.151	-7.151	0.000
CaCl2	3.391e-008	3.391e-008	-7.470	-7.470	0.000
CuCl2	1.230e-008	1.230e-008	-7.910	-7.910	0.000
ZnCl2	4.980e-009	4.980e-009	-8.303	-8.303	0.000
FeCl2+	1.938e-009	1.633e-009	-8.713	-8.787	-0.074
FeCl+2	4.693e-010	2.381e-010	-9.329	-9.623	-0.295
Zn(OH)Cl	2.315e-010	2.315e-010	-9.635	-9.635	0.000
ZnCl3-	2.765e-011	2.329e-011	-10.558	-10.633	-0.074
MnCl3-	2.699e-011	2.274e-011	-10.569	-10.643	-0.074
FeCl+	3.511e-012	2.958e-012	-11.455	-11.529	-0.074
ZnCl4-2	2.997e-012	1.495e-012	-11.523	-11.825	-0.302
FeCl4-	1.671e-016	1.408e-016	-15.777	-15.851	-0.074
FeCl2	1.344e-016	1.344e-016	-15.872	-15.872	0.000
CuCl2-	1.001e-016	8.436e-017	-15.999	-16.074	-0.074
CuCl4-2	3.318e-017	1.656e-017	-16.479	-16.781	-0.302
CuCl3-2	9.194e-018	4.589e-018	-17.036	-17.338	-0.302
FeCl4-2	5.583e-020	2.786e-020	-19.253	-19.555	-0.302
Cl(1)	8.877e-018				
HClO	8.869e-018	8.869e-018	-17.052	-17.052	0.000
ClO-	7.639e-021	6.436e-021	-20.117	-20.191	-0.074
Cl(3)	7.741e-032				
ClO2-	7.399e-032	6.234e-032	-31.131	-31.205	-0.074
HClO2	3.425e-033	3.425e-033	-32.465	-32.465	0.000
Cl(5)	5.122e-029				
ClO3-	5.122e-029	4.296e-029	-28.291	-28.367	-0.076
Cl(7)	1.763e-030				
ClO4-	1.762e-030	1.478e-030	-29.754	-29.830	-0.076
ZnClO4+	1.174e-033	9.891e-034	-32.930	-33.005	-0.074
Cu(1)	1.304e-016				
CuCl2-	1.001e-016	8.436e-017	-15.999	-16.074	-0.074
Cu+	2.107e-017	1.775e-017	-16.676	-16.751	-0.074
CuCl3-2	9.194e-018	4.589e-018	-17.036	-17.338	-0.302
Cu(2)	3.224e-004				
Cu+2	2.242e-004	1.190e-004	-3.649	-3.924	-0.275
CuSO4	9.472e-005	9.472e-005	-4.024	-4.024	0.000
CuCl+	3.273e-006	2.758e-006	-5.485	-5.559	-0.074
CuOH+	1.960e-007	1.651e-007	-6.708	-6.782	-0.074
CuCO3	1.972e-008	1.972e-008	-7.705	-7.705	0.000

CuCl2	1.230e-008	1.230e-008	-7.910	-7.910	0.000
Cu(CO3)2-2	1.223e-015	6.102e-016	-14.913	-15.215	-0.302
CuCl4-2	3.318e-017	1.656e-017	-16.479	-16.781	-0.302
CuCO3(OH)2-2	2.430e-019	1.213e-019	-18.614	-18.916	-0.302
CuO2-2	4.436e-026	2.214e-026	-25.353	-25.655	-0.302
Fe(2)	1.175e-009				
Fe+2	9.028e-010	4.794e-010	-9.044	-9.319	-0.275
FeSO4	2.639e-010	2.639e-010	-9.579	-9.579	0.000
FeHCO3+	4.344e-012	3.660e-012	-11.362	-11.437	-0.074
FeCl+	3.511e-012	2.958e-012	-11.455	-11.529	-0.074
FeOH+	4.839e-015	4.077e-015	-14.315	-14.390	-0.074
FeCO3	4.727e-016	4.727e-016	-15.325	-15.325	0.000
FeCl2	1.344e-016	1.344e-016	-15.872	-15.872	0.000
FeCl4-2	5.583e-020	2.786e-020	-19.253	-19.555	-0.302
Fe(OH)2	8.709e-022	8.709e-022	-21.060	-21.060	0.000
Fe(OH)3-	1.107e-027	9.324e-028	-26.956	-27.030	-0.074
Fe(OH)4-2	5.025e-038	2.508e-038	-37.299	-37.601	-0.302
Fe(3)	3.722e-004				
Fe(OH)2+	3.097e-004	2.609e-004	-3.509	-3.583	-0.074
FeOH+2	5.775e-005	2.930e-005	-4.238	-4.533	-0.295
Fe(OH)3	3.282e-006	3.282e-006	-5.484	-5.484	0.000
Fe+3	5.949e-007	1.687e-007	-6.226	-6.773	-0.547
Fe2(OH)2+4	3.109e-007	2.311e-008	-6.507	-7.636	-1.129
FeSO4+	6.730e-008	5.670e-008	-7.172	-7.246	-0.074
Fe3(OH)4+5	6.696e-008	1.260e-009	-7.174	-8.900	-1.726
FeCO3+	2.009e-008	1.693e-008	-7.697	-7.771	-0.074
Fe(SO4)2-	3.952e-009	3.329e-009	-8.403	-8.478	-0.074
FeCl2+	1.938e-009	1.633e-009	-8.713	-8.787	-0.074
FeCl+2	4.693e-010	2.381e-010	-9.329	-9.623	-0.295
Fe(OH)4-	2.632e-011	2.217e-011	-10.580	-10.654	-0.074
FeCl4-	1.671e-016	1.408e-016	-15.777	-15.851	-0.074
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-43.094	-43.090	0.004
K	9.703e-004				
K+	9.439e-004	7.882e-004	-3.025	-3.103	-0.078
KSO4-	2.622e-005	2.209e-005	-4.581	-4.656	-0.074
KCl	2.242e-007	2.242e-007	-6.649	-6.649	0.000
KHSO4	7.244e-010	7.244e-010	-9.140	-9.140	0.000
KOH	7.350e-014	7.350e-014	-13.134	-13.134	0.000
Mg	5.587e-004				
Mg+2	3.668e-004	2.051e-004	-3.436	-3.688	-0.252
MgSO4	1.903e-004	1.903e-004	-3.721	-3.721	0.000
MgCl+	1.610e-006	1.356e-006	-5.793	-5.868	-0.074
MgHCO3+	4.114e-008	3.466e-008	-7.386	-7.460	-0.074
MgCO3	3.769e-012	3.769e-012	-11.424	-11.424	0.000
Mg4(OH)4+4	2.217e-036	1.647e-037	-35.654	-36.783	-1.129
Mn(2)	2.222e-004				
Mn+2	1.515e-004	8.045e-005	-3.820	-4.094	-0.275
MnSO4	6.894e-005	6.894e-005	-4.162	-4.162	0.000
MnCl+	1.722e-006	1.451e-006	-5.764	-5.838	-0.074
MnHCO3+	1.058e-008	8.912e-009	-7.976	-8.050	-0.074
MnOH+	6.601e-011	5.562e-011	-10.180	-10.255	-0.074
MnCO3	4.892e-011	4.892e-011	-10.311	-10.311	0.000
MnCl3-	2.699e-011	2.274e-011	-10.569	-10.643	-0.074
Mn2OH+3	2.138e-014	4.795e-015	-13.670	-14.319	-0.649
Mn(OH)2	3.672e-018	3.672e-018	-17.435	-17.435	0.000
Mn2(OH)3+	1.881e-019	1.585e-019	-18.726	-18.800	-0.074
Mn(OH)3-	1.099e-025	9.262e-026	-24.959	-25.033	-0.074
Mn(OH)4-2	4.227e-035	2.109e-035	-34.374	-34.676	-0.302
Mn(3)	3.513e-014				
Mn+3	3.513e-014	7.879e-015	-13.454	-14.104	-0.649
Mn(6)	2.871e-025				
MnO4-2	2.871e-025	1.433e-025	-24.542	-24.844	-0.302
Mn(7)	2.762e-019				
MnO4-	2.762e-019	2.317e-019	-18.559	-18.635	-0.076
Na	9.017e-003				
Na+	8.804e-003	7.417e-003	-2.055	-2.130	-0.074

NaSO4-	2.020e-004	1.702e-004	-3.695	-3.769	-0.074
NaCl	1.104e-005	1.104e-005	-4.957	-4.957	0.000
NaHCO3	1.543e-007	1.543e-007	-6.812	-6.812	0.000
NaCO3-	5.350e-013	4.507e-013	-12.272	-12.346	-0.074
NaAlO2	4.049e-013	4.049e-013	-12.393	-12.393	0.000
NaOH	3.316e-013	3.316e-013	-12.479	-12.479	0.000
O(0)	1.909e-006				
O2	9.546e-007	9.625e-007	-6.020	-6.017	0.004
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-130.559	-130.559	0.000
HS-	0.000e+000	0.000e+000	-133.062	-133.139	-0.076
S-2	0.000e+000	0.000e+000	-141.347	-141.635	-0.288
S2-2	0.000e+000	0.000e+000	-235.726	-236.028	-0.302
HAsS2	0.000e+000	0.000e+000	-281.266	-281.266	0.000
S3-2	0.000e+000	0.000e+000	-330.160	-330.462	-0.302
S4-2	0.000e+000	0.000e+000	-424.821	-425.123	-0.302
S5-2	0.000e+000	0.000e+000	-519.699	-520.001	-0.302
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-134.917	-135.219	-0.302
HS2O3-	0.000e+000	0.000e+000	-138.560	-138.635	-0.074
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-122.867	-123.155	-0.288
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-43.193	-43.267	-0.074
H2SO3	0.000e+000	0.000e+000	-45.715	-45.715	0.000
SO3-2	0.000e+000	0.000e+000	-45.774	-46.069	-0.295
SO2	0.000e+000	0.000e+000	-45.815	-45.815	0.000
S2O6-2	0.000e+000	0.000e+000	-61.837	-62.139	-0.302
S3O6-2	0.000e+000	0.000e+000	-158.754	-159.055	-0.302
S4O6-2	0.000e+000	0.000e+000	-239.765	-240.067	-0.302
S5O6-2	0.000e+000	0.000e+000	-349.656	-349.958	-0.302
S(5)	0.000e+000				
S2O5-2	0.000e+000	0.000e+000	-91.062	-91.364	-0.302
S(6)	8.818e-003				
SO4-2	6.959e-003	3.473e-003	-2.157	-2.459	-0.302
CaSO4	9.621e-004	9.621e-004	-3.017	-3.017	0.000
NaSO4-	2.020e-004	1.702e-004	-3.695	-3.769	-0.074
MgSO4	1.903e-004	1.903e-004	-3.721	-3.721	0.000
AlSO4+	1.777e-004	1.497e-004	-3.750	-3.825	-0.074
CuSO4	9.472e-005	9.472e-005	-4.024	-4.024	0.000
MnSO4	6.894e-005	6.894e-005	-4.162	-4.162	0.000
Al(SO4)2-	4.791e-005	4.037e-005	-4.320	-4.394	-0.074
KSO4-	2.622e-005	2.209e-005	-4.581	-4.656	-0.074
ZnSO4	2.582e-005	2.582e-005	-4.588	-4.588	0.000
HSO4-	1.547e-005	1.304e-005	-4.810	-4.885	-0.074
FeSO4+	6.730e-008	5.670e-008	-7.172	-7.246	-0.074
Fe(SO4)2-	3.952e-009	3.329e-009	-8.403	-8.478	-0.074
KHSO4	7.244e-010	7.244e-010	-9.140	-9.140	0.000
FeSO4	2.639e-010	2.639e-010	-9.579	-9.579	0.000
H2SO4	4.571e-013	4.571e-013	-12.340	-12.340	0.000
S(7)	2.298e-039				
S2O8-2	1.149e-039	5.735e-040	-38.940	-39.242	-0.302
S(8)	8.247e-028				
HSO5-	8.247e-028	6.948e-028	-27.084	-27.158	-0.074
Zn	9.306e-005				
Zn+2	6.662e-005	3.538e-005	-4.176	-4.451	-0.275
ZnSO4	2.582e-005	2.582e-005	-4.588	-4.588	0.000
ZnCl+	5.975e-007	5.034e-007	-6.224	-6.298	-0.074
ZnHCO3+	1.575e-008	1.327e-008	-7.803	-7.877	-0.074
ZnCl2	4.980e-009	4.980e-009	-8.303	-8.303	0.000
ZnOH+	1.238e-009	1.043e-009	-8.907	-8.982	-0.074
Zn(OH)Cl	2.315e-010	2.315e-010	-9.635	-9.635	0.000
ZnCl3-	2.765e-011	2.329e-011	-10.558	-10.633	-0.074
ZnCO3	5.160e-012	5.160e-012	-11.287	-11.287	0.000
ZnCl4-2	2.997e-012	1.495e-012	-11.523	-11.825	-0.302
Zn(OH)2	1.202e-013	1.202e-013	-12.920	-12.920	0.000
Zn(OH)3-	1.189e-020	1.002e-020	-19.925	-19.999	-0.074

Zn(OH)4-2	9.204e-029	4.593e-029	-28.036	-28.338	-0.302
ZnClO4+	1.174e-033	9.891e-034	-32.930	-33.005	-0.074

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

Phase	SI	log IAP	log KT	
Al	-136.49	13.43	149.91	Al
Al(g)	-187.19	13.43	200.62	Al
Al2(SO4)3	-35.03	-16.13	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-17.69	-16.13	1.56	Al2(SO4)3:6H2O
Alabandite	-132.38	-132.80	-0.42	MnS
Alum-K	-7.43	-12.40	-4.97	KAl(SO4)2:12H2O
Alunite	5.90	5.43	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.83	-5.18	-4.35	CaSO4
Antarcticite	-10.96	-6.87	4.09	CaCl2:6H2O
Antlerite	-5.24	3.49	8.73	Cu3(SO4)(OH)4
Aphthitalite	-12.47	-16.36	-3.89	NaK3(SO4)2
Aragonite	-5.10	-3.13	1.97	CaCO3
Arcanite	-6.82	-8.67	-1.84	K2SO4
Arsenolite	-53.38	-73.22	-19.84	As2O3
Arsenopyrite	-218.01	-232.46	-14.45	FeAsS
Artinite	-18.55	1.08	19.63	Mg2CO3(OH)2:3H2O
As	-74.78	-32.10	42.68	As
As2O5	-20.31	-18.17	2.14	As2O5
As4O6(cubi)	-106.61	-146.44	-39.82	As4O6
As4O6(mono)	-106.39	-146.44	-40.05	As4O6
Atacamite	-7.53	6.74	14.26	Cu4Cl2(OH)6
Azurite	-12.84	-3.73	9.12	Cu3(CO3)2(OH)2
Bassanite	-1.48	-5.18	-3.71	CaSO4:0.5H2O
Birnessite	8.26	-77.29	-85.55	Mn8O14:5H2O
Bischofite	-12.23	-7.83	4.39	MgCl2:6H2O
Bixbyite	-0.66	-1.63	-0.96	Mn2O3
Bloedite	-10.39	-12.87	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	1.36	8.91	7.55	AlO2H
Bornite	-492.55	-595.08	-102.53	Cu5FeS4
Brochantite	-7.00	8.42	15.42	Cu4(SO4)(OH)6
Brucite	-11.11	5.17	16.28	Mg(OH)2
Burkeite	-27.59	-18.10	9.49	Na6CO3(SO4)2
C	-67.40	-3.25	64.15	C
C(g)	-185.02	-3.25	181.77	C
Ca	-130.69	9.15	139.83	Ca
Ca(g)	-155.93	9.15	165.07	Ca
Ca2Al2O5:8H2O	-29.47	30.10	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-27.02	-0.73	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-17.56	0.24	17.80	Ca3(AsO4)2
Ca3Al2O6	-76.79	36.24	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-85.07	55.41	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-64.88	42.37	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-61.31	42.37	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-56.79	11.54	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-22.94	23.97	46.91	CaAl2O4
CaAl2O4:10H2O	-14.03	23.96	37.99	CaAl2O4:10H2O
CaAl4O7	-26.80	41.79	68.59	CaAl4O7
Calcite	-4.95	-3.13	1.82	CaCO3
Carnallite	-17.28	-13.01	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.65	-5.18	-3.54	CaSO4:0.5H2O
CH4(g)	-138.48	-141.33	-2.84	CH4
Chalcanthite	-3.76	-6.38	-2.63	CuSO4:5H2O
Chalcocite	-127.47	-162.21	-34.74	Cu2S
Chalcocyanite	-9.30	-6.38	2.91	CuSO4
Chalcopyrite	-238.06	-270.66	-32.60	CuFeS2
Chloromagnesite	-29.65	-7.83	21.82	MgCl2
Cl2(g)	-19.01	-16.01	2.99	Cl2
Claudetite	-53.42	-73.22	-19.80	As2O3
CO(g)	-44.94	-47.93	-3.00	CO
CO2(g)	-1.44	-9.27	-7.83	CO2

Corundum	-0.46	17.83	18.29	Al2O3
Covellite	-109.77	-132.63	-22.86	CuS
Cu	-23.55	7.94	31.50	Cu
Cu(g)	-75.71	7.94	83.66	Cu
CuCl2	-11.79	-8.07	3.72	CuCl2
Cuprite	-22.74	-24.64	-1.91	Cu2O
Dawsonite	-2.39	1.95	4.34	NaAlCO3(OH)2
Delafoosite	0.63	-5.80	-6.44	CuFeO2
Diaspore	1.77	8.91	7.15	AlHO2
Dolomite	-9.70	-7.22	2.47	CaMg(CO3)2
Dolomite-dis	-11.24	-7.22	4.01	CaMg(CO3)2
Dolomite-ord	-9.69	-7.22	2.46	CaMg(CO3)2
Epsomite	-4.19	-6.15	-1.96	MgSO4:7H2O
Ettringite	-41.78	20.69	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-56.47	2.55	59.02	Fe
Fe(OH)2	-14.35	-0.46	13.89	Fe(OH)2
Fe(OH)3	0.88	6.52	5.64	Fe(OH)3
Fe2(SO4)3	-23.97	-20.92	3.05	Fe2(SO4)3
FeO	-13.98	-0.46	13.52	FeO
Ferrite-Ca	-2.32	19.17	21.50	CaFe2O4
Ferrite-Cu	7.69	17.97	10.28	CuFe2O4
Ferrite-Dicalcium	-31.49	25.31	56.80	Ca2Fe2O5
Ferrite-Mg	-2.82	18.20	21.02	MgFe2O4
Ferrite-Zn	5.74	17.44	11.70	ZnFe2O4
FeSO4	-14.39	-11.78	2.61	FeSO4
Gaylussite	-18.96	-7.80	11.16	CaNa2(CO3)2:5H2O
Gibbsite	1.17	8.91	7.74	Al(OH)3
Glauberite	-6.43	-11.90	-5.47	Na2Ca(SO4)2
Goethite	5.99	6.52	0.53	FeOOH
Gypsum	-0.65	-5.18	-4.53	CaSO4:2H2O
H2(g)	-39.99	-43.09	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-129.58	-137.57	-7.99	H2S
Halite	-5.76	-4.20	1.56	NaCl
Hausmannite	-7.01	3.14	10.14	Mn3O4
HCl(g)	-12.80	-6.50	6.30	HCl
Hematite	12.96	13.03	0.08	Fe2O3
Hercynite	-11.43	17.37	28.80	FeAl2O4
Hexahydrite	-4.42	-6.15	-1.73	MgSO4:6H2O
Huntite	-25.63	-15.42	10.22	CaMg3(CO3)4
Hydromagnesite	-41.95	-11.21	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-18.61	-6.87	11.75	CaCl2
Hydrozincite	-26.80	3.51	30.31	Zn5(OH)6(CO3)2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	7.65	-1.76	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	4.66	-0.79	-5.45	NaFe3(SO4)2(OH)6
K	-68.15	2.83	70.98	K
K(g)	-78.75	2.83	81.58	K
K2CO3:1.5H2O	-19.99	-6.61	13.38	K2CO3:1.5H2O
K2O	-81.38	2.65	84.04	K2O
K3H(SO4)2	-15.04	-18.66	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-72.70	-44.99	27.71	K8H4(CO3)6:3H2O
Kainite	-11.01	-11.32	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-15.67	-12.40	3.27	KAl(SO4)2
Kalinite	-8.22	-7.94	0.28	KHCO3
Katoite	-42.70	36.24	78.94	Ca3Al2H12O12
Kieserite	-5.88	-6.15	-0.27	MgSO4:H2O
KMgCl3	-34.25	-13.01	21.25	KMgCl3
KMgCl3:2H2O	-26.97	-13.01	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-15.90	-5.64	10.26	KNaCO3:6H2O
Lammerite	-4.92	-3.37	1.55	Cu3(AsO4)2
Lansfordite	-8.94	-4.10	4.84	MgCO3:5H2O
Lawrencite	-22.52	-13.46	9.05	FeCl2
Leonite	-10.70	-14.81	-4.11	K2Mg(SO4)2:4H2O
Lime	-26.43	6.14	32.57	CaO
Magnesite	-6.37	-4.10	2.27	MgCO3
Magnetite	2.16	12.57	10.42	Fe3O4

Malachite	-5.30	0.60	5.90	Cu ₂ CO ₃ (OH) ₂
Manganite	-0.65	-0.81	-0.16	MnO(OH)
Manganosite	-13.15	4.77	17.92	MnO
Mayenite	-295.71	198.45	494.15	Ca ₁₂ Al ₁₄ O ₃₃
Melanterite	-9.38	-11.78	-2.40	FeSO ₄ ·7H ₂ O
Mercallite	-8.55	-9.99	-1.44	KHSO ₄
Mg	-114.34	8.18	122.52	Mg
Mg(g)	-134.07	8.18	142.25	Mg
Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O	-10.05	-4.85	5.20	Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O
Mg _{1.5} SO ₄ (OH)	-12.77	-3.56	9.21	Mg _{1.5} SO ₄ (OH)
MgCl ₂ :2H ₂ O	-20.56	-7.83	12.73	MgCl ₂ :2H ₂ O
MgCl ₂ :4H ₂ O	-15.13	-7.83	7.30	MgCl ₂ :4H ₂ O
MgCl ₂ :H ₂ O	-23.90	-7.83	16.07	MgCl ₂ :H ₂ O
MgOHCl	-17.22	-1.33	15.89	MgOHCl
MgSO ₄	-10.98	-6.15	4.83	MgSO ₄
Mirabilite	-5.57	-6.72	-1.15	Na ₂ SO ₄ :10H ₂ O
Misenite	-57.55	-68.62	-11.08	K ₈ H ₆ (SO ₄) ₇
Mn	-75.16	7.77	82.93	Mn
Mn(OH) ₂ (am)	-10.54	4.76	15.31	Mn(OH) ₂
Mn(OH) ₃	-7.16	-0.81	6.34	Mn(OH) ₃
MnCl ₂ :2H ₂ O	-12.24	-8.24	4.00	MnCl ₂ :2H ₂ O
MnCl ₂ :4H ₂ O	-10.99	-8.24	2.75	MnCl ₂ :4H ₂ O
MnCl ₂ :H ₂ O	-13.78	-8.24	5.54	MnCl ₂ :H ₂ O
MnO ₂ (gamma)	1.66	-14.47	-16.13	MnO ₂
MnSO ₄	-9.16	-6.55	2.61	MnSO ₄
Molysite	-26.46	-12.99	13.47	FeCl ₃
Monohydrocalcite	-5.81	-3.13	2.68	CaCO ₃ :H ₂ O
Na	-63.57	3.80	67.37	Na
Na(g)	-77.05	3.80	80.86	Na
Na ₂ CO ₃	-15.83	-4.67	11.16	Na ₂ CO ₃
Na ₂ CO ₃ :7H ₂ O	-14.61	-4.67	9.94	Na ₂ CO ₃ :7H ₂ O
Na ₂ O	-62.82	4.60	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-14.85	-15.74	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-12.73	-18.62	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
NaFeO ₂	-11.07	8.82	19.88	NaFeO ₂
Nahcolite	-6.83	-6.97	-0.14	NaHCO ₃
Nantokite	-12.06	-18.82	-6.77	CuCl
Natron	-14.26	-4.67	9.59	Na ₂ CO ₃ :10H ₂ O
Nesquehonite	-9.38	-4.10	5.29	MgCO ₃ :3H ₂ O
O ₂ (g)	-3.12	-6.02	-2.89	O ₂
Orpiment	-406.44	-485.92	-79.49	As ₂ S ₃
Oxychloride-Mg	-21.99	3.84	25.83	Mg ₂ Cl(OH) ₃ :4H ₂ O
Pentahydrite	-4.76	-6.15	-1.39	MgSO ₄ :5H ₂ O
Periclase	-16.15	5.17	21.33	MgO
Picromerite	-10.38	-14.81	-4.44	K ₂ Mg(SO ₄) ₂ :6H ₂ O
Pirssonite	-19.12	-7.80	11.32	Na ₂ Ca(CO ₃) ₂ :2H ₂ O
Polyhalite	-10.86	-25.18	-14.31	K ₂ MgCa ₂ (SO ₄) ₄ :2H ₂ O
Portlandite	-16.41	6.14	22.55	Ca(OH) ₂
Pyrite	-219.33	-244.03	-24.70	FeS ₂
Pyrolusite	3.19	-14.47	-17.66	MnO ₂
Pyrrhotite	-134.29	-138.03	-3.74	FeS
Realgar	-157.98	-218.26	-60.28	AsS
Rhodochrosite	-4.28	-4.50	-0.22	MnCO ₃
S	-95.47	-140.58	-45.11	S
S ₂ (g)	-204.82	-212.01	-7.19	S ₂
Scacchite	-16.98	-8.24	8.74	MnCl ₂
Siderite	-9.51	-9.73	-0.22	FeCO ₃
Smithsonite	-5.30	-4.86	0.44	ZnCO ₃
SO ₂ (g)	-45.99	-45.82	0.18	SO ₂
Sphalerite	-121.69	-133.16	-11.47	ZnS
Spinel	-14.61	23.00	37.61	Al ₂ MgO ₄
Starkeyite	-5.15	-6.15	-1.00	MgSO ₄ :4H ₂ O
Sylvite	-6.00	-5.18	0.83	KCl
Syngenite	-6.25	-13.85	-7.60	K ₂ Ca(SO ₄) ₂ :H ₂ O
Tachyhydrite	-39.68	-22.53	17.14	Mg ₂ CaCl ₆ :12H ₂ O
Tenorite	-2.71	4.94	7.65	CuO
Thenardite	-6.36	-6.72	-0.36	Na ₂ SO ₄

Thermonatrite	-15.60	-4.67	10.94	Na2CO3:H2O
Todorokite	7.23	-38.59	-45.82	Mn7O12:3H2O
Troilite	-134.18	-138.03	-3.84	FeS
Trona-K	-25.17	-13.58	11.59	K2NaH(CO3)2:2H2O
Wurtzite	-123.99	-133.16	-9.17	ZnS
Wustite	-12.10	0.30	12.40	Fe.947O
Zincite	-6.79	4.41	11.20	ZnO
Zn	-61.37	7.42	68.79	Zn
Zn(ClO4)2:6H2O	-69.75	-64.11	5.63	Zn(ClO4)2:6H2O
Zn(g)	-77.99	7.42	85.41	Zn
Zn(OH)2(beta)	-7.52	4.41	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-7.25	4.41	11.66	Zn(OH)2
Zn(OH)2(gamma)	-7.48	4.41	11.88	Zn(OH)2
Zn2(OH)3Cl	-12.98	2.31	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-10.08	-2.50	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-14.26	-4.95	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-28.50	-9.41	19.09	Zn3O(SO4)2
ZnCl2	-15.67	-8.60	7.08	ZnCl2
ZnCO3:H2O	-5.00	-4.86	0.14	ZnCO3:H2O
ZnSO4	-10.44	-6.91	3.53	ZnSO4
ZnSO4:6H2O	-5.21	-6.91	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.03	-6.91	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.36	-6.91	-0.55	ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
