
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 1
temp 25
pH 3.098
pe 17
redox pe
units mg/l
density 1
Cl 46.4
S(6) 830
Al 11.6
As 1.7
Ca 78.4
Cu 21.3
Fe 133.5
K 30.3
Mg 8.6
Mn 14.1
Na 19.5
Zn 5.2
C(4) 0
water 1 # kg
SOLUTION 2 AS1
temp 25
units mg/l
pe 10
pH 7.54
Cl 24.2
F 0.25
N(5) 2.9
S(6) 243
Al 0
As 0.0966
Ca 86.82
Cu 0.113
Fe 0
Hg 0
K 3.07
Mg 16.17
Mn 0.181
Na 43.01
Ni 0

```

Pb      0
Zn      0.195
MIX 4
      1      1
      2      3
SELECTED_OUTPUT
file          DAM_AGUASUP
ph            true
percent_error true
totals        Al  As  Cu  Fe  Mg  Mn  Zn
              S(6)

```

Beginning of initial solution calculations.

Initial solution 1. Flujo 1

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

Elements	Molality	Moles
Al	4.304e-004	4.304e-004
As	2.272e-005	2.272e-005
Ca	1.959e-003	1.959e-003
Cl	1.310e-003	1.310e-003
Cu	3.356e-004	3.356e-004
Fe	2.393e-003	2.393e-003
K	7.759e-004	7.759e-004
Mg	3.543e-004	3.543e-004
Mn	2.570e-004	2.570e-004
Na	8.492e-004	8.492e-004
S(6)	8.652e-003	8.652e-003
Zn	7.962e-005	7.962e-005

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

```

pH = 3.098
pe = 17.000
Activity of water = 1.000
Ionic strength = 2.715e-002
Mass of water (kg) = 1.000e+000
Total alkalinity (eq/kg) = -3.600e-003
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = -3.759e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -13.38
Iterations = 9
Total H = 1.110544e+002
Total O = 5.556248e+001

```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	9.068e-004	7.980e-004	-3.042	-3.098	-0.056
OH-	1.417e-011	1.207e-011	-10.849	-10.918	-0.070
H2O	5.553e+001	9.997e-001	1.744	-0.000	0.000
Al	4.304e-004				
AlSO4+	2.135e-004	1.825e-004	-3.671	-3.739	-0.068
Al+3	1.537e-004	4.763e-005	-3.813	-4.322	-0.509
Al(SO4)2-	6.205e-005	5.304e-005	-4.207	-4.275	-0.068
AlOH+2	1.244e-006	6.684e-007	-5.905	-6.175	-0.270
Al(OH)2+	2.275e-009	1.944e-009	-8.643	-8.711	-0.068
Al2(OH)2+4	7.923e-010	7.265e-011	-9.101	-10.139	-1.038
HALO2	3.546e-012	3.546e-012	-11.450	-11.450	0.000

Al3(OH)4+5	1.360e-013	3.505e-015	-12.866	-14.455	-1.589
AlO2-	1.781e-015	1.522e-015	-14.749	-14.818	-0.068
NaAlO2	2.057e-019	2.057e-019	-18.687	-18.687	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-52.670	-55.785	-3.115
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-151.853	-151.853	0.000
As(3)	9.018e-027				
HAsO2	4.812e-027	4.812e-027	-26.318	-26.318	0.000
As(OH)3	4.206e-027	4.206e-027	-26.376	-26.376	0.000
H2AsO3-	3.771e-033	3.223e-033	-32.424	-32.492	-0.068
AsO2-	3.606e-033	3.082e-033	-32.443	-32.511	-0.068
AsO2OH-2	0.000e+000	0.000e+000	-40.128	-40.404	-0.276
As(5)	2.272e-005				
H2AsO4-	2.027e-005	1.733e-005	-4.693	-4.761	-0.068
H3AsO4	2.436e-006	2.436e-006	-5.613	-5.613	0.000
HAsO4-2	6.805e-009	3.605e-009	-8.167	-8.443	-0.276
AsO4-3	4.856e-017	1.159e-017	-16.314	-16.936	-0.622
Ca	1.959e-003				
Ca+2	1.500e-003	8.374e-004	-2.824	-3.077	-0.253
CaSO4	4.580e-004	4.580e-004	-3.339	-3.339	0.000
CaCl+	2.306e-007	1.971e-007	-6.637	-6.705	-0.068
CaCl2	2.574e-010	2.574e-010	-9.589	-9.589	0.000
CaOH+	1.734e-013	1.482e-013	-12.761	-12.829	-0.068
Cl(-1)	1.310e-003				
Cl-	1.309e-003	1.110e-003	-2.883	-2.955	-0.071
CuCl+	4.495e-007	3.842e-007	-6.347	-6.415	-0.068
MnCl+	2.615e-007	2.235e-007	-6.583	-6.651	-0.068
CaCl+	2.306e-007	1.971e-007	-6.637	-6.705	-0.068
HCl	1.990e-007	1.990e-007	-6.701	-6.701	0.000
NaCl	1.382e-007	1.382e-007	-6.859	-6.859	0.000
MgCl+	1.323e-007	1.131e-007	-6.878	-6.946	-0.068
ZnCl+	6.734e-008	5.756e-008	-7.172	-7.240	-0.068
FeCl+2	3.035e-008	1.630e-008	-7.518	-7.788	-0.270
KCl	2.383e-008	2.383e-008	-7.623	-7.623	0.000
FeCl2+	1.715e-008	1.466e-008	-7.766	-7.834	-0.068
CaCl2	2.574e-010	2.574e-010	-9.589	-9.589	0.000
CuCl2	2.247e-010	2.247e-010	-9.648	-9.648	0.000
ZnCl2	7.466e-011	7.466e-011	-10.127	-10.127	0.000
FeCl+	8.697e-012	7.434e-012	-11.061	-11.129	-0.068
Zn(OH)Cl	1.233e-012	1.233e-012	-11.909	-11.909	0.000
MnCl3-	7.044e-014	6.021e-014	-13.152	-13.220	-0.068
ZnCl3-	5.357e-014	4.579e-014	-13.271	-13.339	-0.068
ZnCl4-2	7.275e-016	3.854e-016	-15.138	-15.414	-0.276
FeCl2	4.430e-017	4.430e-017	-16.354	-16.354	0.000
FeCl4-	2.542e-017	2.173e-017	-16.595	-16.663	-0.068
CuCl2-	6.618e-020	5.657e-020	-19.179	-19.247	-0.068
CuCl4-2	9.814e-021	5.199e-021	-20.008	-20.284	-0.276
CuCl3-2	7.615e-022	4.034e-022	-21.118	-21.394	-0.276
FeCl4-2	2.980e-022	1.578e-022	-21.526	-21.802	-0.276
Cl(1)	4.019e-017				
HClO	4.019e-017	4.019e-017	-16.396	-16.396	0.000
ClO-	1.589e-021	1.358e-021	-20.799	-20.867	-0.068
Cl(3)	4.974e-032				
HClO2	2.497e-032	2.497e-032	-31.603	-31.603	0.000
ClO2-	2.476e-032	2.117e-032	-31.606	-31.674	-0.068
Cl(5)	2.757e-029				
ClO3-	2.757e-029	2.348e-029	-28.560	-28.629	-0.070
Cl(7)	1.527e-030				
ClO4-	1.526e-030	1.300e-030	-29.816	-29.886	-0.070
ZnClO4+	8.875e-034	7.586e-034	-33.052	-33.120	-0.068
Cu(1)	8.770e-019				
Cu+	8.101e-019	6.924e-019	-18.091	-18.160	-0.068
CuCl2-	6.618e-020	5.657e-020	-19.179	-19.247	-0.068
CuCl3-2	7.615e-022	4.034e-022	-21.118	-21.394	-0.276
Cu(2)	3.356e-004				
Cu+2	2.266e-004	1.265e-004	-3.645	-3.898	-0.253
CuSO4	1.085e-004	1.085e-004	-3.965	-3.965	0.000

CuCl+	4.495e-007	3.842e-007	-6.347	-6.415	-0.068
CuOH+	9.563e-009	8.174e-009	-8.019	-8.088	-0.068
CuCl2	2.247e-010	2.247e-010	-9.648	-9.648	0.000
CuCl4-2	9.814e-021	5.199e-021	-20.008	-20.284	-0.276
CuO2-2	2.089e-031	1.107e-031	-30.680	-30.956	-0.276
Fe(2)	2.193e-008				
Fe+2	1.647e-008	9.190e-009	-7.783	-8.037	-0.253
FeSO4	5.453e-009	5.453e-009	-8.263	-8.263	0.000
FeCl+	8.697e-012	7.434e-012	-11.061	-11.129	-0.068
FeOH+	4.259e-015	3.641e-015	-14.371	-14.439	-0.068
FeCl2	4.430e-017	4.430e-017	-16.354	-16.354	0.000
FeCl4-2	2.980e-022	1.578e-022	-21.526	-21.802	-0.276
Fe(OH)2	3.623e-023	3.623e-023	-22.441	-22.441	0.000
Fe(OH)3-	2.114e-030	1.807e-030	-29.675	-29.743	-0.068
Fe(OH)4-2	0.000e+000	0.000e+000	-41.369	-41.645	-0.276
Fe(3)	2.393e-003				
FeOH+2	1.327e-003	7.127e-004	-2.877	-3.147	-0.270
Fe(OH)2+	3.459e-004	2.956e-004	-3.461	-3.529	-0.068
Fe+3	2.843e-004	8.811e-005	-3.546	-4.055	-0.509
Fe2(OH)2+4	1.491e-004	1.367e-005	-3.827	-4.864	-1.038
FeSO4+	3.734e-005	3.192e-005	-4.428	-4.496	-0.068
Fe3(OH)4+5	3.276e-005	8.444e-007	-4.485	-6.073	-1.589
Fe(SO4)2-	2.364e-006	2.021e-006	-5.626	-5.695	-0.068
Fe(OH)3	1.732e-007	1.732e-007	-6.761	-6.761	0.000
FeCl+2	3.035e-008	1.630e-008	-7.518	-7.788	-0.270
FeCl2+	1.715e-008	1.466e-008	-7.766	-7.834	-0.068
Fe(OH)4-	6.378e-014	5.452e-014	-13.195	-13.263	-0.068
FeCl4-	2.542e-017	2.173e-017	-16.595	-16.663	-0.068
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-43.299	-43.296	0.003
K	7.759e-004				
K+	7.533e-004	6.391e-004	-3.123	-3.194	-0.071
KSO4-	2.260e-005	1.932e-005	-4.646	-4.714	-0.068
KCl	2.383e-008	2.383e-008	-7.623	-7.623	0.000
KHSO4	1.360e-008	1.360e-008	-7.866	-7.866	0.000
KOH	2.776e-015	2.776e-015	-14.557	-14.557	0.000
Mg	3.543e-004				
Mg+2	2.237e-004	1.305e-004	-3.650	-3.884	-0.234
MgSO4	1.305e-004	1.305e-004	-3.884	-3.884	0.000
MgCl+	1.323e-007	1.131e-007	-6.878	-6.946	-0.068
Mg4(OH)4+4	0.000e+000	0.000e+000	-41.859	-42.896	-1.038
Mn(2)	2.570e-004				
Mn+2	1.694e-004	9.453e-005	-3.771	-4.024	-0.253
MnSO4	8.733e-005	8.733e-005	-4.059	-4.059	0.000
MnCl+	2.615e-007	2.235e-007	-6.583	-6.651	-0.068
MnOH+	3.561e-012	3.044e-012	-11.448	-11.517	-0.068
MnCl3-	7.044e-014	6.021e-014	-13.152	-13.220	-0.068
Mn2OH+3	1.215e-015	3.083e-016	-14.915	-15.511	-0.596
Mn(OH)2	9.361e-021	9.361e-021	-20.029	-20.029	0.000
Mn2(OH)3+	2.588e-023	2.212e-023	-22.587	-22.655	-0.068
Mn(OH)3-	1.287e-029	1.100e-029	-28.890	-28.959	-0.068
Mn(OH)4-2	2.203e-040	1.167e-040	-39.657	-39.933	-0.276
Mn(3)	9.938e-013				
Mn+3	9.938e-013	2.521e-013	-12.003	-12.598	-0.596
Mn(6)	3.873e-030				
MnO4-2	3.873e-030	2.052e-030	-29.412	-29.688	-0.276
Mn(7)	1.061e-022				
MnO4-	1.061e-022	9.036e-023	-21.974	-22.044	-0.070
Na	8.492e-004				
Na+	8.286e-004	7.083e-004	-3.082	-3.150	-0.068
NaSO4-	2.050e-005	1.752e-005	-4.688	-4.756	-0.068
NaCl	1.382e-007	1.382e-007	-6.859	-6.859	0.000
NaOH	1.475e-015	1.475e-015	-14.831	-14.831	0.000
NaAlO2	2.057e-019	2.057e-019	-18.687	-18.687	0.000
O(0)	4.953e-006				
O2	2.476e-006	2.493e-006	-5.606	-5.603	0.003
S(6)	8.652e-003				

SO4-2	7.068e-003	3.744e-003	-2.151	-2.427	-0.276
CaSO4	4.580e-004	4.580e-004	-3.339	-3.339	0.000
HSO4-	3.531e-004	3.018e-004	-3.452	-3.520	-0.068
AlSO4+	2.135e-004	1.825e-004	-3.671	-3.739	-0.068
MgSO4	1.305e-004	1.305e-004	-3.884	-3.884	0.000
CuSO4	1.085e-004	1.085e-004	-3.965	-3.965	0.000
MnSO4	8.733e-005	8.733e-005	-4.059	-4.059	0.000
Al(SO4)2-	6.205e-005	5.304e-005	-4.207	-4.275	-0.068
FeSO4+	3.734e-005	3.192e-005	-4.428	-4.496	-0.068
ZnSO4	2.427e-005	2.427e-005	-4.615	-4.615	0.000
KSO4-	2.260e-005	1.932e-005	-4.646	-4.714	-0.068
NaSO4-	2.050e-005	1.752e-005	-4.688	-4.756	-0.068
Fe(SO4)2-	2.364e-006	2.021e-006	-5.626	-5.695	-0.068
KHSO4	1.360e-008	1.360e-008	-7.866	-7.866	0.000
FeSO4	5.453e-009	5.453e-009	-8.263	-8.263	0.000
H2SO4	2.272e-010	2.272e-010	-9.644	-9.644	0.000
Zn	7.962e-005				
Zn+2	5.528e-005	3.085e-005	-4.257	-4.511	-0.253
ZnSO4	2.427e-005	2.427e-005	-4.615	-4.615	0.000
ZnCl+	6.734e-008	5.756e-008	-7.172	-7.240	-0.068
ZnCl2	7.466e-011	7.466e-011	-10.127	-10.127	0.000
ZnOH+	4.959e-011	4.239e-011	-10.305	-10.373	-0.068
Zn(OH)Cl	1.233e-012	1.233e-012	-11.909	-11.909	0.000
ZnCl3-	5.357e-014	4.579e-014	-13.271	-13.339	-0.068
ZnCl4-2	7.275e-016	3.854e-016	-15.138	-15.414	-0.276
Zn(OH)2	2.274e-016	2.274e-016	-15.643	-15.643	0.000
Zn(OH)3-	1.033e-024	8.831e-025	-23.986	-24.054	-0.068
ZnClO4+	8.875e-034	7.586e-034	-33.052	-33.120	-0.068
Zn(OH)4-2	3.560e-034	1.886e-034	-33.448	-33.724	-0.276

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

Phase	SI	log IAP	log KT	
Al	-140.74	9.17	149.91	Al
Al(g)	-191.44	9.17	200.62	Al
Al2(SO4)3	-34.82	-15.92	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-17.48	-15.92	1.56	Al2(SO4)3:6H2O
Alum-K	-7.40	-12.37	-4.97	KAl(SO4)2:12H2O
Alunite	-1.96	-2.43	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.15	-5.50	-4.35	CaSO4
Antarcticite	-13.08	-8.99	4.09	CaCl2:6H2O
Antlerite	-10.46	-1.73	8.73	Cu3(SO4)(OH)4
Aphthitalite	-13.70	-17.59	-3.89	NaK3(SO4)2
Arcanite	-6.97	-8.82	-1.84	K2SO4
Arsenolite	-51.34	-71.18	-19.84	As2O3
As	-74.07	-31.39	42.68	As
As2O5	-17.85	-15.72	2.14	As2O5
As4O6(cubi)	-102.53	-142.36	-39.82	As4O6
As4O6(mono)	-102.31	-142.36	-40.05	As4O6
Atacamite	-17.18	-2.91	14.26	Cu4Cl2(OH)6
Bassanite	-1.80	-5.50	-3.71	CaSO4:0.5H2O
Birnessite	-11.25	-96.79	-85.55	Mn8O14:5H2O
Bischofite	-14.19	-9.79	4.39	MgCl2:6H2O
Bixbyite	-5.64	-6.61	-0.96	Mn2O3
Bloedite	-12.56	-15.04	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-2.58	4.97	7.55	AlO2H
Brochantite	-14.85	0.57	15.42	Cu4(SO4)(OH)6
Brucite	-13.97	2.31	16.28	Mg(OH)2
Ca	-133.91	5.92	139.83	Ca
Ca(g)	-159.15	5.92	165.07	Ca
Ca2Al2O5:8H2O	-43.39	16.18	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-32.16	-5.87	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-24.16	-6.36	17.80	Ca3(AsO4)2
Ca3Al2O6	-93.73	19.30	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-107.59	32.90	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-84.84	22.42	107.25	Ca4Al2O7:13H2O

Ca4Al2O7:19H2O	-81.27	22.42	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-67.96	0.37	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-33.85	13.06	46.91	CaAl2O4
CaAl2O4:10H2O	-24.93	13.06	37.99	CaAl2O4:10H2O
CaAl4O7	-45.59	23.01	68.59	CaAl4O7
Carnallite	-20.22	-15.94	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.97	-5.50	-3.54	CaSO4:0.5H2O
Chalcanthite	-3.70	-6.33	-2.63	CuSO4:5H2O
Chalcocyanite	-9.24	-6.32	2.91	CuSO4
Chloromagnesite	-31.61	-9.79	21.82	MgCl2
Cl2(g)	-17.90	-14.91	2.99	Cl2
Claudetite	-51.38	-71.18	-19.80	As2O3
Corundum	-8.35	9.94	18.29	Al2O3
Cu	-26.40	5.10	31.50	Cu
Cu(g)	-78.56	5.10	83.66	Cu
CuCl2	-13.53	-9.81	3.72	CuCl2
Cuprite	-28.22	-30.12	-1.91	Cu2O
Delafossite	-3.39	-9.82	-6.44	CuFeO2
Diaspore	-2.17	4.97	7.15	AlHO2
Epsomite	-4.35	-6.31	-1.96	MgSO4:7H2O
Ettringite	-59.68	2.78	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-58.06	0.96	59.02	Fe
Fe(OH)2	-15.74	-1.84	13.89	Fe(OH)2
Fe(OH)3	-0.40	5.24	5.64	Fe(OH)3
Fe2(SO4)3	-18.44	-15.39	3.05	Fe2(SO4)3
FeO	-15.36	-1.84	13.52	FeO
Ferrite-Ca	-7.90	13.60	21.50	CaFe2O4
Ferrite-Cu	2.49	12.78	10.28	CuFe2O4
Ferrite-Dicalcium	-40.08	16.72	56.80	Ca2Fe2O5
Ferrite-Mg	-8.23	12.79	21.02	MgFe2O4
Ferrite-Zn	0.46	12.16	11.70	ZnFe2O4
FeSO4	-13.07	-10.46	2.61	FeSO4
Gibbsite	-2.77	4.97	7.74	Al(OH)3
Glauberite	-8.76	-14.23	-5.47	Na2Ca(SO4)2
Goethite	4.71	5.24	0.53	FeOOH
Gypsum	-0.97	-5.50	-4.53	CaSO4:2H2O
H2(g)	-40.20	-43.30	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.67	-6.10	1.56	NaCl
Hausmannite	-14.58	-4.44	10.14	Mn3O4
HCl(g)	-12.35	-6.05	6.30	HCl
Hematite	10.40	10.48	0.08	Fe2O3
Hercynite	-20.70	8.10	28.80	FeAl2O4
Hexahydrite	-4.59	-6.31	-1.73	MgSO4:6H2O
Hydrophilite	-20.73	-8.99	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	7.79	-1.63	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	3.87	-1.58	-5.45	NaFe3(SO4)2(OH)6
K	-69.67	1.30	70.98	K
K(g)	-80.27	1.30	81.58	K
K2O	-84.23	-0.19	84.04	K2O
K3H(SO4)2	-13.91	-17.53	-3.62	K3H(SO4)2
Kainite	-12.15	-12.46	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-15.64	-12.37	3.27	KAl(SO4)2
Katoite	-59.64	19.30	78.94	Ca3Al2H12O12
Kieserite	-6.04	-6.31	-0.27	MgSO4:H2O
KMgCl3	-37.19	-15.94	21.25	KMgCl3
KMgCl3:2H2O	-29.90	-15.94	13.96	KMgCl3:2H2O
Lammerite	-10.38	-8.82	1.55	Cu3(AsO4)2
Lawrencite	-23.00	-13.95	9.05	FeCl2
Leonite	-11.01	-15.13	-4.11	K2Mg(SO4)2:4H2O
Lime	-29.45	3.12	32.57	CaO
Magnetite	-1.78	8.64	10.42	Fe3O4
Manganite	-3.14	-3.30	-0.16	MnO(OH)
Manganosite	-15.74	2.17	17.92	MnO
Mayenite	-387.12	107.03	494.15	Ca12Al14O33
Melanterite	-8.07	-10.46	-2.40	FeSO4:7H2O

Mercallite	-7.28	-8.72	-1.44	KHSO4
Mg	-117.41	5.11	122.52	Mg
Mg(g)	-137.13	5.11	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.93	-5.73	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-14.36	-5.16	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.53	-9.79	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.10	-9.79	7.30	MgCl2:4H2O
MgCl2:H2O	-25.87	-9.79	16.07	MgCl2:H2O
MgOHCl	-19.63	-3.74	15.89	MgOHCl
MgSO4	-11.14	-6.31	4.83	MgSO4
Mirabilite	-7.57	-8.73	-1.15	Na2SO4:10H2O
Misenite	-50.05	-61.13	-11.08	K8H6(SO4)7
Mn	-77.96	4.97	82.93	Mn
Mn(OH)2(am)	-13.14	2.17	15.31	Mn(OH)2
Mn(OH)3	-9.65	-3.30	6.34	Mn(OH)3
MnCl2:2H2O	-13.93	-9.93	4.00	MnCl2:2H2O
MnCl2:4H2O	-12.69	-9.93	2.75	MnCl2:4H2O
MnCl2:H2O	-15.48	-9.93	5.54	MnCl2:H2O
MnO2(gamma)	-0.73	-16.86	-16.13	MnO2
MnSO4	-9.06	-6.45	2.61	MnSO4
Molysite	-26.39	-12.92	13.47	FeCl3
Na	-66.02	1.35	67.37	Na
Na(g)	-79.51	1.35	80.86	Na
Na2O	-67.52	-0.10	67.42	Na2O
Na3H(SO4)2	-16.51	-17.40	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-17.06	-22.96	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-14.70	5.19	19.88	NaFeO2
Nantokite	-14.35	-21.11	-6.77	CuCl
O2(g)	-2.71	-5.60	-2.89	O2
Oxychloride-Mg	-27.26	-1.43	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.92	-6.31	-1.39	MgSO4:5H2O
Periclase	-19.01	2.31	21.33	MgO
Picromerite	-10.69	-15.13	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-11.82	-26.13	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-19.43	3.12	22.55	Ca(OH)2
Pyrolusite	0.80	-16.86	-17.66	MnO2
Scacchite	-18.67	-9.93	8.74	MnCl2
Spinel	-25.35	12.25	37.61	Al2MgO4
Starkeyite	-5.31	-6.31	-1.00	MgSO4:4H2O
Sylvite	-6.98	-6.15	0.83	KCl
Syngenite	-6.72	-14.32	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-45.72	-28.57	17.14	Mg2CaCl6:12H2O
Tenorite	-5.35	2.30	7.65	CuO
Thenardite	-8.37	-8.73	-0.36	Na2SO4
Todorokite	-9.89	-55.71	-45.82	Mn7O12:3H2O
Wustite	-13.40	-0.99	12.40	Fe.947O
Zincite	-9.51	1.69	11.20	ZnO
Zn	-64.30	4.49	68.79	Zn
Zn(ClO4)2:6H2O	-69.92	-64.28	5.63	Zn(ClO4)2:6H2O
Zn(g)	-80.92	4.49	85.41	Zn
Zn(OH)2(beta)	-10.25	1.69	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-9.98	1.69	11.66	Zn(OH)2
Zn(OH)2(gamma)	-10.20	1.69	11.88	Zn(OH)2
Zn2(OH)3Cl	-17.97	-2.68	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-12.83	-5.25	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-19.97	-10.66	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-31.28	-12.19	19.09	Zn3O(SO4)2
ZnCl2	-17.50	-10.42	7.08	ZnCl2
ZnSO4	-10.47	-6.94	3.53	ZnSO4
ZnSO4:6H2O	-5.24	-6.94	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.06	-6.94	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.39	-6.94	-0.55	ZnSO4:H2O

Initial solution 2. AS1

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

Elements	Molality	Moles
As	1.290e-006	1.290e-006
Ca	2.167e-003	2.167e-003
Cl	6.829e-004	6.829e-004
Cu	1.779e-006	1.779e-006
F	1.316e-005	1.316e-005
K	7.855e-005	7.855e-005
Mg	6.656e-004	6.656e-004
Mn	3.296e-006	3.296e-006
N(5)	2.071e-004	2.071e-004
Na	1.872e-003	1.872e-003
S(6)	2.531e-003	2.531e-003
Zn	2.983e-006	2.983e-006

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

pH = 7.540
 pe = 10.000
 Activity of water = 1.000
 Ionic strength = 1.056e-002
 Mass of water (kg) = 1.000e+000
 Total alkalinity (eq/kg) = 1.343e-006
 Total carbon (mol/kg) = 0.000e+000
 Total CO2 (mol/kg) = 0.000e+000
 Temperature (deg C) = 25.000
 Electrical balance (eq) = 1.664e-003
 Percent error, $100 \cdot (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = 13.88
 Iterations = 24
 Total H = 1.110507e+002
 Total O = 5.553608e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	3.718e-007	3.340e-007	-6.430	-6.476	-0.047
H+	3.161e-008	2.884e-008	-7.500	-7.540	-0.040
H2O	5.553e+001	9.999e-001	1.744	-0.000	0.000
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-172.417	-172.417	0.000
As(3)	0.000e+000				
HAsO2	0.000e+000	0.000e+000	-62.230	-62.230	0.000
As(OH)3	0.000e+000	0.000e+000	-62.288	-62.288	0.000
H2AsO3-	0.000e+000	0.000e+000	-63.916	-63.962	-0.046
AsO2-	0.000e+000	0.000e+000	-63.936	-63.981	-0.046
AsO2OH-2	0.000e+000	0.000e+000	-67.247	-67.432	-0.185
As(5)	1.290e-006				
AsO3F-2	1.270e-006	8.301e-007	-5.896	-6.081	-0.185
HAsO3F-	1.976e-008	1.778e-008	-7.704	-7.750	-0.046
HAsO4-2	0.000e+000	0.000e+000	-40.403	-40.587	-0.185
H2AsO4-	0.000e+000	0.000e+000	-41.302	-41.347	-0.046
AsO4-3	0.000e+000	0.000e+000	-44.222	-44.638	-0.416
H3AsO4	0.000e+000	0.000e+000	-46.642	-46.642	0.000
Ca	2.167e-003				
Ca+2	1.907e-003	1.277e-003	-2.720	-2.894	-0.174
CaSO4	2.583e-004	2.583e-004	-3.588	-3.588	0.000
CaNO3+	1.313e-006	1.181e-006	-5.882	-5.928	-0.046
CaCl+	1.840e-007	1.656e-007	-6.735	-6.781	-0.046
CaF+	7.576e-008	6.817e-008	-7.121	-7.166	-0.046
CaOH+	6.949e-009	6.252e-009	-8.158	-8.204	-0.046
CaCl2	1.192e-010	1.192e-010	-9.924	-9.924	0.000
Cl(-1)	6.829e-004				
Cl-	6.823e-004	6.119e-004	-3.166	-3.213	-0.047
MgCl+	1.928e-007	1.735e-007	-6.715	-6.761	-0.046
CaCl+	1.840e-007	1.656e-007	-6.735	-6.781	-0.046

NaCl	1.795e-007	1.795e-007	-6.746	-6.746	0.000
MnCl+	2.596e-009	2.336e-009	-8.586	-8.632	-0.046
ZnCl+	1.858e-009	1.672e-009	-8.731	-8.777	-0.046
KCl	1.432e-009	1.432e-009	-8.844	-8.844	0.000
Zn(OH)Cl	9.910e-010	9.910e-010	-9.004	-9.004	0.000
CuCl+	8.707e-010	7.835e-010	-9.060	-9.106	-0.046
CaCl2	1.192e-010	1.192e-010	-9.924	-9.924	0.000
HCl	3.964e-012	3.964e-012	-11.402	-11.402	0.000
ZnCl2	1.195e-012	1.195e-012	-11.923	-11.923	0.000
CuCl2	2.525e-013	2.525e-013	-12.598	-12.598	0.000
CuCl2-	7.065e-016	6.357e-016	-15.151	-15.197	-0.046
ZnCl3-	4.488e-016	4.039e-016	-15.348	-15.394	-0.046
MnCl3-	2.124e-016	1.911e-016	-15.673	-15.719	-0.046
CuCl3-2	3.823e-018	2.498e-018	-17.418	-17.602	-0.185
ZnCl4-2	2.866e-018	1.873e-018	-17.543	-17.727	-0.185
CuCl4-2	2.715e-024	1.774e-024	-23.566	-23.751	-0.185
Cl(1)	1.250e-026				
ClO-	6.368e-027	5.730e-027	-26.196	-26.242	-0.046
HClO	6.129e-027	6.129e-027	-26.213	-26.213	0.000
Cl(3)	0.000e+000				
ClO2-	0.000e+000	0.000e+000	-42.119	-42.165	-0.046
HClO2	0.000e+000	0.000e+000	-46.535	-46.535	0.000
Cl(5)	0.000e+000				
ClO3-	0.000e+000	0.000e+000	-44.189	-44.236	-0.047
Cl(7)	0.000e+000				
ClO4-	0.000e+000	0.000e+000	-50.562	-50.609	-0.047
ZnClO4+	0.000e+000	0.000e+000	-55.075	-55.121	-0.046
Cu(1)	2.919e-014				
Cu+	2.848e-014	2.562e-014	-13.546	-13.591	-0.046
CuCl2-	7.065e-016	6.357e-016	-15.151	-15.197	-0.046
CuCl3-2	3.823e-018	2.498e-018	-17.418	-17.602	-0.185
Cu(2)	1.779e-006				
CuOH+	9.303e-007	8.370e-007	-6.031	-6.077	-0.046
Cu+2	6.992e-007	4.681e-007	-6.155	-6.330	-0.174
CuSO4	1.485e-007	1.485e-007	-6.828	-6.828	0.000
CuCl+	8.707e-010	7.835e-010	-9.060	-9.106	-0.046
CuF+	8.661e-011	7.793e-011	-10.062	-10.108	-0.046
CuCl2	2.525e-013	2.525e-013	-12.598	-12.598	0.000
CuO2-2	3.675e-016	2.402e-016	-15.435	-15.620	-0.185
CuCl4-2	2.715e-024	1.774e-024	-23.566	-23.751	-0.185
F	1.316e-005				
F-	1.169e-005	1.050e-005	-4.932	-4.979	-0.047
AsO3F-2	1.270e-006	8.301e-007	-5.896	-6.081	-0.185
MgF+	1.023e-007	9.206e-008	-6.990	-7.036	-0.046
CaF+	7.576e-008	6.817e-008	-7.121	-7.166	-0.046
HAsO3F-	1.976e-008	1.778e-008	-7.704	-7.750	-0.046
NaF	1.875e-009	1.875e-009	-8.727	-8.727	0.000
MnF+	5.633e-010	5.068e-010	-9.249	-9.295	-0.046
HF	4.651e-010	4.651e-010	-9.332	-9.332	0.000
ZnF+	2.681e-010	2.413e-010	-9.572	-9.617	-0.046
CuF+	8.661e-011	7.793e-011	-10.062	-10.108	-0.046
HF2-	1.315e-015	1.183e-015	-14.881	-14.927	-0.046
H2F2	5.380e-019	5.380e-019	-18.269	-18.269	0.000
H(0)	1.317e-038				
H2	6.583e-039	6.600e-039	-38.182	-38.180	0.001
K	7.855e-005				
K+	7.769e-005	6.967e-005	-4.110	-4.157	-0.047
KSO4-	8.657e-007	7.790e-007	-6.063	-6.108	-0.046
KCl	1.432e-009	1.432e-009	-8.844	-8.844	0.000
KOH	8.375e-012	8.375e-012	-11.077	-11.077	0.000
KHSO4	1.982e-014	1.982e-014	-13.703	-13.703	0.000
Mg	6.656e-004				
Mg+2	5.310e-004	3.631e-004	-3.275	-3.440	-0.165
MgSO4	1.343e-004	1.343e-004	-3.872	-3.872	0.000
MgCl+	1.928e-007	1.735e-007	-6.715	-6.761	-0.046
MgF+	1.023e-007	9.206e-008	-6.990	-7.036	-0.046
Mg4(OH)4+4	2.283e-023	4.466e-024	-22.642	-23.350	-0.709

Mn(2)	3.296e-006					
Mn+2	2.678e-006	1.793e-006	-5.572	-5.747	-0.174	
MnSO4	6.126e-007	6.126e-007	-6.213	-6.213	0.000	
MnCl+	2.596e-009	2.336e-009	-8.586	-8.632	-0.046	
MnOH+	1.775e-009	1.597e-009	-8.751	-8.797	-0.046	
MnNO3+	5.828e-010	5.244e-010	-9.234	-9.280	-0.046	
MnF+	5.633e-010	5.068e-010	-9.249	-9.295	-0.046	
Mn(NO3)2	2.432e-013	2.432e-013	-12.614	-12.614	0.000	
Mn2(OH)3+	1.873e-013	1.686e-013	-12.727	-12.773	-0.046	
Mn(OH)2	1.359e-013	1.359e-013	-12.867	-12.867	0.000	
Mn2OH+3	7.780e-015	3.068e-015	-14.109	-14.513	-0.404	
MnCl3-	2.124e-016	1.911e-016	-15.673	-15.719	-0.046	
Mn(OH)3-	4.913e-018	4.421e-018	-17.309	-17.355	-0.046	
Mn(OH)4-2	1.986e-024	1.298e-024	-23.702	-23.887	-0.185	
Mn(3)	1.212e-021					
Mn+3	1.212e-021	4.781e-022	-20.916	-21.320	-0.404	
Mn(6)	2.047e-024					
MnO4-2	2.047e-024	1.338e-024	-23.689	-23.874	-0.185	
Mn(7)	6.557e-024					
MnO4-	6.557e-024	5.890e-024	-23.183	-23.230	-0.047	
N(5)	2.071e-004					
NO3-	2.058e-004	1.846e-004	-3.687	-3.734	-0.047	
CaNO3+	1.313e-006	1.181e-006	-5.882	-5.928	-0.046	
MnNO3+	5.828e-010	5.244e-010	-9.234	-9.280	-0.046	
HNO3	2.784e-013	2.784e-013	-12.555	-12.555	0.000	
Mn(NO3)2	2.432e-013	2.432e-013	-12.614	-12.614	0.000	
Na	1.872e-003					
Na+	1.854e-003	1.669e-003	-2.732	-2.778	-0.046	
NaSO4-	1.697e-005	1.527e-005	-4.770	-4.816	-0.046	
NaCl	1.795e-007	1.795e-007	-6.746	-6.746	0.000	
NaF	1.875e-009	1.875e-009	-8.727	-8.727	0.000	
NaOH	9.616e-011	9.616e-011	-10.017	-10.017	0.000	
O(0)	2.916e-016					
O2	1.458e-016	1.462e-016	-15.836	-15.835	0.001	
S(6)	2.531e-003					
SO4-2	2.119e-003	1.385e-003	-2.674	-2.858	-0.185	
CaSO4	2.583e-004	2.583e-004	-3.588	-3.588	0.000	
MgSO4	1.343e-004	1.343e-004	-3.872	-3.872	0.000	
NaSO4-	1.697e-005	1.527e-005	-4.770	-4.816	-0.046	
KSO4-	8.657e-007	7.790e-007	-6.063	-6.108	-0.046	
MnSO4	6.126e-007	6.126e-007	-6.213	-6.213	0.000	
ZnSO4	4.733e-007	4.733e-007	-6.325	-6.325	0.000	
CuSO4	1.485e-007	1.485e-007	-6.828	-6.828	0.000	
HSO4-	4.485e-009	4.035e-009	-8.348	-8.394	-0.046	
KHSO4	1.982e-014	1.982e-014	-13.703	-13.703	0.000	
H2SO4	1.098e-019	1.098e-019	-18.959	-18.959	0.000	
Zn	2.983e-006					
Zn+2	2.429e-006	1.626e-006	-5.615	-5.789	-0.174	
ZnSO4	4.733e-007	4.733e-007	-6.325	-6.325	0.000	
ZnOH+	6.871e-008	6.182e-008	-7.163	-7.209	-0.046	
Zn(OH)2	9.179e-009	9.179e-009	-8.037	-8.037	0.000	
ZnCl+	1.858e-009	1.672e-009	-8.731	-8.777	-0.046	
Zn(OH)Cl	9.910e-010	9.910e-010	-9.004	-9.004	0.000	
ZnF+	2.681e-010	2.413e-010	-9.572	-9.617	-0.046	
ZnCl2	1.195e-012	1.195e-012	-11.923	-11.923	0.000	
Zn(OH)3-	1.096e-012	9.864e-013	-11.960	-12.006	-0.046	
ZnCl3-	4.488e-016	4.039e-016	-15.348	-15.394	-0.046	
Zn(OH)4-2	8.921e-018	5.830e-018	-17.050	-17.234	-0.185	
ZnCl4-2	2.866e-018	1.873e-018	-17.543	-17.727	-0.185	
ZnClO4+	0.000e+000	0.000e+000	-55.075	-55.121	-0.046	

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

Phase	SI	log IAP	log KT	
Anhydrite	-1.40	-5.75	-4.35	CaSO4
Antarcticite	-13.41	-9.32	4.09	CaCl2:6H2O

Antlerite	-0.42	8.31	8.73	Cu ₃ (SO ₄)(OH) ₄
Aphthitalite	-17.08	-20.97	-3.89	NaK ₃ (SO ₄) ₂
Arcanite	-9.33	-11.17	-1.84	K ₂ SO ₄
Arsenolite	-123.16	-143.00	-19.84	As ₂ O ₃
As	-102.31	-59.63	42.68	As
As ₂ O ₅	-99.91	-97.77	2.14	As ₂ O ₅
As ₄ O ₆ (cubi)	-246.18	-286.01	-39.82	As ₄ O ₆
As ₄ O ₆ (mono)	-245.96	-286.01	-40.05	As ₄ O ₆
Atacamite	-0.77	13.49	14.26	Cu ₄ Cl ₂ (OH) ₆
Bassanite	-2.05	-5.75	-3.71	CaSO ₄ :0.5H ₂ O
Birnessite	15.35	-70.19	-85.55	Mn ₈ O ₁₄ :5H ₂ O
Bischofite	-14.26	-9.87	4.39	MgCl ₂ :6H ₂ O
Bixbyite	3.56	2.60	-0.96	Mn ₂ O ₃
Bloedite	-12.23	-14.71	-2.48	Na ₂ Mg(SO ₄) ₂ :4H ₂ O
Brochantite	1.64	17.06	15.42	Cu ₄ (SO ₄)(OH) ₆
Brucite	-4.64	11.64	16.28	Mg(OH) ₂
Ca	-119.73	20.10	139.83	Ca
Ca(g)	-144.97	20.10	165.07	Ca
Ca ₂ Cl ₂ (OH) ₂ :H ₂ O	-23.42	2.87	26.29	Ca ₂ Cl ₂ (OH) ₂ :H ₂ O
Ca ₃ (AsO ₄) ₂	-79.02	-61.22	17.80	Ca ₃ (AsO ₄) ₂
Ca ₄ Cl ₂ (OH) ₆ :13H ₂ O	-41.09	27.24	68.33	Ca ₄ Cl ₂ (OH) ₆ :13H ₂ O
Carnallite	-21.51	-17.24	4.27	KMgCl ₃ :6H ₂ O
CaSO ₄ :0.5H ₂ O(beta)	-2.22	-5.75	-3.54	CaSO ₄ :0.5H ₂ O
Chalcanthite	-6.56	-9.19	-2.63	CuSO ₄ :5H ₂ O
Chalcocyanite	-12.10	-9.19	2.91	CuSO ₄
Chloromagnesite	-31.68	-9.87	21.82	MgCl ₂
Cl ₂ (g)	-32.42	-29.42	2.99	Cl ₂
Claudetite	-123.21	-143.00	-19.80	As ₂ O ₃
Cu	-14.83	16.67	31.50	Cu
Cu(g)	-66.99	16.67	83.66	Cu
CuCl ₂	-16.48	-12.76	3.72	CuCl ₂
CuF	-25.65	-18.57	7.08	CuF
CuF ₂	-15.67	-16.29	-0.62	CuF ₂
CuF ₂ :2H ₂ O	-11.74	-16.29	-4.55	CuF ₂ :2H ₂ O
Cuprite	-10.20	-12.10	-1.91	Cu ₂ O
Epsomite	-4.34	-6.30	-1.96	MgSO ₄ :7H ₂ O
F ₂ (g)	-88.67	-32.95	55.71	F ₂
Fluorite	-2.78	-12.85	-10.07	CaF ₂
Glauberite	-8.70	-14.17	-5.47	Na ₂ Ca(SO ₄) ₂
Gypsum	-1.22	-5.75	-4.53	CaSO ₄ :2H ₂ O
H ₂ (g)	-35.08	-38.18	-3.10	H ₂
H ₂ O(g)	-1.59	-0.00	1.59	H ₂ O
Halite	-7.55	-5.99	1.56	NaCl
Hausmannite	1.79	11.93	10.14	Mn ₃ O ₄
HCl(g)	-17.06	-10.75	6.30	HCl
Hexahydrate	-4.57	-6.30	-1.73	MgSO ₄ :6H ₂ O
Hydrophilite	-21.07	-9.32	11.75	CaCl ₂
Ice	-0.14	-0.00	0.14	H ₂ O
K	-63.63	7.34	70.98	K
K(g)	-74.24	7.34	81.58	K
K ₂ O	-77.27	6.77	84.04	K ₂ O
K ₃ H(SO ₄) ₂	-22.10	-25.73	-3.62	K ₃ H(SO ₄) ₂
Kainite	-13.36	-13.67	-0.31	KMgClSO ₄ :3H ₂ O
Kieserite	-6.03	-6.30	-0.27	MgSO ₄ :H ₂ O
KMgCl ₃	-38.48	-17.24	21.25	KMgCl ₃
KMgCl ₃ :2H ₂ O	-31.20	-17.24	13.96	KMgCl ₃ :2H ₂ O
Lammerite	-73.08	-71.52	1.55	Cu ₃ (AsO ₄) ₂
Leonite	-13.36	-17.47	-4.11	K ₂ Mg(SO ₄) ₂ :4H ₂ O
Lime	-20.38	12.19	32.57	CaO
Manganite	1.46	1.30	-0.16	MnO(OH)
Manganosite	-8.58	9.33	17.92	MnO
Mercallite	-13.12	-14.56	-1.44	KHSO ₄
Mg	-102.96	19.56	122.52	Mg
Mg(g)	-122.69	19.56	142.25	Mg
Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O	-8.58	-3.39	5.20	Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O
Mg _{1.5} SO ₄ (OH)	-9.69	-0.48	9.21	Mg _{1.5} SO ₄ (OH)
MgCl ₂ :2H ₂ O	-22.60	-9.87	12.73	MgCl ₂ :2H ₂ O

MgCl2:4H2O	-17.17	-9.87	7.30	MgCl2:4H2O
MgCl2:H2O	-25.94	-9.87	16.07	MgCl2:H2O
MgOHCl	-15.00	0.89	15.89	MgOHCl
MgSO4	-11.13	-6.30	4.83	MgSO4
Mirabilite	-7.26	-8.41	-1.15	Na2SO4:10H2O
Misenite	-87.43	-98.50	-11.08	K8H6(SO4)7
Mn	-65.68	17.25	82.93	Mn
Mn(OH)2(am)	-5.97	9.33	15.31	Mn(OH)2
Mn(OH)3	-5.04	1.30	6.34	Mn(OH)3
MnCl2:2H2O	-16.17	-12.17	4.00	MnCl2:2H2O
MnCl2:4H2O	-14.92	-12.17	2.75	MnCl2:4H2O
MnCl2:H2O	-17.71	-12.17	5.54	MnCl2:H2O
MnO2(gamma)	1.32	-14.81	-16.13	MnO2
MnSO4	-11.21	-8.61	2.61	MnSO4
Na	-58.65	8.72	67.37	Na
Na(g)	-72.14	8.72	80.86	Na
Na2O	-57.89	9.52	67.42	Na2O
Na3H(SO4)2	-20.70	-21.59	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.69	-22.58	-5.89	Na4Ca(SO4)3:2H2O
Nantokite	-10.04	-16.80	-6.77	CuCl
Niter	-7.67	-7.89	-0.22	KNO3
NO2(g)	-15.66	-7.31	8.35	NO2
O2(g)	-12.94	-15.84	-2.89	O2
Oxychloride-Mg	-13.31	12.53	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.91	-6.30	-1.39	MgSO4:5H2O
Periclase	-9.69	11.64	21.33	MgO
Picromerite	-13.03	-17.47	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-14.66	-28.98	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-10.36	12.19	22.55	Ca(OH)2
Pyrolusite	2.85	-14.81	-17.66	MnO2
Scacchite	-20.91	-12.17	8.74	MnCl2
Sellaite	-3.95	-13.40	-9.44	MgF2
Starkeyite	-5.30	-6.30	-1.00	MgSO4:4H2O
Sylvite	-8.20	-7.37	0.83	KCl
Syngenite	-9.32	-16.92	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-46.20	-29.05	17.14	Mg2CaCl6:12H2O
Tenorite	1.10	8.75	7.65	CuO
Thenardite	-8.06	-8.41	-0.36	Na2SO4
Todorokite	14.67	-31.16	-45.82	Mn7O12:3H2O
Zincite	-1.91	9.29	11.20	ZnO
Zn	-51.58	17.21	68.79	Zn
Zn(ClO4)2:6H2O	-112.64	-107.01	5.63	Zn(ClO4)2:6H2O
Zn(g)	-68.20	17.21	85.41	Zn
Zn(NO3)2:6H2O	-16.66	-13.26	3.40	Zn(NO3)2:6H2O
Zn(OH)2(beta)	-2.64	9.29	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-2.37	9.29	11.66	Zn(OH)2
Zn(OH)2(gamma)	-2.59	9.29	11.88	Zn(OH)2
Zn2(OH)3Cl	-7.46	7.83	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-6.94	0.64	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-79.21	-69.90	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-27.09	-8.00	19.09	Zn3O(SO4)2
Zn5(NO3)2(OH)8	-18.76	23.91	42.67	Zn5(NO3)2(OH)8
ZnCl2	-19.29	-12.22	7.08	ZnCl2
ZnF2	-15.25	-15.75	-0.49	ZnF2
ZnSO4	-12.18	-8.65	3.53	ZnSO4
ZnSO4:6H2O	-6.95	-8.65	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-6.77	-8.65	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-8.10	-8.65	-0.55	ZnSO4:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using mix 4.

Mixture 4.

1.000e+000 Solution 1 Flujo 1
 3.000e+000 Solution 2 AS1

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

Elements	Molality	Moles
Al	1.076e-004	4.304e-004
As	6.647e-006	2.659e-005
Ca	2.115e-003	8.460e-003
Cl	8.398e-004	3.359e-003
Cu	8.523e-005	3.409e-004
F	9.873e-006	3.949e-005
Fe	5.983e-004	2.393e-003
K	2.529e-004	1.012e-003
Mg	5.877e-004	2.351e-003
Mn	6.671e-005	2.668e-004
N	1.553e-004	6.214e-004
Na	1.616e-003	6.464e-003
S	4.062e-003	1.625e-002
Zn	2.214e-005	8.857e-005

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

pH	=	3.447	Charge balance
pe	=	16.531	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	1.429e-002	
Mass of water (kg)	=	4.000e+000	
Total alkalinity (eq/kg)	=	-8.988e-004	
Total carbon (mol/kg)	=	0.000e+000	
Total CO2 (mol/kg)	=	0.000e+000	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	1.232e-003	
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	1.93	
Iterations	=	12	
Total H	=	4.442064e+002	
Total O	=	2.221707e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	3.961e-004	3.575e-004	-3.402	-3.447	-0.045
OH-	3.046e-011	2.695e-011	-10.516	-10.570	-0.053
H2O	5.553e+001	9.998e-001	1.744	-0.000	0.000
Al	1.076e-004				
Al+3	4.960e-005	1.948e-005	-4.304	-4.710	-0.406
AlSO4+	4.639e-005	4.113e-005	-4.334	-4.386	-0.052
Al(SO4)2-	7.430e-006	6.588e-006	-5.129	-5.181	-0.052
AlF+2	3.188e-006	1.979e-006	-5.496	-5.704	-0.207
AlOH+2	9.836e-007	6.104e-007	-6.007	-6.214	-0.207
AlF2+	9.023e-009	8.000e-009	-8.045	-8.097	-0.052
Al(OH)2+	4.471e-009	3.964e-009	-8.350	-8.402	-0.052
Al2(OH)2+4	3.856e-010	6.059e-011	-9.414	-10.218	-0.804
HALO2	1.614e-011	1.614e-011	-10.792	-10.792	0.000
AlF3	1.023e-012	1.023e-012	-11.990	-11.990	0.000
Al3(OH)4+5	1.027e-013	5.960e-015	-12.989	-14.225	-1.236
AlO2-	1.744e-014	1.546e-014	-13.758	-13.811	-0.052
NaAlO2	4.169e-018	4.169e-018	-17.380	-17.380	0.000
AlF4-	2.943e-018	2.610e-018	-17.531	-17.583	-0.052
Al13O4(OH)24+7	0.000e+000	0.000e+000	-47.248	-49.671	-2.424
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-186.387	-186.387	0.000

As(3)	0.000e+000					
HAsO2	0.000e+000	0.000e+000	-61.573	-61.573	0.000	
As(OH)3	0.000e+000	0.000e+000	-61.631	-61.631	0.000	
H2AsO3-	0.000e+000	0.000e+000	-67.346	-67.398	-0.052	
AsO2-	0.000e+000	0.000e+000	-67.365	-67.418	-0.052	
AsO2OH-2	0.000e+000	0.000e+000	-74.751	-74.961	-0.211	
HAsS2	0.000e+000	0.000e+000	-311.751	-311.751	0.000	
As(5)	6.647e-006					
HAsO3F-	6.611e-006	5.862e-006	-5.180	-5.232	-0.052	
AsO3F-2	3.588e-008	2.208e-008	-7.445	-7.656	-0.211	
H2AsO4-	1.394e-040	1.236e-040	-39.856	-39.908	-0.052	
H3AsO4	0.000e+000	0.000e+000	-41.109	-41.109	0.000	
HAsO4-2	0.000e+000	0.000e+000	-43.030	-43.241	-0.211	
AsO4-3	0.000e+000	0.000e+000	-50.910	-51.385	-0.475	
Ca	2.115e-003					
Ca+2	1.774e-003	1.127e-003	-2.751	-2.948	-0.197	
CaSO4	3.395e-004	3.395e-004	-3.469	-3.469	0.000	
CaNO3+	8.674e-007	7.691e-007	-6.062	-6.114	-0.052	
CaCl+	1.995e-007	1.769e-007	-6.700	-6.752	-0.052	
CaCl2	1.541e-010	1.541e-010	-9.812	-9.812	0.000	
CaF+	6.560e-011	5.816e-011	-10.183	-10.235	-0.052	
CaOH+	5.020e-013	4.451e-013	-12.299	-12.352	-0.052	
Cl(-1)	8.398e-004					
Cl-	8.390e-004	7.407e-004	-3.076	-3.130	-0.054	
CaCl+	1.995e-007	1.769e-007	-6.700	-6.752	-0.052	
NaCl	1.840e-007	1.840e-007	-6.735	-6.735	0.000	
MgCl+	1.839e-007	1.631e-007	-6.735	-6.788	-0.052	
CuCl+	9.499e-008	8.423e-008	-7.022	-7.075	-0.052	
HCl	5.947e-008	5.947e-008	-7.226	-7.226	0.000	
MnCl+	5.688e-008	5.043e-008	-7.245	-7.297	-0.052	
ZnCl+	1.546e-008	1.371e-008	-7.811	-7.863	-0.052	
KCl	5.463e-009	5.463e-009	-8.263	-8.263	0.000	
FeCl+2	2.277e-009	1.413e-009	-8.643	-8.850	-0.207	
FeCl2+	9.558e-010	8.475e-010	-9.020	-9.072	-0.052	
CaCl2	1.541e-010	1.541e-010	-9.812	-9.812	0.000	
CuCl2	3.285e-011	3.285e-011	-10.483	-10.483	0.000	
ZnCl2	1.186e-011	1.186e-011	-10.926	-10.926	0.000	
FeCl+	2.140e-012	1.897e-012	-11.670	-11.722	-0.052	
Zn(OH)Cl	6.556e-013	6.556e-013	-12.183	-12.183	0.000	
MnCl3-	6.817e-015	6.044e-015	-14.166	-14.219	-0.052	
ZnCl3-	5.472e-015	4.852e-015	-14.262	-14.314	-0.052	
ZnCl4-2	4.425e-017	2.724e-017	-16.354	-16.565	-0.211	
FeCl2	7.541e-018	7.541e-018	-17.123	-17.123	0.000	
FeCl4-	6.304e-019	5.590e-019	-18.200	-18.253	-0.052	
CuCl2-	2.746e-020	2.435e-020	-19.561	-19.613	-0.052	
CuCl4-2	5.495e-022	3.383e-022	-21.260	-21.471	-0.211	
CuCl3-2	1.882e-022	1.158e-022	-21.725	-21.936	-0.211	
FeCl4-2	1.942e-023	1.195e-023	-22.712	-22.922	-0.211	
Cl(1)	6.906e-018					
HClO	6.905e-018	6.905e-018	-17.161	-17.161	0.000	
ClO-	5.874e-022	5.208e-022	-21.231	-21.283	-0.052	
Cl(3)	7.733e-033					
ClO2-	5.265e-033	4.669e-033	-32.279	-32.331	-0.052	
HClO2	2.467e-033	2.467e-033	-32.608	-32.608	0.000	
Cl(5)	3.366e-030					
ClO3-	3.366e-030	2.978e-030	-29.473	-29.526	-0.053	
Cl(7)	1.072e-031					
ClO4-	1.071e-031	9.480e-032	-30.970	-31.023	-0.053	
ZnClO4+	2.228e-035	1.975e-035	-34.652	-34.704	-0.052	
Cu(1)	7.833e-019					
Cu+	7.556e-019	6.700e-019	-18.122	-18.174	-0.052	
CuCl2-	2.746e-020	2.435e-020	-19.561	-19.613	-0.052	
CuCl3-2	1.882e-022	1.158e-022	-21.725	-21.936	-0.211	
Cu(2)	8.523e-005					
Cu+2	6.548e-005	4.157e-005	-4.184	-4.381	-0.197	
CuSO4	1.965e-005	1.965e-005	-4.707	-4.707	0.000	
CuCl+	9.499e-008	8.423e-008	-7.022	-7.075	-0.052	

	CuOH+	6.764e-009	5.998e-009	-8.170	-8.222	-0.052
	CuCl2	3.285e-011	3.285e-011	-10.483	-10.483	0.000
	CuF+	7.547e-012	6.692e-012	-11.122	-11.174	-0.052
	CuNO2+	4.308e-019	3.819e-019	-18.366	-18.418	-0.052
	CuCl4-2	5.495e-022	3.383e-022	-21.260	-21.471	-0.211
	CuO2-2	1.468e-030	9.034e-031	-29.833	-30.044	-0.211
	Cu(NO2)2	3.429e-034	3.429e-034	-33.465	-33.465	0.000
	CuNH3+2	0.000e+000	0.000e+000	-57.347	-57.554	-0.207
	Cu(NH3)2+2	0.000e+000	0.000e+000	-111.126	-111.333	-0.207
	Cu(NH3)3+2	0.000e+000	0.000e+000	-165.518	-165.725	-0.207
F		9.873e-006				
	HAsO3F-	6.611e-006	5.862e-006	-5.180	-5.232	-0.052
	AlF+2	3.188e-006	1.979e-006	-5.496	-5.704	-0.207
	AsO3F-2	3.588e-008	2.208e-008	-7.445	-7.656	-0.211
	F-	1.148e-008	1.016e-008	-7.940	-7.993	-0.053
	AlF2+	9.023e-009	8.000e-009	-8.045	-8.097	-0.052
	HF	5.574e-009	5.574e-009	-8.254	-8.254	0.000
	FeF+2	2.811e-009	1.744e-009	-8.551	-8.758	-0.207
	MgF+	7.795e-011	6.912e-011	-10.108	-10.160	-0.052
	CaF+	6.560e-011	5.816e-011	-10.183	-10.235	-0.052
	MnF+	9.859e-012	8.742e-012	-11.006	-11.058	-0.052
	CuF+	7.547e-012	6.692e-012	-11.122	-11.174	-0.052
	ZnF+	1.782e-012	1.580e-012	-11.749	-11.801	-0.052
	NaF	1.535e-012	1.535e-012	-11.814	-11.814	0.000
	AlF3	1.023e-012	1.023e-012	-11.990	-11.990	0.000
	FeF2+	3.233e-013	2.867e-013	-12.490	-12.543	-0.052
	FeF+	9.226e-016	8.181e-016	-15.035	-15.087	-0.052
	H2F2	7.727e-017	7.727e-017	-16.112	-16.112	0.000
	HF2-	1.547e-017	1.371e-017	-16.811	-16.863	-0.052
	AlF4-	2.943e-018	2.610e-018	-17.531	-17.583	-0.052
Fe(2)		6.690e-009				
	Fe+2	5.538e-009	3.516e-009	-8.257	-8.454	-0.197
	FeSO4	1.150e-009	1.150e-009	-8.939	-8.939	0.000
	FeCl+	2.140e-012	1.897e-012	-11.670	-11.722	-0.052
	FeOH+	3.507e-015	3.110e-015	-14.455	-14.507	-0.052
	FeF+	9.226e-016	8.181e-016	-15.035	-15.087	-0.052
	FeCl2	7.541e-018	7.541e-018	-17.123	-17.123	0.000
	Fe(OH)2	6.908e-023	6.908e-023	-22.161	-22.161	0.000
	FeCl4-2	1.942e-023	1.195e-023	-22.712	-22.922	-0.211
	Fe(OH)3-	8.675e-030	7.692e-030	-29.062	-29.114	-0.052
	Fe(OH)4-2	0.000e+000	0.000e+000	-40.457	-40.667	-0.211
Fe(3)		5.983e-004				
	FeOH+2	3.332e-004	2.068e-004	-3.477	-3.684	-0.207
	Fe(OH)2+	2.160e-004	1.915e-004	-3.666	-3.718	-0.052
	Fe+3	2.916e-005	1.145e-005	-4.535	-4.941	-0.406
	Fe2(OH)2+4	7.324e-006	1.151e-006	-5.135	-5.939	-0.804
	FeSO4+	2.578e-006	2.286e-006	-5.589	-5.641	-0.052
	Fe3(OH)4+5	7.932e-007	4.605e-008	-6.101	-7.337	-1.236
	Fe(OH)3	2.505e-007	2.505e-007	-6.601	-6.601	0.000
	Fe(SO4)2-	8.993e-008	7.974e-008	-7.046	-7.098	-0.052
	FeNO3+2	2.514e-008	1.560e-008	-7.600	-7.807	-0.207
	FeF+2	2.811e-009	1.744e-009	-8.551	-8.758	-0.207
	FeCl+2	2.277e-009	1.413e-009	-8.643	-8.850	-0.207
	FeCl2+	9.558e-010	8.475e-010	-9.020	-9.072	-0.052
	FeF2+	3.233e-013	2.867e-013	-12.490	-12.543	-0.052
	Fe(OH)4-	1.985e-013	1.760e-013	-12.702	-12.755	-0.052
	FeNO2+2	2.287e-018	1.419e-018	-17.641	-17.848	-0.207
	FeCl4-	6.304e-019	5.590e-019	-18.200	-18.253	-0.052
H(0)		0.000e+000				
	H2	0.000e+000	0.000e+000	-43.058	-43.056	0.002
K		2.529e-004				
	K+	2.488e-004	2.196e-004	-3.604	-3.658	-0.054
	KSO4-	4.125e-006	3.658e-006	-5.385	-5.437	-0.052
	KCl	5.463e-009	5.463e-009	-8.263	-8.263	0.000
	KHSO4	1.154e-009	1.154e-009	-8.938	-8.938	0.000
	KOH	2.130e-015	2.130e-015	-14.672	-14.672	0.000
Mg		5.877e-004				

Mg+2	4.322e-004	2.820e-004	-3.364	-3.550	-0.185
MgSO4	1.554e-004	1.554e-004	-3.809	-3.809	0.000
MgCl+	1.839e-007	1.631e-007	-6.735	-6.788	-0.052
MgF+	7.795e-011	6.912e-011	-10.108	-10.160	-0.052
Mg4(OH)4+4	4.378e-040	0.000e+000	-39.359	-40.162	-0.804
Mn(2)	6.671e-005				
Mn+2	5.037e-005	3.198e-005	-4.298	-4.495	-0.197
MnSO4	1.628e-005	1.628e-005	-4.788	-4.788	0.000
MnCl+	5.688e-008	5.043e-008	-7.245	-7.297	-0.052
MnNO3+	7.786e-009	6.904e-009	-8.109	-8.161	-0.052
MnF+	9.859e-012	8.742e-012	-11.006	-11.058	-0.052
MnOH+	2.593e-012	2.299e-012	-11.586	-11.638	-0.052
Mn(NO3)2	2.362e-012	2.362e-012	-11.627	-11.627	0.000
MnCl3-	6.817e-015	6.044e-015	-14.166	-14.219	-0.052
Mn2OH+3	2.268e-016	7.877e-017	-15.644	-16.104	-0.459
Mn(OH)2	1.578e-020	1.578e-020	-19.802	-19.802	0.000
Mn2(OH)3+	3.176e-023	2.816e-023	-22.498	-22.550	-0.052
Mn(OH)3-	4.670e-029	4.140e-029	-28.331	-28.383	-0.052
Mn(OH)4-2	1.593e-039	9.806e-040	-38.798	-39.009	-0.211
Mn(3)	8.342e-014				
Mn+3	8.342e-014	2.897e-014	-13.079	-13.538	-0.459
Mn(6)	9.260e-030				
MnO4-2	9.260e-030	5.700e-030	-29.033	-29.244	-0.211
Mn(7)	9.636e-023				
MnO4-	9.636e-023	8.526e-023	-22.016	-22.069	-0.053
N(-03)	0.000e+000				
HN3	0.000e+000	0.000e+000	-82.157	-82.157	0.000
N3-	0.000e+000	0.000e+000	-83.360	-83.413	-0.052
ZnN3+	0.000e+000	0.000e+000	-87.876	-87.929	-0.052
Zn(N3)2	0.000e+000	0.000e+000	-170.588	-170.588	0.000
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-51.364	-51.420	-0.055
NH3	0.000e+000	0.000e+000	-57.213	-57.213	0.000
CuNH3+2	0.000e+000	0.000e+000	-57.347	-57.554	-0.207
Zn(NH3)+2	0.000e+000	0.000e+000	-59.911	-60.118	-0.207
NH4SO4-	0.000e+000	0.000e+000	-62.353	-62.405	-0.052
Cu(NH3)2+2	0.000e+000	0.000e+000	-111.126	-111.333	-0.207
Zn(NH3)2+2	0.000e+000	0.000e+000	-114.917	-115.124	-0.207
Cu(NH3)3+2	0.000e+000	0.000e+000	-165.518	-165.725	-0.207
Zn(NH3)3+2	0.000e+000	0.000e+000	-169.924	-170.131	-0.207
Zn(NH3)4+2	0.000e+000	0.000e+000	-225.204	-225.411	-0.207
N(0)	1.616e-007				
N2	8.080e-008	8.080e-008	-7.093	-7.093	0.000
N(3)	1.556e-016				
NO2-	9.938e-017	8.774e-017	-16.003	-16.057	-0.054
HNO2	5.353e-017	5.353e-017	-16.271	-16.271	0.000
FeNO2+2	2.287e-018	1.419e-018	-17.641	-17.848	-0.207
CuNO2+	4.308e-019	3.819e-019	-18.366	-18.418	-0.052
Cu(NO2)2	3.429e-034	3.429e-034	-33.465	-33.465	0.000
N(5)	1.552e-004				
NO3-	1.543e-004	1.362e-004	-3.812	-3.866	-0.054
CaNO3+	8.674e-007	7.691e-007	-6.062	-6.114	-0.052
FeNO3+2	2.514e-008	1.560e-008	-7.600	-7.807	-0.207
MnNO3+	7.786e-009	6.904e-009	-8.109	-8.161	-0.052
HNO3	2.547e-009	2.547e-009	-8.594	-8.594	0.000
Mn(NO3)2	2.362e-012	2.362e-012	-11.627	-11.627	0.000
Na	1.616e-003				
Na+	1.594e-003	1.413e-003	-2.797	-2.850	-0.052
NaSO4-	2.173e-005	1.927e-005	-4.663	-4.715	-0.052
NaCl	1.840e-007	1.840e-007	-6.735	-6.735	0.000
NaF	1.535e-012	1.535e-012	-11.814	-11.814	0.000
NaOH	6.571e-015	6.571e-015	-14.182	-14.182	0.000
NaAlO2	4.169e-018	4.169e-018	-17.380	-17.380	0.000
O(0)	1.643e-006				
O2	8.214e-007	8.243e-007	-6.085	-6.084	0.002
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-128.684	-128.684	0.000

HS-	0.000e+000	0.000e+000	-132.194	-132.247	-0.053
S-2	0.000e+000	0.000e+000	-141.522	-141.726	-0.204
S2-2	0.000e+000	0.000e+000	-234.067	-234.278	-0.211
HAsS2	0.000e+000	0.000e+000	-311.751	-311.751	0.000
S3-2	0.000e+000	0.000e+000	-326.661	-326.871	-0.211
S4-2	0.000e+000	0.000e+000	-419.481	-419.692	-0.211
S5-2	0.000e+000	0.000e+000	-512.518	-512.729	-0.211
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-133.359	-133.570	-0.211
HS2O3-	0.000e+000	0.000e+000	-135.951	-136.003	-0.052
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-121.337	-121.540	-0.204
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-42.424	-42.476	-0.052
H2SO3	0.000e+000	0.000e+000	-43.942	-43.942	0.000
SO2	0.000e+000	0.000e+000	-44.042	-44.042	0.000
SO3-2	0.000e+000	0.000e+000	-46.054	-46.261	-0.207
S2O6-2	0.000e+000	0.000e+000	-60.380	-60.591	-0.211
S3O6-2	0.000e+000	0.000e+000	-155.456	-155.667	-0.211
S4O6-2	0.000e+000	0.000e+000	-234.627	-234.837	-0.211
S5O6-2	0.000e+000	0.000e+000	-342.676	-342.887	-0.211
S(5)	0.000e+000				
S2O5-2	0.000e+000	0.000e+000	-89.572	-89.783	-0.211
S(6)	4.062e-003				
SO4-2	3.352e-003	2.063e-003	-2.475	-2.685	-0.211
CaSO4	3.395e-004	3.395e-004	-3.469	-3.469	0.000
MgSO4	1.554e-004	1.554e-004	-3.809	-3.809	0.000
HSO4-	8.403e-005	7.451e-005	-4.076	-4.128	-0.052
AlSO4+	4.639e-005	4.113e-005	-4.334	-4.386	-0.052
NaSO4-	2.173e-005	1.927e-005	-4.663	-4.715	-0.052
CuSO4	1.965e-005	1.965e-005	-4.707	-4.707	0.000
MnSO4	1.628e-005	1.628e-005	-4.788	-4.788	0.000
Al(SO4)2-	7.430e-006	6.588e-006	-5.129	-5.181	-0.052
ZnSO4	4.776e-006	4.776e-006	-5.321	-5.321	0.000
KSO4-	4.125e-006	3.658e-006	-5.385	-5.437	-0.052
FeSO4+	2.578e-006	2.286e-006	-5.589	-5.641	-0.052
Fe(SO4)2-	8.993e-008	7.974e-008	-7.046	-7.098	-0.052
KHSO4	1.154e-009	1.154e-009	-8.938	-8.938	0.000
FeSO4	1.150e-009	1.150e-009	-8.939	-8.939	0.000
H2SO4	2.513e-011	2.513e-011	-10.600	-10.600	0.000
NH4SO4-	0.000e+000	0.000e+000	-62.353	-62.405	-0.052
S(7)	5.629e-038				
S2O8-2	2.815e-038	1.733e-038	-37.551	-37.761	-0.211
S(8)	4.144e-027				
HSO5-	4.144e-027	3.675e-027	-26.383	-26.435	-0.052
Zn	2.214e-005				
Zn+2	1.735e-005	1.102e-005	-4.761	-4.958	-0.197
ZnSO4	4.776e-006	4.776e-006	-5.321	-5.321	0.000
ZnCl+	1.546e-008	1.371e-008	-7.811	-7.863	-0.052
ZnOH+	3.811e-011	3.379e-011	-10.419	-10.471	-0.052
ZnCl2	1.186e-011	1.186e-011	-10.926	-10.926	0.000
ZnF+	1.782e-012	1.580e-012	-11.749	-11.801	-0.052
Zn(OH)Cl	6.556e-013	6.556e-013	-12.183	-12.183	0.000
ZnCl3-	5.472e-015	4.852e-015	-14.262	-14.314	-0.052
Zn(OH)2	4.047e-016	4.047e-016	-15.393	-15.393	0.000
ZnCl4-2	4.425e-017	2.724e-017	-16.354	-16.565	-0.211
Zn(OH)3-	3.957e-024	3.508e-024	-23.403	-23.455	-0.052
Zn(OH)4-2	2.718e-033	1.673e-033	-32.566	-32.777	-0.211
ZnClO4+	2.228e-035	1.975e-035	-34.652	-34.704	-0.052
Zn(NH3)+2	0.000e+000	0.000e+000	-59.911	-60.118	-0.207
ZnN3+	0.000e+000	0.000e+000	-87.876	-87.929	-0.052
Zn(NH3)2+2	0.000e+000	0.000e+000	-114.917	-115.124	-0.207
Zn(NH3)3+2	0.000e+000	0.000e+000	-169.924	-170.131	-0.207
Zn(N3)2	0.000e+000	0.000e+000	-170.588	-170.588	0.000
Zn(NH3)4+2	0.000e+000	0.000e+000	-225.204	-225.411	-0.207

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

Phase	SI	log IAP	log KT	
Al	-139.72	10.19	149.91	Al
Al(g)	-190.43	10.19	200.62	Al
Al2(SO4)3	-36.38	-17.48	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-19.03	-17.48	1.56	Al2(SO4)3:6H2O
Alabandite	-132.88	-133.30	-0.42	MnS
AlF3	-11.42	-28.69	-17.27	AlF3
Alum-K	-8.77	-13.74	-4.97	KAl(SO4)2:12H2O
Alunite	-2.01	-2.48	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.28	-5.63	-4.35	CaSO4
Antarcticite	-13.30	-9.21	4.09	CaCl2:6H2O
Antlerite	-10.77	-2.04	8.73	Cu3(SO4)(OH)4
Aphthitalite	-15.31	-19.20	-3.89	NaK3(SO4)2
Arcanite	-8.16	-10.00	-1.84	K2SO4
Arsenolite	-121.85	-141.69	-19.84	As2O3
Arsenopyrite	-251.42	-265.87	-14.45	FeAsS
As	-108.96	-66.28	42.68	As
As2O5	-88.84	-86.71	2.14	As2O5
As4O6(cubi)	-243.55	-283.38	-39.82	As4O6
As4O6(mono)	-243.33	-283.38	-40.05	As4O6
Atacamite	-17.37	-3.11	14.26	Cu4Cl2(OH)6
Bassanite	-1.93	-5.63	-3.71	CaSO4:0.5H2O
Birnessite	-10.88	-96.42	-85.55	Mn8O14:5H2O
Bischofite	-14.20	-9.81	4.39	MgCl2:6H2O
Bixbyite	-5.43	-6.40	-0.96	Mn2O3
Bloedite	-12.14	-14.62	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-1.92	5.63	7.55	AlO2H
Bornite	-498.20	-600.73	-102.53	Cu5FeS4
Brochantite	-14.95	0.47	15.42	Cu4(SO4)(OH)6
Brucite	-12.94	3.34	16.28	Mg(OH)2
Ca	-132.84	6.99	139.83	Ca
Ca(g)	-158.08	6.99	165.07	Ca
Ca2Al2O5:8H2O	-40.42	19.15	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-31.55	-5.26	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-92.68	-74.87	17.80	Ca3(AsO4)2
Ca3Al2O6	-89.94	23.09	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-102.64	37.84	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-80.21	27.04	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-76.64	27.04	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-65.70	2.63	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-31.70	15.20	46.91	CaAl2O4
CaAl2O4:10H2O	-22.79	15.20	37.99	CaAl2O4:10H2O
CaAl4O7	-42.13	26.46	68.59	CaAl4O7
Carnallite	-20.87	-16.60	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-2.10	-5.63	-3.54	CaSO4:0.5H2O
Chalcanthite	-4.44	-7.07	-2.63	CuSO4:5H2O
Chalcocite	-130.40	-165.15	-34.74	Cu2S
Chalcocyanite	-9.98	-7.07	2.91	CuSO4
Chalcopyrite	-237.83	-270.44	-32.60	CuFeS2
Chloromagnesite	-31.63	-9.81	21.82	MgCl2
Cl2(g)	-19.19	-16.20	2.99	Cl2
Claudetite	-121.89	-141.69	-19.80	As2O3
Corundum	-7.03	11.26	18.29	Al2O3
Covellite	-110.32	-133.18	-22.86	CuS
Cu	-25.94	5.55	31.50	Cu
Cu(g)	-78.10	5.55	83.66	Cu
CuCl2	-14.36	-10.64	3.72	CuCl2
CuF	-33.25	-26.17	7.08	CuF
CuF2	-19.75	-20.37	-0.62	CuF2
CuF2:2H2O	-15.82	-20.37	-4.55	CuF2:2H2O
Cuprite	-27.55	-29.45	-1.91	Cu2O
Delafoosite	-2.89	-9.33	-6.44	CuFeO2
Diaspore	-1.52	5.63	7.15	AlHO2
Epsomite	-4.27	-6.24	-1.96	MgSO4:7H2O
Ettringite	-56.27	6.19	62.46	Ca6Al2(SO4)3(OH)12:26H2O

F2(g)	-81.63	-25.92	55.71	F2
Fe	-57.54	1.48	59.02	Fe
Fe(OH)2	-15.45	-1.56	13.89	Fe(OH)2
Fe(OH)3	-0.24	5.40	5.64	Fe(OH)3
Fe2(SO4)3	-20.99	-17.94	3.05	Fe2(SO4)3
FeF2	-22.02	-24.44	-2.42	FeF2
FeF3	-9.66	-28.92	-19.26	FeF3
FeO	-15.08	-1.56	13.52	FeO
Ferrite-Ca	-6.75	14.74	21.50	CaFe2O4
Ferrite-Cu	3.03	13.31	10.28	CuFe2O4
Ferrite-Dicalcium	-38.11	18.69	56.80	Ca2Fe2O5
Ferrite-Mg	-6.88	14.14	21.02	MgFe2O4
Ferrite-Zn	1.03	12.73	11.70	ZnFe2O4
FeSO4	-13.75	-11.14	2.61	FeSO4
Fluorite	-8.87	-18.93	-10.07	CaF2
Gibbsite	-2.11	5.63	7.74	Al(OH)3
Glauberite	-8.55	-14.02	-5.47	Na2Ca(SO4)2
Goethite	4.87	5.40	0.53	FeOOH
Gypsum	-1.10	-5.63	-4.53	CaSO4:2H2O
H2(g)	-39.96	-43.06	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-127.70	-135.69	-7.99	H2S
Halite	-7.54	-5.98	1.56	NaCl
Hausmannite	-14.14	-4.00	10.14	Mn3O4
HCl(g)	-12.88	-6.58	6.30	HCl
Hematite	10.72	10.80	0.08	Fe2O3
Hercynite	-19.10	9.70	28.80	FeAl2O4
Hexahydrate	-4.51	-6.24	-1.73	MgSO4:6H2O
Hydrophilite	-20.95	-9.21	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	6.24	-3.17	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	3.08	-2.36	-5.45	NaFe3(SO4)2(OH)6
K	-69.67	1.31	70.98	K
K(g)	-80.27	1.31	81.58	K
K2O	-84.46	-0.42	84.04	K2O
K3H(SO4)2	-16.17	-19.79	-3.62	K3H(SO4)2
Kainite	-12.71	-13.02	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-17.01	-13.74	3.27	KAl(SO4)2
Katoite	-55.85	23.09	78.94	Ca3Al2H12O12
Kieserite	-5.97	-6.24	-0.27	MgSO4:H2O
KMgCl3	-37.85	-16.60	21.25	KMgCl3
KMgCl3:2H2O	-30.56	-16.60	13.96	KMgCl3:2H2O
Lammerite	-80.73	-79.17	1.55	Cu3(AsO4)2
Lawrencite	-23.77	-14.71	9.05	FeCl2
Leonite	-12.13	-16.24	-4.11	K2Mg(SO4)2:4H2O
Lime	-28.62	3.95	32.57	CaO
Magnetite	-1.18	9.24	10.42	Fe3O4
Manganite	-3.03	-3.20	-0.16	MnO(OH)
Manganosite	-15.52	2.40	17.92	MnO
Mayenite	-367.99	126.16	494.15	Ca12Al14O33
Melanterite	-8.74	-11.14	-2.40	FeSO4:7H2O
Mercallite	-8.35	-9.79	-1.44	KHSO4
Mg	-116.13	6.39	122.52	Mg
Mg(g)	-135.86	6.39	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.59	-5.40	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-13.77	-4.56	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.54	-9.81	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.11	-9.81	7.30	MgCl2:4H2O
MgCl2:H2O	-25.88	-9.81	16.07	MgCl2:H2O
MgOHCl	-19.12	-3.23	15.89	MgOHCl
MgSO4	-11.06	-6.24	4.83	MgSO4
Mirabilite	-7.23	-8.39	-1.15	Na2SO4:10H2O
Misenite	-57.67	-68.75	-11.08	K8H6(SO4)7
Mn	-77.49	5.44	82.93	Mn
Mn(OH)2(am)	-12.91	2.40	15.31	Mn(OH)2
Mn(OH)3	-9.54	-3.20	6.34	Mn(OH)3
MnCl2:2H2O	-14.75	-10.76	4.00	MnCl2:2H2O

MnCl2:4H2O	-13.51	-10.76	2.75	MnCl2:4H2O
MnCl2:H2O	-16.30	-10.76	5.54	MnCl2:H2O
MnO2 (gamma)	-0.74	-16.87	-16.13	MnO2
MnSO4	-9.79	-7.18	2.61	MnSO4
Molysite	-27.80	-14.33	13.47	FeCl3
N2(g)	-3.91	-7.09	-3.18	N2
Na	-65.25	2.12	67.37	Na
Na(g)	-78.74	2.12	80.86	Na
Na2O	-66.22	1.19	67.42	Na2O
Na3H(SO4)2	-16.48	-17.37	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.51	-22.40	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-13.89	6.00	19.88	NaFeO2
Nantokite	-14.54	-21.30	-6.77	CuCl
NH3(g)	-59.01	-57.21	1.80	NH3
Niter	-7.30	-7.52	-0.22	KNO3
NO(g)	-18.72	-17.98	0.74	NO
NO2(g)	-14.14	-5.79	8.35	NO2
O2(g)	-3.19	-6.08	-2.89	O2
Orpiment	-469.28	-548.77	-79.49	As2S3
Oxychloride-Mg	-25.72	0.11	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.85	-6.24	-1.39	MgSO4:5H2O
Periclase	-17.98	3.34	21.33	MgO
Picromerite	-11.80	-16.24	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-13.19	-27.50	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-18.60	3.95	22.55	Ca(OH)2
Pyrite	-216.72	-241.42	-24.70	FeS2
Pyrolusite	0.79	-16.87	-17.66	MnO2
Pyrrhotite	-133.52	-137.25	-3.74	FeS
Realgar	-190.33	-250.60	-60.28	AsS
S	-93.63	-138.74	-45.11	S
S2(g)	-201.14	-208.33	-7.19	S2
Scacchite	-19.50	-10.76	8.74	MnCl2
Sellaite	-10.09	-19.54	-9.44	MgF2
SO2(g)	-44.22	-44.04	0.18	SO2
Sphalerite	-122.29	-133.76	-11.47	ZnS
Spinel	-23.00	14.60	37.61	Al2MgO4
Starkeyite	-5.24	-6.24	-1.00	MgSO4:4H2O
Sylvite	-7.62	-6.79	0.83	KCl
Syngenite	-8.04	-15.64	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-45.97	-28.83	17.14	Mg2CaCl6:12H2O
Tenorite	-5.13	2.51	7.65	CuO
Thenardite	-8.03	-8.38	-0.36	Na2SO4
Todorokite	-9.50	-55.33	-45.82	Mn7O12:3H2O
Troilite	-133.41	-137.25	-3.84	FeS
Wurtzite	-124.59	-133.76	-9.17	ZnS
Wustite	-13.14	-0.74	12.40	Fe.947O
Zincite	-9.26	1.94	11.20	ZnO
Zn	-63.81	4.98	68.79	Zn
Zn(ClO4)2:6H2O	-72.64	-67.00	5.63	Zn(ClO4)2:6H2O
Zn(g)	-80.43	4.98	85.41	Zn
Zn(NO3)2:6H2O	-16.09	-12.69	3.40	Zn(NO3)2:6H2O
Zn(OH)2(beta)	-10.00	1.94	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-9.72	1.94	11.66	Zn(OH)2
Zn(OH)2(gamma)	-9.95	1.94	11.88	Zn(OH)2
Zn2(OH)3Cl	-18.00	-2.71	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-13.29	-5.71	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-90.21	-80.90	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-32.44	-13.35	19.09	Zn3O(SO4)2
Zn5(NO3)2(OH)8	-47.62	-4.95	42.67	Zn5(NO3)2(OH)8
ZnCl2	-18.30	-11.22	7.08	ZnCl2
ZnCl2(NH3)2	-118.64	-125.64	-7.01	ZnCl2(NH3)2
ZnCl2(NH3)4	-233.36	-240.07	-6.71	ZnCl2(NH3)4
ZnCl2(NH3)6	-349.75	-354.50	-4.74	ZnCl2(NH3)6
ZnF2	-20.45	-20.94	-0.49	ZnF2
ZnSO4	-11.18	-7.64	3.53	ZnSO4
ZnSO4:6H2O	-5.94	-7.64	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.77	-7.64	-1.88	ZnSO4:7H2O

ZnSO4:H2O -7.09 -7.64 -0.55 ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
