
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 4 AS3
temp 25
units mg/l
pe 10
pH 7.74
Cl 24.2
S(6) 243.00
Al 0.00
As 0.0966
Ca 86.82
Cu 0.113
Fe 0.00
K 3.07
Mg 16.17
Mn 0.181
Na 43.01
Zn 0.195
C(4) 115.9
MIX 4
1 1

```

4      3
SELECTED_OUTPUT
file          DAM_AGUASUP
ph            true
percent_error true
totals        Al As Cu Fe Mg Mn Zn
              S(6)

```

Beginning of initial solution calculations.

Initial solution 1. Flujo 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 4. AS3

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

Elements	Molality	Moles
As	1.290e-006	1.290e-006
C(4)	1.901e-003	1.901e-003

Ca	2.167e-003	2.167e-003
Cl	6.830e-004	6.830e-004
Cu	1.779e-006	1.779e-006
K	7.856e-005	7.856e-005
Mg	6.656e-004	6.656e-004
Mn	3.296e-006	3.296e-006
Na	1.872e-003	1.872e-003
S(6)	2.531e-003	2.531e-003
Zn	2.984e-006	2.984e-006

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

pH	=	7.740
pe	=	10.000
Activity of water	=	1.000
Ionic strength	=	1.132e-002
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	1.857e-003
Total CO2 (mol/kg)	=	1.901e-003
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	2.892e-005
Percent error, 100*(Cat- An)/(Cat+ An)	=	0.21
Iterations	=	4
Total H	=	1.110525e+002
Total O	=	5.554109e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	5.913e-007	5.294e-007	-6.228	-6.276	-0.048
H+	1.999e-008	1.820e-008	-7.699	-7.740	-0.041
H2O	5.553e+001	9.998e-001	1.744	-0.000	0.000
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-139.943	-139.943	0.000
As(3)	5.393e-029				
HAsO2	2.782e-029	2.782e-029	-28.556	-28.556	0.000
As(OH)3	2.432e-029	2.432e-029	-28.614	-28.614	0.000
H2AsO3-	9.114e-031	8.174e-031	-30.040	-30.088	-0.047
AsO2-	8.714e-031	7.815e-031	-30.060	-30.107	-0.047
AsO2OH-2	6.804e-034	4.389e-034	-33.167	-33.358	-0.190
As(5)	1.290e-006				
HAsO4-2	1.195e-006	7.711e-007	-5.922	-6.113	-0.190
H2AsO4-	9.424e-008	8.452e-008	-7.026	-7.073	-0.047
AsO4-3	2.920e-010	1.087e-010	-9.535	-9.964	-0.429
H3AsO4	2.709e-013	2.709e-013	-12.567	-12.567	0.000
C(4)	1.901e-003				
HCO3-	1.776e-003	1.593e-003	-2.751	-2.798	-0.047
CO2	6.706e-005	6.724e-005	-4.174	-4.172	0.001
CaHCO3+	2.618e-005	2.348e-005	-4.582	-4.629	-0.047
CaCO3	1.119e-005	1.119e-005	-4.951	-4.951	0.000
MgHCO3+	7.342e-006	6.584e-006	-5.134	-5.181	-0.047
CO3-2	5.981e-006	3.883e-006	-5.223	-5.411	-0.188
NaHCO3	3.782e-006	3.782e-006	-5.422	-5.422	0.000
CuCO3	1.553e-006	1.553e-006	-5.809	-5.809	0.000
MgCO3	1.462e-006	1.462e-006	-5.835	-5.835	0.000
MnCO3	2.237e-007	2.237e-007	-6.650	-6.650	0.000
ZnHCO3+	6.961e-008	6.243e-008	-7.157	-7.205	-0.047
ZnCO3	4.958e-008	4.958e-008	-7.305	-7.305	0.000
NaCO3-	2.515e-008	2.256e-008	-7.599	-7.647	-0.047
MnHCO3+	2.225e-008	1.996e-008	-7.653	-7.700	-0.047
Cu(CO3)2-2	1.666e-008	1.075e-008	-7.778	-7.969	-0.190
CuCO3(OH)2-2	6.181e-011	3.987e-011	-10.209	-10.399	-0.190
Ca	2.167e-003				
Ca+2	1.880e-003	1.244e-003	-2.726	-2.905	-0.179
CaSO4	2.499e-004	2.499e-004	-3.602	-3.602	0.000

CaHCO ₃ ⁺	2.618e-005	2.348e-005	-4.582	-4.629	-0.047
CaCO ₃	1.119e-005	1.119e-005	-4.951	-4.951	0.000
CaCl ⁺	1.793e-007	1.608e-007	-6.746	-6.794	-0.047
CaOH ⁺	1.076e-008	9.653e-009	-7.968	-8.015	-0.047
CaCl ₂	1.153e-010	1.153e-010	-9.938	-9.938	0.000
Cl(-1)	6.830e-004				
Cl ⁻	6.824e-004	6.099e-004	-3.166	-3.215	-0.049
MgCl ⁺	1.890e-007	1.695e-007	-6.724	-6.771	-0.047
CaCl ⁺	1.793e-007	1.608e-007	-6.746	-6.794	-0.047
NaCl	1.780e-007	1.780e-007	-6.750	-6.750	0.000
MnCl ⁺	2.383e-009	2.137e-009	-8.623	-8.670	-0.047
ZnCl ⁺	1.737e-009	1.558e-009	-8.760	-8.807	-0.047
Zn(OH)Cl	1.464e-009	1.464e-009	-8.835	-8.835	0.000
KCl	1.422e-009	1.422e-009	-8.847	-8.847	0.000
CaCl ₂	1.153e-010	1.153e-010	-9.938	-9.938	0.000
CuCl ⁺	7.800e-011	6.996e-011	-10.108	-10.155	-0.047
HCl	2.493e-012	2.493e-012	-11.603	-11.603	0.000
ZnCl ₂	1.110e-012	1.110e-012	-11.955	-11.955	0.000
CuCl ₂	2.247e-014	2.247e-014	-13.648	-13.648	0.000
ZnCl ₃ ⁻	4.169e-016	3.739e-016	-15.380	-15.427	-0.047
MnCl ₃ ⁻	1.936e-016	1.737e-016	-15.713	-15.760	-0.047
CuCl ₂ ⁻	6.308e-017	5.658e-017	-16.200	-16.247	-0.047
ZnCl ₄ ⁻²	2.680e-018	1.729e-018	-17.572	-17.762	-0.190
CuCl ₃ ⁻²	3.436e-019	2.216e-019	-18.464	-18.654	-0.190
CuCl ₄ ⁻²	2.432e-025	1.569e-025	-24.614	-24.804	-0.190
Cl(1)	2.568e-026				
ClO ⁻	1.599e-026	1.435e-026	-25.796	-25.843	-0.047
HClO	9.681e-027	9.681e-027	-26.014	-26.014	0.000
Cl(3)	0.000e+000				
ClO ₂ ⁻	0.000e+000	0.000e+000	-41.319	-41.366	-0.047
HClO ₂	0.000e+000	0.000e+000	-45.937	-45.937	0.000
Cl(5)	0.000e+000				
ClO ₃ ⁻	0.000e+000	0.000e+000	-42.989	-43.037	-0.048
Cl(7)	0.000e+000				
ClO ₄ ⁻	0.000e+000	0.000e+000	-48.962	-49.010	-0.048
ZnClO ₄ ⁺	0.000e+000	0.000e+000	-53.504	-53.551	-0.047
Cu(1)	2.623e-015				
Cu ⁺	2.560e-015	2.296e-015	-14.592	-14.639	-0.047
CuCl ₂ ⁻	6.308e-017	5.658e-017	-16.200	-16.247	-0.047
CuCl ₃ ⁻²	3.436e-019	2.216e-019	-18.464	-18.654	-0.190
Cu(2)	1.779e-006				
CuCO ₃	1.553e-006	1.553e-006	-5.809	-5.809	0.000
CuOH ⁺	1.325e-007	1.189e-007	-6.878	-6.925	-0.047
Cu ²	6.339e-008	4.193e-008	-7.198	-7.377	-0.179
Cu(CO ₃) ₂ ⁻²	1.666e-008	1.075e-008	-7.778	-7.969	-0.190
CuSO ₄	1.321e-008	1.321e-008	-7.879	-7.879	0.000
CuCl ⁺	7.800e-011	6.996e-011	-10.108	-10.155	-0.047
CuCO ₃ (OH) ₂ ⁻²	6.181e-011	3.987e-011	-10.209	-10.399	-0.190
CuCl ₂	2.247e-014	2.247e-014	-13.648	-13.648	0.000
CuO ₂ ⁻²	2.105e-016	1.357e-016	-15.677	-15.867	-0.190
CuCl ₄ ⁻²	2.432e-025	1.569e-025	-24.614	-24.804	-0.190
H(0)	5.241e-039				
H ₂	2.620e-039	2.628e-039	-38.582	-38.580	0.001
K	7.856e-005				
K ⁺	7.770e-005	6.945e-005	-4.110	-4.158	-0.049
KSO ₄ ⁻	8.595e-007	7.709e-007	-6.066	-6.113	-0.047
KCl	1.422e-009	1.422e-009	-8.847	-8.847	0.000
KOH	1.323e-011	1.323e-011	-10.878	-10.878	0.000
KHSO ₄	1.238e-014	1.238e-014	-13.907	-13.907	0.000
Mg	6.656e-004				
Mg ²	5.259e-004	3.559e-004	-3.279	-3.449	-0.170
MgSO ₄	1.307e-004	1.307e-004	-3.884	-3.884	0.000
MgHCO ₃ ⁺	7.342e-006	6.584e-006	-5.134	-5.181	-0.047
MgCO ₃	1.462e-006	1.462e-006	-5.835	-5.835	0.000
MgCl ⁺	1.890e-007	1.695e-007	-6.724	-6.771	-0.047
Mg ₄ (OH) ₄ ⁴⁺	1.396e-022	2.601e-023	-21.855	-22.585	-0.730
Mn(2)	3.296e-006				

Mn+2	2.487e-006	1.645e-006	-5.604	-5.784	-0.179
MnSO4	5.583e-007	5.583e-007	-6.253	-6.253	0.000
MnCO3	2.237e-007	2.237e-007	-6.650	-6.650	0.000
MnHCO3+	2.225e-008	1.996e-008	-7.653	-7.700	-0.047
MnOH+	2.591e-009	2.324e-009	-8.587	-8.634	-0.047
MnCl+	2.383e-009	2.137e-009	-8.623	-8.670	-0.047
Mn2(OH)3+	6.304e-013	5.654e-013	-12.200	-12.248	-0.047
Mn(OH)2	3.134e-013	3.134e-013	-12.504	-12.504	0.000
Mn2OH+3	1.069e-014	4.097e-015	-13.971	-14.388	-0.416
MnCl3-	1.936e-016	1.737e-016	-15.713	-15.760	-0.047
Mn(OH)3-	1.801e-017	1.615e-017	-16.744	-16.792	-0.047
Mn(OH)4-2	1.165e-023	7.516e-024	-22.934	-23.124	-0.190
Mn(3)	1.145e-021				
Mn+3	1.145e-021	4.389e-022	-20.941	-21.358	-0.416
Mn(6)	7.578e-023				
MnO4-2	7.578e-023	4.888e-023	-22.120	-22.311	-0.190
Mn(7)	2.404e-022				
MnO4-	2.404e-022	2.152e-022	-21.619	-21.667	-0.048
Na	1.872e-003				
Na+	1.851e-003	1.660e-003	-2.733	-2.780	-0.047
NaSO4-	1.682e-005	1.508e-005	-4.774	-4.821	-0.047
NaHCO3	3.782e-006	3.782e-006	-5.422	-5.422	0.000
NaCl	1.780e-007	1.780e-007	-6.750	-6.750	0.000
NaCO3-	2.515e-008	2.256e-008	-7.599	-7.647	-0.047
NaOH	1.516e-010	1.516e-010	-9.819	-9.819	0.000
O(0)	1.839e-015				
O2	9.196e-016	9.221e-016	-15.036	-15.035	0.001
S(6)	2.531e-003				
SO4-2	2.132e-003	1.375e-003	-2.671	-2.862	-0.190
CaSO4	2.499e-004	2.499e-004	-3.602	-3.602	0.000
MgSO4	1.307e-004	1.307e-004	-3.884	-3.884	0.000
NaSO4-	1.682e-005	1.508e-005	-4.774	-4.821	-0.047
KSO4-	8.595e-007	7.709e-007	-6.066	-6.113	-0.047
MnSO4	5.583e-007	5.583e-007	-6.253	-6.253	0.000
ZnSO4	4.394e-007	4.394e-007	-6.357	-6.357	0.000
CuSO4	1.321e-008	1.321e-008	-7.879	-7.879	0.000
HSO4-	2.818e-009	2.528e-009	-8.550	-8.597	-0.047
KHSO4	1.238e-014	1.238e-014	-13.907	-13.907	0.000
H2SO4	4.340e-020	4.340e-020	-19.363	-19.363	0.000
Zn	2.984e-006				
Zn+2	2.298e-006	1.520e-006	-5.639	-5.818	-0.179
ZnSO4	4.394e-007	4.394e-007	-6.357	-6.357	0.000
ZnOH+	1.022e-007	9.162e-008	-6.991	-7.038	-0.047
ZnHCO3+	6.961e-008	6.243e-008	-7.157	-7.205	-0.047
ZnCO3	4.958e-008	4.958e-008	-7.305	-7.305	0.000
Zn(OH)2	2.156e-008	2.156e-008	-7.666	-7.666	0.000
ZnCl+	1.737e-009	1.558e-009	-8.760	-8.807	-0.047
Zn(OH)Cl	1.464e-009	1.464e-009	-8.835	-8.835	0.000
Zn(OH)3-	4.094e-012	3.672e-012	-11.388	-11.435	-0.047
ZnCl2	1.110e-012	1.110e-012	-11.955	-11.955	0.000
ZnCl3-	4.169e-016	3.739e-016	-15.380	-15.427	-0.047
Zn(OH)4-2	5.333e-017	3.439e-017	-16.273	-16.464	-0.190
ZnCl4-2	2.680e-018	1.729e-018	-17.572	-17.762	-0.190
ZnClO4+	0.000e+000	0.000e+000	-53.504	-53.551	-0.047

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

Phase	SI	log IAP	log KT	
Anhydrite	-1.42	-5.77	-4.35	CaSO4
Antarcticite	-13.43	-9.34	4.09	CaCl2:6H2O
Antlerite	-2.76	5.97	8.73	Cu3(SO4)(OH)4
Aphthitalite	-17.09	-20.98	-3.89	NaK3(SO4)2
Aragonite	0.07	2.04	1.97	CaCO3
Arcanite	-9.33	-11.18	-1.84	K2SO4
Arsenolite	-55.81	-75.65	-19.84	As2O3
Artinite	-6.10	13.52	19.63	Mg2CO3(OH)2:3H2O

As	-69.23	-26.55	42.68	As
As2O5	-31.76	-29.63	2.14	As2O5
As4O6(cubi)	-111.49	-151.31	-39.82	As4O6
As4O6(mono)	-111.26	-151.31	-40.05	As4O6
Atacamite	-3.76	10.50	14.26	Cu4Cl2(OH)6
Azurite	-5.88	3.23	9.12	Cu3(CO3)2(OH)2
Bassanite	-2.06	-5.77	-3.71	CaSO4:0.5H2O
Birnessite	20.65	-64.89	-85.55	Mn8O14:5H2O
Bischofite	-14.27	-9.88	4.39	MgCl2:6H2O
Bixbyite	4.69	3.72	-0.96	Mn2O3
Bloedite	-12.25	-14.73	-2.48	Na2Mg(SO4)2:4H2O
Brochantite	-1.35	14.07	15.42	Cu4(SO4)(OH)6
Brucite	-4.25	12.03	16.28	Mg(OH)2
Burkeite	-26.95	-17.46	9.49	Na6CO3(SO4)2
C	-59.65	4.50	64.15	C
C(g)	-177.27	4.50	181.77	C
Ca	-119.74	20.09	139.83	Ca
Ca(g)	-144.98	20.09	165.07	Ca
Ca2Cl2(OH)2:H2O	-23.05	3.24	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-9.70	8.10	17.80	Ca3(AsO4)2
Ca4Cl2(OH)6:13H2O	-39.94	28.39	68.33	Ca4Cl2(OH)6:13H2O
Calcite	0.21	2.04	1.82	CaCO3
Carnallite	-21.52	-17.25	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-2.23	-5.77	-3.54	CaSO4:0.5H2O
Chalcanthite	-7.61	-10.24	-2.63	CuSO4:5H2O
Chalcocyanite	-13.15	-10.24	2.91	CuSO4
Chloromagnesite	-31.69	-9.88	21.82	MgCl2
Cl2(g)	-32.42	-29.43	2.99	Cl2
Claudetite	-55.86	-75.65	-19.80	As2O3
CO2(g)	-2.71	-10.54	-7.83	CO2
Cu	-15.88	15.62	31.50	Cu
Cu(g)	-68.04	15.62	83.66	Cu
CuCl2	-17.53	-13.81	3.72	CuCl2
Cuprite	-11.89	-13.80	-1.91	Cu2O
Dolomite	1.06	3.53	2.47	CaMg(CO3)2
Dolomite-dis	-0.48	3.53	4.01	CaMg(CO3)2
Dolomite-ord	1.07	3.53	2.46	CaMg(CO3)2
Epsomite	-4.35	-6.31	-1.96	MgSO4:7H2O
Gaylussite	-9.75	1.42	11.16	CaNa2(CO3)2:5H2O
Glauberite	-8.72	-14.19	-5.47	Na2Ca(SO4)2
Gypsum	-1.24	-5.77	-4.53	CaSO4:2H2O
H2(g)	-35.48	-38.58	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.56	-5.99	1.56	NaCl
Hausmannite	3.28	13.42	10.14	Mn3O4
HCl(g)	-17.26	-10.95	6.30	HCl
Hexahydrate	-4.58	-6.31	-1.73	MgSO4:6H2O
Huntite	-3.70	6.52	10.22	CaMg3(CO3)4
Hydromagnesite	-12.73	18.01	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-21.08	-9.33	11.75	CaCl2
Hydrozincite	-3.07	27.23	30.31	Zn5(OH)6(CO3)2
Ice	-0.14	-0.00	0.14	H2O
K	-63.64	7.34	70.98	K
K(g)	-74.24	7.34	81.58	K
K2CO3:1.5H2O	-16.75	-3.37	13.38	K2CO3:1.5H2O
K2O	-76.87	7.16	84.04	K2O
K3H(SO4)2	-22.32	-25.94	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-62.28	-34.57	27.71	K8H4(CO3)6:3H2O
Kainite	-13.37	-13.68	-0.31	KMgClSO4:3H2O
Kaliginite	-7.24	-6.96	0.28	KHCO3
Kieserite	-6.04	-6.31	-0.27	MgSO4:H2O
KMgCl3	-38.50	-17.25	21.25	KMgCl3
KMgCl3:2H2O	-31.21	-17.25	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-12.26	-2.00	10.26	KNaCO3:6H2O
Lammerite	-6.87	-5.32	1.55	Cu3(AsO4)2
Lansfordite	-3.35	1.49	4.84	MgCO3:5H2O
Leonite	-13.38	-17.49	-4.11	K2Mg(SO4)2:4H2O

Lime	-19.99	12.57	32.57	CaO
Magnesite	-0.78	1.49	2.27	MgCO ₃
Malachite	-0.23	5.67	5.90	Cu ₂ CO ₃ (OH) ₂
Manganite	2.03	1.86	-0.16	MnO(OH)
Manganosite	-8.22	9.70	17.92	MnO
Mercallite	-13.32	-14.76	-1.44	KHSO ₄
Mg	-102.97	19.55	122.52	Mg
Mg(g)	-122.70	19.55	142.25	Mg
Mg1.25SO ₄ (OH)0.5:0.5H ₂ O	-8.50	-3.30	5.20	Mg1.25SO ₄ (OH)0.5:0.5H ₂ O
Mg1.5SO ₄ (OH)	-9.50	-0.29	9.21	Mg1.5SO ₄ (OH)
MgCl ₂ :2H ₂ O	-22.61	-9.88	12.73	MgCl ₂ :2H ₂ O
MgCl ₂ :4H ₂ O	-17.18	-9.88	7.30	MgCl ₂ :4H ₂ O
MgCl ₂ :H ₂ O	-25.95	-9.88	16.07	MgCl ₂ :H ₂ O
MgOHCl	-14.81	1.08	15.89	MgOHCl
MgSO ₄	-11.14	-6.31	4.83	MgSO ₄
Mirabilite	-7.27	-8.42	-1.15	Na ₂ SO ₄ :10H ₂ O
Misenite	-88.66	-99.74	-11.08	K ₈ H ₆ (SO ₄) ₇
Mn	-65.72	17.21	82.93	Mn
Mn(OH) ₂ (am)	-5.61	9.70	15.31	Mn(OH) ₂
Mn(OH) ₃	-4.48	1.86	6.34	Mn(OH) ₃
MnCl ₂ :2H ₂ O	-16.21	-12.21	4.00	MnCl ₂ :2H ₂ O
MnCl ₂ :4H ₂ O	-14.97	-12.21	2.75	MnCl ₂ :4H ₂ O
MnCl ₂ :H ₂ O	-17.76	-12.21	5.54	MnCl ₂ :H ₂ O
MnO ₂ (gamma)	2.08	-14.05	-16.13	MnO ₂
MnSO ₄	-11.25	-8.65	2.61	MnSO ₄
Monohydrocalcite	-0.64	2.04	2.68	CaCO ₃ :H ₂ O
Na	-58.65	8.72	67.37	Na
Na(g)	-72.14	8.72	80.86	Na
Na ₂ CO ₃	-11.78	-0.62	11.16	Na ₂ CO ₃
Na ₂ CO ₃ :7H ₂ O	-10.56	-0.62	9.94	Na ₂ CO ₃ :7H ₂ O
Na ₂ O	-57.50	9.92	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-20.91	-21.80	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-16.72	-22.61	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
Nahcolite	-5.44	-5.58	-0.14	NaHCO ₃
Nantokite	-11.09	-17.85	-6.77	CuCl
Natron	-10.21	-0.62	9.59	Na ₂ CO ₃ :10H ₂ O
Nesquehonite	-3.80	1.49	5.29	MgCO ₃ :3H ₂ O
O ₂ (g)	-12.14	-15.04	-2.89	O ₂
Oxychloride-Mg	-12.72	13.11	25.83	Mg ₂ Cl(OH) ₃ :4H ₂ O
Pentahydrate	-4.92	-6.31	-1.39	MgSO ₄ :5H ₂ O
Periclase	-9.29	12.03	21.33	MgO
Picromerite	-13.05	-17.49	-4.44	K ₂ Mg(SO ₄) ₂ :6H ₂ O
Pirssonite	-9.90	1.42	11.32	Na ₂ Ca(CO ₃) ₂ :2H ₂ O
Polyhalite	-14.71	-29.02	-14.31	K ₂ MgCa ₂ (SO ₄) ₄ :2H ₂ O
Portlandite	-9.97	12.57	22.55	Ca(OH) ₂
Pyrolusite	3.61	-14.05	-17.66	MnO ₂
Rhodochrosite	-0.62	-0.84	-0.22	MnCO ₃
Scacchite	-20.95	-12.21	8.74	MnCl ₂
Smithsonite	-1.32	-0.88	0.44	ZnCO ₃
Starkeyite	-5.31	-6.31	-1.00	MgSO ₄ :4H ₂ O
Sylvite	-8.20	-7.37	0.83	KCl
Syngenite	-9.35	-16.95	-7.60	K ₂ Ca(SO ₄) ₂ :H ₂ O
Tachyhydrate	-46.24	-29.09	17.14	Mg ₂ CaCl ₆ :12H ₂ O
Tenorite	0.46	8.10	7.65	CuO
Thenardite	-8.06	-8.42	-0.36	Na ₂ SO ₄
Thermonatrite	-11.55	-0.62	10.94	Na ₂ CO ₃ :H ₂ O
Todorokite	19.21	-26.62	-45.82	Mn ₇ O ₁₂ :3H ₂ O
Trona-K	-20.54	-8.95	11.59	K ₂ NaH(CO ₃) ₂ :2H ₂ O
Zincite	-1.54	9.66	11.20	ZnO
Zn	-51.61	17.18	68.79	Zn
Zn(ClO ₄) ₂ :6H ₂ O	-109.47	-103.84	5.63	Zn(ClO ₄) ₂ :6H ₂ O
Zn(g)	-68.23	17.18	85.41	Zn
Zn(OH) ₂ (beta)	-2.27	9.66	11.93	Zn(OH) ₂
Zn(OH) ₂ (epsilon)	-2.00	9.66	11.66	Zn(OH) ₂
Zn(OH) ₂ (gamma)	-2.22	9.66	11.88	Zn(OH) ₂
Zn ₂ (OH) ₃ Cl	-6.92	8.37	15.29	Zn ₂ (OH) ₃ Cl
Zn ₂ SO ₄ (OH) ₂	-6.60	0.98	7.58	Zn ₂ SO ₄ (OH) ₂

Zn3(AsO4)2	-9.95	-0.64	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-26.79	-7.70	19.09	Zn3O(SO4)2
ZnCl2	-19.33	-12.25	7.08	ZnCl2
ZnCO3:H2O	-1.02	-0.88	0.14	ZnCO3:H2O
ZnSO4	-12.21	-8.68	3.53	ZnSO4
ZnSO4:6H2O	-6.98	-8.68	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-6.80	-8.68	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-8.13	-8.68	-0.55	ZnSO4:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using mix 4.

Mixture 4.

1.000e+000 Solution 1 Flujo 3
3.000e+000 Solution 4 AS3

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

Elements	Molality	Moles
Al	2.005e-004	8.019e-004
As	1.374e-005	5.494e-005
C	1.426e-003	5.703e-003
Ca	2.405e-003	9.621e-003
Cl	8.012e-004	3.205e-003
Cu	1.625e-004	6.502e-004
Fe	1.861e-004	7.445e-004
K	2.831e-004	1.133e-003
Mg	6.375e-004	2.550e-003
Mn	1.131e-004	4.522e-004
Na	1.631e-003	6.526e-003
S	5.194e-003	2.078e-002
Zn	3.942e-005	1.577e-004

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

pH	=	5.718	Charge balance
pe	=	14.201	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	1.598e-002	
Mass of water (kg)	=	4.000e+000	
Total alkalinity (eq/kg)	=	8.259e-004	
Total CO2 (mol/kg)	=	1.426e-003	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	-1.045e-002	
Percent error, 100*(Cat- An)/(Cat+ An)	=	-15.09	
Iterations	=	17	
Total H	=	4.442104e+002	
Total O	=	2.222023e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	2.132e-006	1.916e-006	-5.671	-5.718	-0.046
OH-	5.717e-009	5.028e-009	-8.243	-8.299	-0.056
H2O	5.553e+001	9.998e-001	1.744	-0.000	0.000
Al	2.005e-004				
Al13O4(OH)24+7	1.521e-005	4.439e-008	-4.818	-7.353	-2.535
AlOH+2	8.691e-007	5.271e-007	-6.061	-6.278	-0.217

Al(OH)2+	7.246e-007	6.387e-007	-6.140	-6.195	-0.055
HAIO2	4.852e-007	4.852e-007	-6.314	-6.314	0.000
AlSO4+	2.774e-007	2.445e-007	-6.557	-6.612	-0.055
Al+3	2.386e-007	9.015e-008	-6.622	-7.045	-0.423
AlO2-	9.842e-008	8.676e-008	-7.007	-7.062	-0.055
Al(SO4)2-	5.706e-008	5.030e-008	-7.244	-7.298	-0.055
Al2(OH)2+4	3.134e-010	4.517e-011	-9.504	-10.345	-0.841
NaAlO2	2.338e-011	2.338e-011	-10.631	-10.631	0.000
Al3(OH)4+5	1.406e-011	7.160e-013	-10.852	-12.145	-1.293
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-153.248	-153.248	0.000
As(3)	3.061e-029				
HAsO2	1.633e-029	1.633e-029	-28.787	-28.787	0.000
As(OH)3	1.427e-029	1.427e-029	-28.845	-28.845	0.000
H2AsO3-	5.169e-033	4.557e-033	-32.287	-32.341	-0.055
AsO2-	4.943e-033	4.357e-033	-32.306	-32.361	-0.055
AsO2OH-2	3.866e-038	2.324e-038	-37.413	-37.634	-0.221
HAsS2	0.000e+000	0.000e+000	-286.889	-286.889	0.000
As(5)	1.374e-005				
H2AsO4-	1.218e-005	1.074e-005	-4.914	-4.969	-0.055
HAsO4-2	1.548e-006	9.306e-007	-5.810	-6.031	-0.221
H3AsO4	3.624e-009	3.624e-009	-8.441	-8.441	0.000
AsO4-3	3.925e-012	1.246e-012	-11.406	-11.904	-0.498
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-254.082	-254.082	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-225.033	-225.033	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-140.764	-140.764	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-47.826	-47.826	0.000
C(4)	1.426e-003				
CO2	1.127e-003	1.131e-003	-2.948	-2.946	0.002
HCO3-	2.888e-004	2.546e-004	-3.539	-3.594	-0.055
CaHCO3+	4.118e-006	3.630e-006	-5.385	-5.440	-0.055
CuCO3	3.967e-006	3.967e-006	-5.402	-5.402	0.000
MgHCO3+	9.408e-007	8.293e-007	-6.026	-6.081	-0.055
NaHCO3	5.144e-007	5.144e-007	-6.289	-6.289	0.000
ZnHCO3+	1.350e-007	1.190e-007	-6.870	-6.925	-0.055
MnHCO3+	1.097e-007	9.669e-008	-6.960	-7.015	-0.055
CaCO3	1.644e-008	1.644e-008	-7.784	-7.784	0.000
MnCO3	1.030e-008	1.030e-008	-7.987	-7.987	0.000
CO3-2	9.721e-009	5.895e-009	-8.012	-8.229	-0.217
FeCO3+	8.894e-009	7.840e-009	-8.051	-8.106	-0.055
MgCO3	1.749e-009	1.749e-009	-8.757	-8.757	0.000
ZnCO3	8.975e-010	8.975e-010	-9.047	-9.047	0.000
Cu(CO3)2-2	6.931e-011	4.166e-011	-10.159	-10.380	-0.221
NaCO3-	3.306e-011	2.914e-011	-10.481	-10.536	-0.055
FeHCO3+	2.290e-012	2.019e-012	-11.640	-11.695	-0.055
CuCO3(OH)2-2	1.528e-014	9.185e-015	-13.816	-14.037	-0.221
FeCO3	5.057e-015	5.057e-015	-14.296	-14.296	0.000
Ca	2.405e-003				
Ca+2	1.935e-003	1.203e-003	-2.713	-2.920	-0.206
CaSO4	4.659e-004	4.659e-004	-3.332	-3.332	0.000
CaHCO3+	4.118e-006	3.630e-006	-5.385	-5.440	-0.055
CaCl+	2.032e-007	1.791e-007	-6.692	-6.747	-0.055
CaCO3	1.644e-008	1.644e-008	-7.784	-7.784	0.000
CaCl2	1.479e-010	1.479e-010	-9.830	-9.830	0.000
CaOH+	1.006e-010	8.871e-011	-9.997	-10.052	-0.055
Cl(-1)	8.012e-004				
Cl-	8.004e-004	7.022e-004	-3.097	-3.154	-0.057
CaCl+	2.032e-007	1.791e-007	-6.692	-6.747	-0.055
MgCl+	1.744e-007	1.538e-007	-6.758	-6.813	-0.055
NaCl	1.743e-007	1.743e-007	-6.759	-6.759	0.000
CuCl+	1.537e-007	1.355e-007	-6.813	-6.868	-0.055
MnCl+	8.461e-008	7.459e-008	-7.073	-7.127	-0.055
ZnCl+	2.426e-008	2.139e-008	-7.615	-7.670	-0.055

KCl	5.736e-009	5.736e-009	-8.241	-8.241	0.000
HCl	3.021e-010	3.021e-010	-9.520	-9.520	0.000
Zn(OH)Cl	1.909e-010	1.909e-010	-9.719	-9.719	0.000
CaCl2	1.479e-010	1.479e-010	-9.830	-9.830	0.000
CuCl2	5.010e-011	5.010e-011	-10.300	-10.300	0.000
ZnCl2	1.754e-011	1.754e-011	-10.756	-10.756	0.000
FeCl+2	4.442e-014	2.694e-014	-13.352	-13.570	-0.217
FeCl2+	1.737e-014	1.532e-014	-13.760	-13.815	-0.055
MnCl3-	9.114e-015	8.034e-015	-14.040	-14.095	-0.055
FeCl+	8.768e-015	7.729e-015	-14.057	-14.112	-0.055
ZnCl3-	7.718e-015	6.803e-015	-14.113	-14.167	-0.055
ZnCl4-2	6.024e-017	3.621e-017	-16.220	-16.441	-0.221
CuCl2-	9.004e-018	7.937e-018	-17.046	-17.100	-0.055
CuCl3-2	5.955e-020	3.579e-020	-19.225	-19.446	-0.221
FeCl2	2.912e-020	2.912e-020	-19.536	-19.536	0.000
CuCl4-2	7.713e-022	4.636e-022	-21.113	-21.334	-0.221
FeCl4-	1.030e-023	9.079e-024	-22.987	-23.042	-0.055
FeCl4-2	6.904e-026	4.150e-026	-25.161	-25.382	-0.221
Cl(1)	2.717e-020				
HClO	2.674e-020	2.674e-020	-19.573	-19.573	0.000
ClO-	4.270e-022	3.764e-022	-21.370	-21.424	-0.055
Cl(3)	2.925e-033				
ClO2-	2.918e-033	2.572e-033	-32.535	-32.590	-0.055
HClO2	7.285e-036	7.285e-036	-35.138	-35.138	0.000
Cl(5)	1.422e-030				
ClO3-	1.422e-030	1.251e-030	-29.847	-29.903	-0.056
Cl(7)	3.453e-032				
ClO4-	3.452e-032	3.036e-032	-31.462	-31.518	-0.056
ZnClO4+	1.181e-035	1.041e-035	-34.928	-34.983	-0.055
Cu(1)	2.847e-016				
Cu+	2.756e-016	2.430e-016	-15.560	-15.614	-0.055
CuCl2-	9.004e-018	7.937e-018	-17.046	-17.100	-0.055
CuCl3-2	5.955e-020	3.579e-020	-19.225	-19.446	-0.221
Cu(2)	1.625e-004				
Cu+2	1.134e-004	7.054e-005	-3.945	-4.152	-0.206
CuSO4	4.283e-005	4.283e-005	-4.368	-4.368	0.000
CuCO3	3.967e-006	3.967e-006	-5.402	-5.402	0.000
CuOH+	2.154e-006	1.899e-006	-5.667	-5.721	-0.055
CuCl+	1.537e-007	1.355e-007	-6.813	-6.868	-0.055
Cu(CO3)2-2	6.931e-011	4.166e-011	-10.159	-10.380	-0.221
CuCl2	5.010e-011	5.010e-011	-10.300	-10.300	0.000
CuCO3(OH)2-2	1.528e-014	9.185e-015	-13.816	-14.037	-0.221
CuO2-2	3.092e-021	1.859e-021	-20.510	-20.731	-0.221
CuCl4-2	7.713e-022	4.636e-022	-21.113	-21.334	-0.221
Fe(2)	3.295e-011				
Fe+2	2.430e-011	1.511e-011	-10.614	-10.821	-0.206
FeSO4	6.347e-012	6.347e-012	-11.197	-11.197	0.000
FeHCO3+	2.290e-012	2.019e-012	-11.640	-11.695	-0.055
FeCl+	8.768e-015	7.729e-015	-14.057	-14.112	-0.055
FeCO3	5.057e-015	5.057e-015	-14.296	-14.296	0.000
FeOH+	2.829e-015	2.494e-015	-14.548	-14.603	-0.055
FeCl2	2.912e-020	2.912e-020	-19.536	-19.536	0.000
Fe(OH)2	1.034e-020	1.034e-020	-19.986	-19.986	0.000
Fe(OH)3-	2.436e-025	2.148e-025	-24.613	-24.668	-0.055
FeCl4-2	6.904e-026	4.150e-026	-25.161	-25.382	-0.221
Fe(OH)4-2	1.865e-034	1.121e-034	-33.729	-33.950	-0.221
Fe(3)	1.861e-004				
Fe(OH)2+	1.521e-004	1.341e-004	-3.818	-3.873	-0.055
Fe(OH)3	3.273e-005	3.273e-005	-4.485	-4.485	0.000
FeOH+2	1.279e-006	7.759e-007	-5.893	-6.110	-0.217
FeCO3+	8.894e-009	7.840e-009	-8.051	-8.106	-0.055
Fe(OH)4-	4.867e-009	4.290e-009	-8.313	-8.368	-0.055
Fe+3	6.095e-010	2.303e-010	-9.215	-9.638	-0.423
Fe2(OH)2+4	1.124e-010	1.620e-011	-9.949	-10.790	-0.841
FeSO4+	6.698e-011	5.904e-011	-10.174	-10.229	-0.055
Fe3(OH)4+5	8.910e-012	4.539e-013	-11.050	-12.343	-1.293
Fe(SO4)2-	3.001e-012	2.646e-012	-11.523	-11.577	-0.055

FeCl+2	4.442e-014	2.694e-014	-13.352	-13.570	-0.217
FeCl2+	1.737e-014	1.532e-014	-13.760	-13.815	-0.055
FeCl4-	1.030e-023	9.079e-024	-22.987	-23.042	-0.055
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-42.940	-42.938	0.002
K	2.831e-004				
K+	2.772e-004	2.432e-004	-3.557	-3.614	-0.057
KSO4-	5.903e-006	5.203e-006	-5.229	-5.284	-0.055
KCl	5.736e-009	5.736e-009	-8.241	-8.241	0.000
KHSO4	8.795e-012	8.795e-012	-11.056	-11.056	0.000
KOH	4.401e-013	4.401e-013	-12.356	-12.356	0.000
Mg	6.375e-004				
Mg+2	4.379e-004	2.805e-004	-3.359	-3.552	-0.193
MgSO4	1.985e-004	1.985e-004	-3.702	-3.702	0.000
MgHCO3+	9.408e-007	8.293e-007	-6.026	-6.081	-0.055
MgCl+	1.744e-007	1.538e-007	-6.758	-6.813	-0.055
MgCO3	1.749e-009	1.749e-009	-8.757	-8.757	0.000
Mg4(OH)4+4	5.666e-031	8.166e-032	-30.247	-31.088	-0.841
Mn(2)	1.131e-004				
Mn+2	8.022e-005	4.989e-005	-4.096	-4.302	-0.206
MnSO4	3.262e-005	3.262e-005	-4.486	-4.486	0.000
MnHCO3+	1.097e-007	9.669e-008	-6.960	-7.015	-0.055
MnCl+	8.461e-008	7.459e-008	-7.073	-7.127	-0.055
MnCO3	1.030e-008	1.030e-008	-7.987	-7.987	0.000
MnOH+	7.591e-010	6.692e-010	-9.120	-9.174	-0.055
Mn2OH+3	1.083e-013	3.577e-014	-12.965	-13.446	-0.481
MnCl3-	9.114e-015	8.034e-015	-14.040	-14.095	-0.055
Mn(OH)2	8.573e-016	8.573e-016	-15.067	-15.067	0.000
Mn2(OH)3+	5.052e-016	4.453e-016	-15.297	-15.351	-0.055
Mn(OH)3-	4.761e-022	4.197e-022	-21.322	-21.377	-0.055
Mn(OH)4-2	3.086e-030	1.855e-030	-29.511	-29.732	-0.221
Mn(3)	6.403e-016				
Mn+3	6.403e-016	2.115e-016	-15.194	-15.675	-0.481
Mn(6)	1.042e-020				
MnO4-2	1.042e-020	6.266e-021	-19.982	-20.203	-0.221
Mn(7)	4.986e-016				
MnO4-	4.986e-016	4.385e-016	-15.302	-15.358	-0.056
Na	1.631e-003				
Na+	1.603e-003	1.413e-003	-2.795	-2.850	-0.055
NaSO4-	2.806e-005	2.474e-005	-4.552	-4.607	-0.055
NaHCO3	5.144e-007	5.144e-007	-6.289	-6.289	0.000
NaCl	1.743e-007	1.743e-007	-6.759	-6.759	0.000
NaCO3-	3.306e-011	2.914e-011	-10.481	-10.536	-0.055
NaAlO2	2.338e-011	2.338e-011	-10.631	-10.631	0.000
NaOH	1.226e-012	1.226e-012	-11.912	-11.912	0.000
O(0)	9.543e-007				
O2	4.772e-007	4.790e-007	-6.321	-6.320	0.002
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-132.646	-132.646	0.000
HS-	0.000e+000	0.000e+000	-133.882	-133.938	-0.056
S-2	0.000e+000	0.000e+000	-140.933	-141.146	-0.213
S2-2	0.000e+000	0.000e+000	-237.556	-237.778	-0.221
HAsS2	0.000e+000	0.000e+000	-286.889	-286.889	0.000
S3-2	0.000e+000	0.000e+000	-334.229	-334.450	-0.221
S4-2	0.000e+000	0.000e+000	-431.129	-431.350	-0.221
S5-2	0.000e+000	0.000e+000	-528.246	-528.467	-0.221
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-137.202	-137.423	-0.221
HS2O3-	0.000e+000	0.000e+000	-142.072	-142.127	-0.055
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-125.298	-125.511	-0.213
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-44.466	-44.521	-0.055
SO3-2	0.000e+000	0.000e+000	-45.818	-46.035	-0.217
H2SO3	0.000e+000	0.000e+000	-48.257	-48.257	0.000
SO2	0.000e+000	0.000e+000	-48.357	-48.357	0.000
S2O6-2	0.000e+000	0.000e+000	-64.576	-64.797	-0.221

S306-2	0.000e+000	0.000e+000	-163.732	-163.953	-0.221
S406-2	0.000e+000	0.000e+000	-246.982	-247.203	-0.221
S506-2	0.000e+000	0.000e+000	-359.111	-359.332	-0.221
S(5)	0.000e+000				
S205-2	0.000e+000	0.000e+000	-93.651	-93.872	-0.221
S(6)	5.194e-003				
SO4-2	4.409e-003	2.650e-003	-2.356	-2.577	-0.221
CaSO4	4.659e-004	4.659e-004	-3.332	-3.332	0.000
MgSO4	1.985e-004	1.985e-004	-3.702	-3.702	0.000
CuSO4	4.283e-005	4.283e-005	-4.368	-4.368	0.000
MnSO4	3.262e-005	3.262e-005	-4.486	-4.486	0.000
NaSO4-	2.806e-005	2.474e-005	-4.552	-4.607	-0.055
ZnSO4	1.010e-005	1.010e-005	-4.996	-4.996	0.000
KSO4-	5.903e-006	5.203e-006	-5.229	-5.284	-0.055
HSO4-	5.818e-007	5.129e-007	-6.235	-6.290	-0.055
AlSO4+	2.774e-007	2.445e-007	-6.557	-6.612	-0.055
Al(SO4)2-	5.706e-008	5.030e-008	-7.244	-7.298	-0.055
FeSO4+	6.698e-011	5.904e-011	-10.174	-10.229	-0.055
KHSO4	8.795e-012	8.795e-012	-11.056	-11.056	0.000
FeSO4	6.347e-012	6.347e-012	-11.197	-11.197	0.000
Fe(SO4)2-	3.001e-012	2.646e-012	-11.523	-11.577	-0.055
H2SO4	9.270e-016	9.270e-016	-15.033	-15.033	0.000
S(7)	0.000e+000				
S208-2	0.000e+000	0.000e+000	-41.982	-42.204	-0.221
S(8)	2.187e-029				
HSO5-	2.187e-029	1.928e-029	-28.660	-28.715	-0.055
Zn	3.942e-005				
Zn+2	2.915e-005	1.813e-005	-4.535	-4.742	-0.206
ZnSO4	1.010e-005	1.010e-005	-4.996	-4.996	0.000
ZnHCO3+	1.350e-007	1.190e-007	-6.870	-6.925	-0.055
ZnCl+	2.426e-008	2.139e-008	-7.615	-7.670	-0.055
ZnOH+	1.177e-008	1.038e-008	-7.929	-7.984	-0.055
ZnCO3	8.975e-010	8.975e-010	-9.047	-9.047	0.000
Zn(OH)Cl	1.909e-010	1.909e-010	-9.719	-9.719	0.000
Zn(OH)2	2.319e-011	2.319e-011	-10.635	-10.635	0.000
ZnCl2	1.754e-011	1.754e-011	-10.756	-10.756	0.000
ZnCl3-	7.718e-015	6.803e-015	-14.113	-14.167	-0.055
ZnCl4-2	6.024e-017	3.621e-017	-16.220	-16.441	-0.221
Zn(OH)3-	4.256e-017	3.751e-017	-16.371	-16.426	-0.055
Zn(OH)4-2	5.553e-024	3.338e-024	-23.255	-23.477	-0.221
ZnClO4+	1.181e-035	1.041e-035	-34.928	-34.983	-0.055

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

Phase	SI	log IAP	log KT	
Al	-135.07	14.85	149.91	Al
Al(g)	-185.77	14.85	200.62	Al
Al2(SO4)3	-40.72	-21.82	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-23.38	-21.82	1.56	Al2(SO4)3:6H2O
Alabandite	-132.10	-132.52	-0.42	MnS
Alum-K	-10.84	-15.81	-4.97	KAl(SO4)2:12H2O
Alunite	4.87	4.40	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.15	-5.50	-4.35	CaSO4
Antarcticite	-13.32	-9.23	4.09	CaCl2:6H2O
Antlerite	-0.89	7.84	8.73	Cu3(SO4)(OH)4
Aphthitalite	-14.96	-18.85	-3.89	NaK3(SO4)2
Aragonite	-2.77	-0.80	1.97	CaCO3
Arcanite	-7.96	-9.80	-1.84	K2SO4
Arsenolite	-56.28	-76.12	-19.84	As2O3
Arsenopyrite	-220.25	-234.69	-14.45	FeAsS
Artinite	-13.17	6.45	19.63	Mg2CO3(OH)2:3H2O
As	-76.00	-33.32	42.68	As
As2O5	-23.51	-21.37	2.14	As2O5
As4O6(cubi)	-112.41	-152.24	-39.82	As4O6
As4O6(mono)	-112.19	-152.24	-40.05	As4O6
Atacamite	-2.87	11.39	14.26	Cu4Cl2(OH)6

Azurite	-5.89	3.23	9.12	$\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$
Bassanite	-1.79	-5.50	-3.71	$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$
Birnessite	26.30	-59.25	-85.55	$\text{Mn}_8\text{O}_{14} \cdot 5\text{H}_2\text{O}$
Bischofite	-14.25	-9.86	4.39	$\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$
Bixbyite	3.92	2.96	-0.96	Mn_2O_3
Bloedite	-11.93	-14.41	-2.48	$\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$
Boehmite	2.56	10.11	7.55	AlO_2H
Bornite	-487.78	-590.31	-102.53	Cu_5FeS_4
Brochantite	-0.30	15.12	15.42	$\text{Cu}_4(\text{SO}_4)(\text{OH})_6$
Brucite	-8.40	7.88	16.28	$\text{Mg}(\text{OH})_2$
Burkeite	-29.62	-20.13	9.49	$\text{Na}_6\text{CO}_3(\text{SO}_4)_2$
C	-67.14	-2.99	64.15	C
C(g)	-184.76	-2.99	181.77	C
Ca	-128.16	11.68	139.83	Ca
Ca(g)	-153.40	11.68	165.07	Ca
$\text{Ca}_2\text{Al}_2\text{O}_5 \cdot 8\text{H}_2\text{O}$	-22.32	37.25	59.57	$\text{Ca}_2\text{Al}_2\text{O}_5 \cdot 8\text{H}_2\text{O}$
$\text{Ca}_2\text{Cl}_2(\text{OH})_2 \cdot \text{H}_2\text{O}$	-27.00	-0.71	26.29	$\text{Ca}_2\text{Cl}_2(\text{OH})_2 \cdot \text{H}_2\text{O}$
$\text{Ca}_3(\text{AsO}_4)_2$	-13.63	4.17	17.80	$\text{Ca}_3(\text{AsO}_4)_2$
$\text{Ca}_3\text{Al}_2\text{O}_6$	-67.27	45.76	113.03	$\text{Ca}_3\text{Al}_2\text{O}_6$
$\text{Ca}_4\text{Al}_2\text{Fe}_2\text{O}_{10}$	-71.17	69.31	140.48	$\text{Ca}_4\text{Al}_2\text{Fe}_2\text{O}_{10}$
$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 13\text{H}_2\text{O}$	-52.98	54.28	107.25	$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 13\text{H}_2\text{O}$
$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 19\text{H}_2\text{O}$	-49.40	54.28	103.68	$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 19\text{H}_2\text{O}$
$\text{Ca}_4\text{Cl}_2(\text{OH})_6 \cdot 13\text{H}_2\text{O}$	-52.01	16.32	68.33	$\text{Ca}_4\text{Cl}_2(\text{OH})_6 \cdot 13\text{H}_2\text{O}$
CaAl_2O_4	-18.18	28.73	46.91	CaAl_2O_4
$\text{CaAl}_2\text{O}_4 \cdot 10\text{H}_2\text{O}$	-9.26	28.73	37.99	$\text{CaAl}_2\text{O}_4 \cdot 10\text{H}_2\text{O}$
CaAl_4O_7	-19.64	48.95	68.59	CaAl_4O_7
Calcite	-2.62	-0.80	1.82	CaCO_3
Carnallite	-20.90	-16.63	4.27	$\text{KMgCl}_3 \cdot 6\text{H}_2\text{O}$
$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}(\text{beta})$	-1.96	-5.50	-3.54	$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$
$\text{CH}_4(\text{g})$	-137.92	-140.76	-2.84	CH_4
Chalcanthite	-4.10	-6.73	-2.63	$\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$
Chalcocite	-124.71	-159.45	-34.74	Cu_2S
Chalcocyanite	-9.64	-6.73	2.91	CuSO_4
Chalcopyrite	-238.81	-271.41	-32.60	CuFeS_2
Chloromagnesite	-31.67	-9.86	21.82	MgCl_2
$\text{Cl}_2(\text{g})$	-23.90	-20.90	2.99	Cl_2
Claudetite	-56.32	-76.12	-19.80	As_2O_3
$\text{CO}(\text{g})$	-44.83	-47.83	-3.00	CO
$\text{CO}_2(\text{g})$	-1.48	-9.31	-7.83	CO_2
Corundum	1.92	20.22	18.29	Al_2O_3
Covellite	-109.51	-132.37	-22.86	CuS
Cu	-21.05	10.44	31.50	Cu
$\text{Cu}(\text{g})$	-73.21	10.44	83.66	Cu
CuCl_2	-14.18	-10.46	3.72	CuCl_2
Cuprite	-17.89	-19.79	-1.91	Cu_2O
Dawsonite	-0.68	3.66	4.34	$\text{NaAlCO}_3(\text{OH})_2$
Delafossite	4.05	-2.38	-6.44	CuFeO_2
Diaspore	2.96	10.11	7.15	AlHO_2
Dolomite	-4.70	-2.22	2.47	$\text{CaMg}(\text{CO}_3)_2$
Dolomite-dis	-6.24	-2.22	4.01	$\text{CaMg}(\text{CO}_3)_2$
Dolomite-ord	-4.69	-2.22	2.46	$\text{CaMg}(\text{CO}_3)_2$
Epsomite	-4.17	-6.13	-1.96	$\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$
Ettringite	-33.19	29.27	62.46	$\text{Ca}_6\text{Al}_2(\text{SO}_4)_3(\text{OH})_{12} \cdot 26\text{H}_2\text{O}$
Fe	-55.24	3.77	59.02	Fe
$\text{Fe}(\text{OH})_2$	-13.28	0.61	13.89	$\text{Fe}(\text{OH})_2$
$\text{Fe}(\text{OH})_3$	1.88	7.51	5.64	$\text{Fe}(\text{OH})_3$
$\text{Fe}_2(\text{SO}_4)_3$	-30.05	-27.01	3.05	$\text{Fe}_2(\text{SO}_4)_3$
FeO	-12.91	0.61	13.52	FeO
Ferrite-Ca	2.05	23.55	21.50	CaFe_2O_4
Ferrite-Cu	12.03	22.31	10.28	CuFe_2O_4
Ferrite-Dicalcium	-24.74	32.06	56.80	$\text{Ca}_2\text{Fe}_2\text{O}_5$
Ferrite-Mg	1.89	22.91	21.02	MgFe_2O_4
Ferrite-Zn	10.02	21.72	11.70	ZnFe_2O_4
FeSO_4	-16.00	-13.40	2.61	FeSO_4
Gaylussite	-15.54	-4.37	11.16	$\text{CaNa}_2(\text{CO}_3)_2 \cdot 5\text{H}_2\text{O}$
Gibbsite	2.37	10.11	7.74	$\text{Al}(\text{OH})_3$
Glauberite	-8.30	-13.77	-5.47	$\text{Na}_2\text{Ca}(\text{SO}_4)_2$

Goethite	6.98	7.52	0.53	FeOOH
Gypsum	-0.97	-5.50	-4.53	CaSO4:2H2O
H2(g)	-39.84	-42.94	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-131.66	-139.66	-7.99	H2S
Halite	-7.57	-6.00	1.56	NaCl
Hausmannite	-0.05	10.09	10.14	Mn3O4
HCl(g)	-15.17	-8.87	6.30	HCl
Hematite	14.96	15.03	0.08	Fe2O3
Hercynite	-7.97	20.83	28.80	FeAl2O4
Hexahydrite	-4.40	-6.13	-1.73	MgSO4:6H2O
Huntite	-15.30	-5.08	10.22	CaMg3(CO3)4
Hydromagnesite	-28.57	2.17	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-20.97	-9.23	11.75	CaCl2
Hydrozincite	-15.46	14.84	30.31	Zn5(OH)6(CO3)2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	6.04	-3.38	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	2.84	-2.61	-5.45	NaFe3(SO4)2(OH)6
K	-67.29	3.68	70.98	K
K(g)	-77.89	3.68	81.58	K
K2CO3:1.5H2O	-18.48	-5.10	13.38	K2CO3:1.5H2O
K2O	-79.83	4.21	84.04	K2O
K3H(SO4)2	-18.09	-21.71	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-66.75	-39.04	27.71	K8H4(CO3)6:3H2O
Kainite	-12.59	-12.90	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-19.09	-15.81	3.27	KAl(SO4)2
Kalinite	-7.49	-7.21	0.28	KHCO3
Katoite	-33.18	45.76	78.94	Ca3Al2H12O12
Kieserite	-5.86	-6.13	-0.27	MgSO4:H2O
KMgCl3	-37.87	-16.63	21.25	KMgCl3
KMgCl3:2H2O	-30.59	-16.63	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-14.60	-4.34	10.26	KNaCO3:6H2O
Lammerite	-1.08	0.48	1.55	Cu3(AsO4)2
Lansfordite	-6.27	-1.43	4.84	MgCO3:5H2O
Lawrencite	-26.18	-17.13	9.05	FeCl2
Leonite	-11.82	-15.93	-4.11	K2Mg(SO4)2:4H2O
Lime	-24.05	8.52	32.57	CaO
Magnesite	-3.70	-1.43	2.27	MgCO3
Magnetite	5.23	15.64	10.42	Fe3O4
Malachite	-0.64	5.26	5.90	Cu2CO3(OH)2
Manganite	1.64	1.48	-0.16	MnO(OH)
Manganosite	-10.78	7.13	17.92	MnO
Mayenite	-250.45	243.70	494.15	Ca12Al14O33
Melanterite	-11.00	-13.40	-2.40	FeSO4:7H2O
Mercallite	-10.47	-11.91	-1.44	KHSO4
Mg	-111.48	11.04	122.52	Mg
Mg(g)	-131.20	11.04	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-9.35	-4.16	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-11.40	-2.19	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.59	-9.86	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.16	-9.86	7.30	MgCl2:4H2O
MgCl2:H2O	-25.93	-9.86	16.07	MgCl2:H2O
MgOHCl	-16.88	-0.99	15.89	MgOHCl
MgSO4	-10.96	-6.13	4.83	MgSO4
Mirabilite	-7.12	-8.28	-1.15	Na2SO4:10H2O
Misenite	-70.18	-81.25	-11.08	K8H6(SO4)7
Mn	-72.64	10.29	82.93	Mn
Mn(OH)2(am)	-8.18	7.13	15.31	Mn(OH)2
Mn(OH)3	-4.86	1.48	6.34	Mn(OH)3
MnCl2:2H2O	-14.61	-10.61	4.00	MnCl2:2H2O
MnCl2:4H2O	-13.36	-10.61	2.75	MnCl2:4H2O
MnCl2:H2O	-16.15	-10.61	5.54	MnCl2:H2O
MnO2(gamma)	3.87	-12.25	-16.13	MnO2
MnSO4	-9.49	-6.88	2.61	MnSO4
Molysite	-32.57	-19.10	13.47	FeCl3
Monohydrocalcite	-3.47	-0.80	2.68	CaCO3:H2O
Na	-62.92	4.45	67.37	Na

Na(g)	-76.41	4.45	80.86	Na
Na2CO3	-14.74	-3.58	11.16	Na2CO3
Na2CO3:7H2O	-13.52	-3.58	9.94	Na2CO3:7H2O
Na2O	-61.68	5.74	67.42	Na2O
Na3H(SO4)2	-18.53	-19.42	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.16	-22.05	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-9.50	10.38	19.88	NaFeO2
Nahcolite	-6.30	-6.44	-0.14	NaHCO3
Nantokite	-12.00	-18.77	-6.77	CuCl
Natron	-13.17	-3.58	9.59	Na2CO3:10H2O
Nesquehonite	-6.72	-1.43	5.29	MgCO3:3H2O
O2(g)	-3.43	-6.32	-2.89	O2
Orpiment	-415.60	-495.08	-79.49	As2S3
Oxychloride-Mg	-18.94	6.89	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.74	-6.13	-1.39	MgSO4:5H2O
Periclase	-13.44	7.88	21.33	MgO
Picromerite	-11.49	-15.93	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-15.70	-4.37	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-12.61	-26.93	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-14.03	8.52	22.55	Ca(OH)2
Pyrite	-222.59	-247.29	-24.70	FeS2
Pyrolusite	5.41	-12.25	-17.66	MnO2
Pyrrhotite	-135.30	-139.04	-3.74	FeS
Realgar	-161.44	-221.72	-60.28	AsS
Rhodochrosite	-1.96	-2.18	-0.22	MnCO3
S	-97.70	-142.82	-45.11	S
S2(g)	-209.30	-216.49	-7.19	S2
Scacchite	-19.35	-10.61	8.74	MnCl2
Siderite	-8.48	-8.70	-0.22	FeCO3
Smithsonite	-3.06	-2.62	0.44	ZnCO3
SO2(g)	-48.53	-48.36	0.18	SO2
Sphalerite	-121.49	-132.96	-11.47	ZnS
Spinel	-9.51	28.10	37.61	Al2MgO4
Starkeyite	-5.13	-6.13	-1.00	MgSO4:4H2O
Sylvite	-7.59	-6.77	0.83	KCl
Syngenite	-7.70	-15.30	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-46.09	-28.95	17.14	Mg2CaCl6:12H2O
Tenorite	-0.36	7.28	7.65	CuO
Thenardite	-7.92	-8.28	-0.36	Na2SO4
Thermonatrite	-14.51	-3.58	10.94	Na2CO3:H2O
Todorokite	23.05	-22.77	-45.82	Mn7O12:3H2O
Troilite	-135.20	-139.04	-3.84	FeS
Trona-K	-23.14	-11.55	11.59	K2NaH(CO3)2:2H2O
Wurtzite	-123.79	-132.96	-9.17	ZnS
Wustite	-11.09	1.31	12.40	Fe.947O
Zincite	-4.51	6.69	11.20	ZnO
Zn	-58.93	9.85	68.79	Zn
Zn(ClO4)2:6H2O	-73.41	-67.78	5.63	Zn(ClO4)2:6H2O
Zn(g)	-75.55	9.85	85.41	Zn
Zn(OH)2(beta)	-5.24	6.69	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-4.97	6.69	11.66	Zn(OH)2
Zn(OH)2(gamma)	-5.19	6.69	11.88	Zn(OH)2
Zn2(OH)3Cl	-10.78	4.52	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-8.21	-0.62	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-10.60	-1.29	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-27.03	-7.94	19.09	Zn3O(SO4)2
ZnCl2	-18.13	-11.05	7.08	ZnCl2
ZnCO3:H2O	-2.76	-2.62	0.14	ZnCO3:H2O
ZnSO4	-10.85	-7.32	3.53	ZnSO4
ZnSO4:6H2O	-5.62	-7.32	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.44	-7.32	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.77	-7.32	-0.55	ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
