
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      1
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.

WARNING: Maximum iterations exceeded, 100

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying smaller step size, pe step size 10, 5 ...

Using mix 4.

Mixture 4.

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

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

Elements	Molality	Moles
Al	2.152e-004	4.304e-004
As	1.200e-005	2.401e-005
Ca	2.063e-003	4.126e-003
Cl	9.966e-004	1.993e-003
Cu	1.687e-004	3.374e-004
F	6.582e-006	1.316e-005
Fe	1.197e-003	2.393e-003
K	4.272e-004	8.545e-004
Mg	5.099e-004	1.020e-003
Mn	1.301e-004	2.603e-004
N	1.036e-004	2.071e-004
Na	1.360e-003	2.721e-003
S	5.592e-003	1.118e-002
Zn	4.130e-005	8.260e-005

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

pH	=	3.262	Charge balance
pe	=	16.766	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	1.840e-002	
Mass of water (kg)	=	2.000e+000	
Total alkalinity (eq/kg)	=	-1.799e-003	
Total carbon (mol/kg)	=	0.000e+000	
Total CO2 (mol/kg)	=	0.000e+000	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	-2.095e-003	
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	-5.24	
Iterations	=	65	
Total H	=	2.221051e+002	
Total O	=	1.110986e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	6.125e-004	5.475e-004	-3.213	-3.262	-0.049
OH-	2.017e-011	1.760e-011	-10.695	-10.755	-0.059
H2O	5.553e+001	9.998e-001	1.744	-0.000	0.000
Al	2.152e-004				
AlSO4+	1.020e-004	8.927e-005	-3.991	-4.049	-0.058
Al+3	9.086e-005	3.263e-005	-4.042	-4.486	-0.445
Al(SO4)2-	2.118e-005	1.853e-005	-4.674	-4.732	-0.058
AlOH+2	1.135e-006	6.676e-007	-5.945	-6.175	-0.230
Al(OH)2+	3.236e-009	2.831e-009	-8.490	-8.548	-0.058
Al2(OH)2+4	5.632e-010	7.247e-011	-9.249	-10.140	-0.891
HALO2	7.525e-012	7.525e-012	-11.123	-11.123	0.000
Al3(OH)4+5	1.186e-013	5.091e-015	-12.926	-14.293	-1.367
AlO2-	5.383e-015	4.709e-015	-14.269	-14.327	-0.058
NaAlO2	1.050e-018	1.050e-018	-17.979	-17.979	0.000
AlF+2	1.018e-040	0.000e+000	-39.992	-40.223	-0.230

Al13O4(OH)24+7	0.000e+000	0.000e+000	-50.002	-52.683	-2.681
AlF2+	0.000e+000	0.000e+000	-77.301	-77.359	-0.058
AlF3	0.000e+000	0.000e+000	-115.995	-115.995	0.000
AlF4-	0.000e+000	0.000e+000	-156.273	-156.331	-0.058
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-152.055	-152.055	0.000
As(3)	2.154e-027				
HAsO2	1.149e-027	1.149e-027	-26.940	-26.940	0.000
As(OH)3	1.004e-027	1.004e-027	-26.998	-26.998	0.000
H2AsO3-	1.283e-033	1.122e-033	-32.892	-32.950	-0.058
AsO2-	1.227e-033	1.073e-033	-32.911	-32.969	-0.058
AsO2OH-2	0.000e+000	0.000e+000	-40.464	-40.698	-0.235
HAsS2	0.000e+000	0.000e+000	-276.956	-276.956	0.000
As(5)	1.200e-005				
HAsO3F-	6.558e-006	5.737e-006	-5.183	-5.241	-0.058
H2AsO4-	4.998e-006	4.372e-006	-5.301	-5.359	-0.058
H3AsO4	4.216e-007	4.216e-007	-6.375	-6.375	0.000
AsO3F-2	2.423e-008	1.411e-008	-7.616	-7.850	-0.235
HAsO4-2	2.276e-009	1.326e-009	-8.643	-8.878	-0.235
AsO4-3	2.100e-017	6.212e-018	-16.678	-17.207	-0.529
Ca	2.063e-003				
Ca+2	1.668e-003	1.009e-003	-2.778	-2.996	-0.218
CaSO4	3.942e-004	3.942e-004	-3.404	-3.404	0.000
CaNO3+	5.179e-007	4.531e-007	-6.286	-6.344	-0.058
CaCl+	2.119e-007	1.853e-007	-6.674	-6.732	-0.058
CaCl2	1.888e-010	1.888e-010	-9.724	-9.724	0.000
CaOH+	2.977e-013	2.604e-013	-12.526	-12.584	-0.058
CaF+	0.000e+000	0.000e+000	-44.968	-45.026	-0.058
Cl(-1)	9.966e-004				
Cl-	9.956e-004	8.663e-004	-3.002	-3.062	-0.060
CaCl+	2.119e-007	1.853e-007	-6.674	-6.732	-0.058
CuCl+	2.015e-007	1.762e-007	-6.696	-6.754	-0.058
NaCl	1.780e-007	1.780e-007	-6.750	-6.750	0.000
MgCl+	1.704e-007	1.491e-007	-6.768	-6.827	-0.058
MnCl+	1.186e-007	1.037e-007	-6.926	-6.984	-0.058
HCl	1.065e-007	1.065e-007	-6.973	-6.973	0.000
ZnCl+	3.101e-008	2.713e-008	-7.509	-7.567	-0.058
KCl	1.059e-008	1.059e-008	-7.975	-7.975	0.000
FeCl+2	8.676e-009	5.105e-009	-8.062	-8.292	-0.230
FeCl2+	4.092e-009	3.580e-009	-8.388	-8.446	-0.058
CaCl2	1.888e-010	1.888e-010	-9.724	-9.724	0.000
CuCl2	8.040e-011	8.040e-011	-10.095	-10.095	0.000
ZnCl2	2.745e-011	2.745e-011	-10.561	-10.561	0.000
FeCl+	4.557e-012	3.986e-012	-11.341	-11.399	-0.058
Zn(OH)Cl	8.470e-013	8.470e-013	-12.072	-12.072	0.000
MnCl3-	1.944e-014	1.700e-014	-13.711	-13.770	-0.058
ZnCl3-	1.501e-014	1.313e-014	-13.824	-13.882	-0.058
ZnCl4-2	1.480e-016	8.623e-017	-15.830	-16.064	-0.235
FeCl2	1.853e-017	1.853e-017	-16.732	-16.732	0.000
FeCl4-	3.692e-018	3.230e-018	-17.433	-17.491	-0.058
CuCl2-	3.963e-020	3.467e-020	-19.402	-19.460	-0.058
CuCl4-2	1.944e-021	1.132e-021	-20.711	-20.946	-0.235
CuCl3-2	3.311e-022	1.929e-022	-21.480	-21.715	-0.235
FeCl4-2	6.898e-023	4.018e-023	-22.161	-22.396	-0.235
Cl(1)	1.559e-017				
HClO	1.559e-017	1.559e-017	-16.807	-16.807	0.000
ClO-	8.776e-022	7.677e-022	-21.057	-21.115	-0.058
Cl(3)	1.693e-032				
ClO2-	9.913e-033	8.671e-033	-32.004	-32.062	-0.058
HClO2	7.018e-033	7.018e-033	-32.154	-32.154	0.000
Cl(5)	7.989e-030				
ClO3-	7.989e-030	6.970e-030	-29.098	-29.157	-0.059
Cl(7)	3.206e-031				
ClO4-	3.205e-031	2.796e-031	-30.494	-30.553	-0.059
ZnClO4+	1.127e-034	9.858e-035	-33.948	-34.006	-0.058
Cu(1)	8.371e-019				
Cu+	7.971e-019	6.973e-019	-18.098	-18.157	-0.058

CuCl2-	3.963e-020	3.467e-020	-19.402	-19.460	-0.058
CuCl3-2	3.311e-022	1.929e-022	-21.480	-21.715	-0.235
Cu(2)	1.687e-004				
Cu+2	1.229e-004	7.438e-005	-3.910	-4.129	-0.218
CuSO4	4.556e-005	4.556e-005	-4.341	-4.341	0.000
CuCl+	2.015e-007	1.762e-007	-6.696	-6.754	-0.058
CuOH+	8.010e-009	7.007e-009	-8.096	-8.154	-0.058
CuCl2	8.040e-011	8.040e-011	-10.095	-10.095	0.000
CuNO2+	4.076e-019	3.565e-019	-18.390	-18.448	-0.058
CuCl4-2	1.944e-021	1.132e-021	-20.711	-20.946	-0.235
CuO2-2	5.045e-031	2.939e-031	-30.297	-30.532	-0.235
Cu(NO2)2	1.670e-034	1.670e-034	-33.777	-33.777	0.000
CuF+	0.000e+000	0.000e+000	-45.607	-45.665	-0.058
CuNH3+2	0.000e+000	0.000e+000	-57.470	-57.700	-0.230
Cu(NH3)2+2	0.000e+000	0.000e+000	-111.648	-111.878	-0.230
Cu(NH3)3+2	0.000e+000	0.000e+000	-166.439	-166.669	-0.230
F	6.582e-006				
HAsO3F-	6.558e-006	5.737e-006	-5.183	-5.241	-0.058
AsO3F-2	2.423e-008	1.411e-008	-7.616	-7.850	-0.235
AlF+2	1.018e-040	0.000e+000	-39.992	-40.223	-0.230
F-	0.000e+000	0.000e+000	-42.677	-42.736	-0.059
FeF+2	0.000e+000	0.000e+000	-42.781	-43.012	-0.230
HF	0.000e+000	0.000e+000	-42.812	-42.812	0.000
MgF+	0.000e+000	0.000e+000	-44.952	-45.010	-0.058
CaF+	0.000e+000	0.000e+000	-44.968	-45.026	-0.058
MnF+	0.000e+000	0.000e+000	-45.498	-45.556	-0.058
CuF+	0.000e+000	0.000e+000	-45.607	-45.665	-0.058
ZnF+	0.000e+000	0.000e+000	-46.258	-46.316	-0.058
NaF	0.000e+000	0.000e+000	-46.639	-46.639	0.000
FeF+	0.000e+000	0.000e+000	-49.518	-49.576	-0.058
AlF2+	0.000e+000	0.000e+000	-77.301	-77.359	-0.058
FeF2+	0.000e+000	0.000e+000	-81.481	-81.539	-0.058
H2F2	0.000e+000	0.000e+000	-85.228	-85.228	0.000
HF2-	0.000e+000	0.000e+000	-86.106	-86.164	-0.058
AlF3	0.000e+000	0.000e+000	-115.995	-115.995	0.000
AlF4-	0.000e+000	0.000e+000	-156.273	-156.331	-0.058
Fe(2)	1.312e-008				
Fe+2	1.044e-008	6.316e-009	-7.981	-8.200	-0.218
FeSO4	2.676e-009	2.676e-009	-8.572	-8.572	0.000
FeCl+	4.557e-012	3.986e-012	-11.341	-11.399	-0.058
FeOH+	4.170e-015	3.648e-015	-14.380	-14.438	-0.058
FeCl2	1.853e-017	1.853e-017	-16.732	-16.732	0.000
FeCl4-2	6.898e-023	4.018e-023	-22.161	-22.396	-0.235
Fe(OH)2	5.291e-023	5.291e-023	-22.276	-22.276	0.000
Fe(OH)3-	4.398e-030	3.847e-030	-29.357	-29.415	-0.058
Fe(OH)4-2	0.000e+000	0.000e+000	-40.919	-41.153	-0.235
FeF+	0.000e+000	0.000e+000	-49.518	-49.576	-0.058
Fe(3)	1.197e-003				
FeOH+2	7.087e-004	4.170e-004	-3.150	-3.380	-0.230
Fe(OH)2+	2.883e-004	2.522e-004	-3.540	-3.598	-0.058
Fe+3	9.847e-005	3.537e-005	-4.007	-4.451	-0.445
Fe2(OH)2+4	3.637e-005	4.680e-006	-4.439	-5.330	-0.891
FeSO4+	1.046e-005	9.148e-006	-4.981	-5.039	-0.058
Fe3(OH)4+5	5.745e-006	2.466e-007	-5.241	-6.608	-1.367
Fe(SO4)2-	4.727e-007	4.135e-007	-6.325	-6.384	-0.058
Fe(OH)3	2.154e-007	2.154e-007	-6.667	-6.667	0.000
FeNO3+2	5.383e-008	3.167e-008	-7.269	-7.499	-0.230
FeCl+2	8.676e-009	5.105e-009	-8.062	-8.292	-0.230
FeCl2+	4.092e-009	3.580e-009	-8.388	-8.446	-0.058
Fe(OH)4-	1.130e-013	9.881e-014	-12.947	-13.005	-0.058
FeNO2+2	3.886e-018	2.287e-018	-17.410	-17.641	-0.230
FeCl4-	3.692e-018	3.230e-018	-17.433	-17.491	-0.058
FeF+2	0.000e+000	0.000e+000	-42.781	-43.012	-0.230
FeF2+	0.000e+000	0.000e+000	-81.481	-81.539	-0.058
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-43.158	-43.157	0.002
K	4.272e-004				

K+	4.182e-004	3.639e-004	-3.379	-3.439	-0.060
KSO4-	8.977e-006	7.853e-006	-5.047	-5.105	-0.058
KCl	1.059e-008	1.059e-008	-7.975	-7.975	0.000
KHSO4	3.793e-009	3.793e-009	-8.421	-8.421	0.000
KOH	2.304e-015	2.304e-015	-14.637	-14.637	0.000
Mg	5.099e-004				
Mg+2	3.524e-004	2.204e-004	-3.453	-3.657	-0.204
MgSO4	1.574e-004	1.574e-004	-3.803	-3.803	0.000
MgCl+	1.704e-007	1.491e-007	-6.768	-6.827	-0.058
Mg4(OH)4+4	0.000e+000	0.000e+000	-40.440	-41.331	-0.891
MgF+	0.000e+000	0.000e+000	-44.952	-45.010	-0.058
Mn(2)	1.301e-004				
Mn+2	9.291e-005	5.623e-005	-4.032	-4.250	-0.218
MnSO4	3.709e-005	3.709e-005	-4.431	-4.431	0.000
MnCl+	1.186e-007	1.037e-007	-6.926	-6.984	-0.058
MnNO3+	9.124e-009	7.981e-009	-8.040	-8.098	-0.058
MnOH+	3.017e-012	2.639e-012	-11.520	-11.579	-0.058
Mn(NO3)2	1.795e-012	1.795e-012	-11.746	-11.746	0.000
MnCl3-	1.944e-014	1.700e-014	-13.711	-13.770	-0.058
Mn2OH+3	5.142e-016	1.590e-016	-15.289	-15.799	-0.510
Mn(OH)2	1.183e-020	1.183e-020	-19.927	-19.927	0.000
Mn2(OH)3+	2.771e-023	2.424e-023	-22.557	-22.615	-0.058
Mn(OH)3-	2.317e-029	2.027e-029	-28.635	-28.693	-0.058
Mn(OH)4-2	5.381e-040	3.134e-040	-39.269	-39.504	-0.235
MnF+	0.000e+000	0.000e+000	-45.498	-45.556	-0.058
Mn(3)	2.832e-013				
Mn+3	2.832e-013	8.758e-014	-12.548	-13.058	-0.510
Mn(6)	4.968e-030				
MnO4-2	4.968e-030	2.894e-030	-29.304	-29.539	-0.235
Mn(7)	8.529e-023				
MnO4-	8.529e-023	7.441e-023	-22.069	-22.128	-0.059
N(-03)	0.000e+000				
HN3	0.000e+000	0.000e+000	-82.952	-82.952	0.000
N3-	0.000e+000	0.000e+000	-84.334	-84.392	-0.058
ZnN3+	0.000e+000	0.000e+000	-88.622	-88.680	-0.058
Zn(N3)2	0.000e+000	0.000e+000	-172.319	-172.319	0.000
N(-3)	0.000e+000				
NH4+	0.000e+000	0.000e+000	-51.572	-51.633	-0.062
CuNH3+2	0.000e+000	0.000e+000	-57.470	-57.700	-0.230
NH3	0.000e+000	0.000e+000	-57.612	-57.612	0.000
Zn(NH3)+2	0.000e+000	0.000e+000	-60.058	-60.288	-0.230
NH4SO4-	0.000e+000	0.000e+000	-62.448	-62.506	-0.058
Cu(NH3)2+2	0.000e+000	0.000e+000	-111.648	-111.878	-0.230
Zn(NH3)2+2	0.000e+000	0.000e+000	-115.463	-115.694	-0.230
Cu(NH3)3+2	0.000e+000	0.000e+000	-166.439	-166.669	-0.230
Zn(NH3)3+2	0.000e+000	0.000e+000	-170.869	-171.099	-0.230
Zn(NH3)4+2	0.000e+000	0.000e+000	-226.548	-226.778	-0.230
N(0)	5.155e-008				
N2	2.578e-008	2.578e-008	-7.589	-7.589	0.000
N(3)	9.967e-017				
NO2-	5.261e-017	4.578e-017	-16.279	-16.339	-0.060
HNO2	4.277e-017	4.277e-017	-16.369	-16.369	0.000
FeNO2+2	3.886e-018	2.287e-018	-17.410	-17.641	-0.230
CuNO2+	4.076e-019	3.565e-019	-18.390	-18.448	-0.058
Cu(NO2)2	1.670e-034	1.670e-034	-33.777	-33.777	0.000
N(5)	1.035e-004				
NO3-	1.029e-004	8.956e-005	-3.987	-4.048	-0.060
CaNO3+	5.179e-007	4.531e-007	-6.286	-6.344	-0.058
FeNO3+2	5.383e-008	3.167e-008	-7.269	-7.499	-0.230
MnNO3+	9.124e-009	7.981e-009	-8.040	-8.098	-0.058
HNO3	2.564e-009	2.564e-009	-8.591	-8.591	0.000
Mn(NO3)2	1.795e-012	1.795e-012	-11.746	-11.746	0.000
Na	1.360e-003				
Na+	1.337e-003	1.169e-003	-2.874	-2.932	-0.058
NaSO4-	2.361e-005	2.065e-005	-4.627	-4.685	-0.058
NaCl	1.780e-007	1.780e-007	-6.750	-6.750	0.000
NaOH	3.549e-015	3.549e-015	-14.450	-14.450	0.000

NaAlO2	1.050e-018	1.050e-018	-17.979	-17.979	0.000
NaF	0.000e+000	0.000e+000	-46.639	-46.639	0.000
O(0)	2.606e-006				
O2	1.303e-006	1.309e-006	-5.885	-5.883	0.002
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-128.603	-128.603	0.000
HS-	0.000e+000	0.000e+000	-132.292	-132.351	-0.059
S-2	0.000e+000	0.000e+000	-141.789	-142.015	-0.226
S2-2	0.000e+000	0.000e+000	-234.151	-234.386	-0.235
HAsS2	0.000e+000	0.000e+000	-276.956	-276.956	0.000
S3-2	0.000e+000	0.000e+000	-326.563	-326.798	-0.235
S4-2	0.000e+000	0.000e+000	-419.202	-419.437	-0.235
S5-2	0.000e+000	0.000e+000	-512.058	-512.292	-0.235
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-133.142	-133.377	-0.235
HS2O3-	0.000e+000	0.000e+000	-135.566	-135.624	-0.058
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-121.020	-121.246	-0.226
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-42.221	-42.279	-0.058
H2SO3	0.000e+000	0.000e+000	-43.559	-43.559	0.000
SO2	0.000e+000	0.000e+000	-43.660	-43.660	0.000
SO3-2	0.000e+000	0.000e+000	-46.019	-46.249	-0.230
S2O6-2	0.000e+000	0.000e+000	-59.861	-60.096	-0.235
S3O6-2	0.000e+000	0.000e+000	-154.756	-154.991	-0.235
S4O6-2	0.000e+000	0.000e+000	-233.745	-233.980	-0.235
S5O6-2	0.000e+000	0.000e+000	-341.614	-341.848	-0.235
S(5)	0.000e+000				
S2O5-2	0.000e+000	0.000e+000	-89.154	-89.389	-0.235
S(6)	5.592e-003				
SO4-2	4.590e-003	2.673e-003	-2.338	-2.573	-0.235
CaSO4	3.942e-004	3.942e-004	-3.404	-3.404	0.000
HSO4-	1.690e-004	1.478e-004	-3.772	-3.830	-0.058
MgSO4	1.574e-004	1.574e-004	-3.803	-3.803	0.000
AlSO4+	1.020e-004	8.927e-005	-3.991	-4.049	-0.058
CuSO4	4.556e-005	4.556e-005	-4.341	-4.341	0.000
MnSO4	3.709e-005	3.709e-005	-4.431	-4.431	0.000
NaSO4-	2.361e-005	2.065e-005	-4.627	-4.685	-0.058
Al(SO4)2-	2.118e-005	1.853e-005	-4.674	-4.732	-0.058
ZnSO4	1.047e-005	1.047e-005	-4.980	-4.980	0.000
FeSO4+	1.046e-005	9.148e-006	-4.981	-5.039	-0.058
KSO4-	8.977e-006	7.853e-006	-5.047	-5.105	-0.058
Fe(SO4)2-	4.727e-007	4.135e-007	-6.325	-6.384	-0.058
KHSO4	3.793e-009	3.793e-009	-8.421	-8.421	0.000
FeSO4	2.676e-009	2.676e-009	-8.572	-8.572	0.000
H2SO4	7.636e-011	7.636e-011	-10.117	-10.117	0.000
NH4SO4-	0.000e+000	0.000e+000	-62.448	-62.506	-0.058
S(7)	2.952e-037				
S2O8-2	1.476e-037	8.597e-038	-36.831	-37.066	-0.235
S(8)	1.050e-026				
HSO5-	1.050e-026	9.189e-027	-25.979	-26.037	-0.058
Zn	4.130e-005				
Zn+2	3.080e-005	1.864e-005	-4.511	-4.730	-0.218
ZnSO4	1.047e-005	1.047e-005	-4.980	-4.980	0.000
ZnCl+	3.101e-008	2.713e-008	-7.509	-7.567	-0.058
ZnOH+	4.267e-011	3.733e-011	-10.370	-10.428	-0.058
ZnCl2	2.745e-011	2.745e-011	-10.561	-10.561	0.000
Zn(OH)Cl	8.470e-013	8.470e-013	-12.072	-12.072	0.000
ZnCl3-	1.501e-014	1.313e-014	-13.824	-13.882	-0.058
Zn(OH)2	2.920e-016	2.920e-016	-15.535	-15.535	0.000
ZnCl4-2	1.480e-016	8.623e-017	-15.830	-16.064	-0.235
Zn(OH)3-	1.889e-024	1.653e-024	-23.724	-23.782	-0.058
Zn(OH)4-2	8.834e-034	5.145e-034	-33.054	-33.289	-0.235
ZnClO4+	1.127e-034	9.858e-035	-33.948	-34.006	-0.058
ZnF+	0.000e+000	0.000e+000	-46.258	-46.316	-0.058
Zn(NH3)+2	0.000e+000	0.000e+000	-60.058	-60.288	-0.230
ZnN3+	0.000e+000	0.000e+000	-88.622	-88.680	-0.058

Zn(NH3)2+2	0.000e+000	0.000e+000	-115.463	-115.694	-0.230
Zn(NH3)3+2	0.000e+000	0.000e+000	-170.869	-171.099	-0.230
Zn(N3)2	0.000e+000	0.000e+000	-172.319	-172.319	0.000
Zn(NH3)4+2	0.000e+000	0.000e+000	-226.548	-226.778	-0.230

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

Phase	SI	log IAP	log KT	
Al	-140.20	9.71	149.91	Al
Al(g)	-190.91	9.71	200.62	Al
Al2(SO4)3	-35.59	-16.69	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-18.25	-16.69	1.56	Al2(SO4)3:6H2O
Alabandite	-132.92	-133.34	-0.42	MnS
AlF3	-115.43	-132.70	-17.27	AlF3
Alum-K	-8.10	-13.07	-4.97	KAl(SO4)2:12H2O
Alunite	-2.01	-2.47	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.22	-5.57	-4.35	CaSO4
Antarcticite	-13.21	-9.12	4.09	CaCl2:6H2O
Antlerite	-10.64	-1.91	8.73	Cu3(SO4)(OH)4
Aphthitalite	-14.51	-18.39	-3.89	NaK3(SO4)2
Arcanite	-7.61	-9.45	-1.84	K2SO4
Arsenolite	-52.58	-72.42	-19.84	As2O3
Arsenopyrite	-216.98	-231.42	-14.45	FeAsS
As	-74.48	-31.80	42.68	As
As2O5	-19.38	-17.24	2.14	As2O5
As4O6(cubi)	-105.02	-144.85	-39.82	As4O6
As4O6(mono)	-104.80	-144.85	-40.05	As4O6
Atacamite	-17.33	-3.07	14.26	Cu4Cl2(OH)6
Bassanite	-1.86	-5.57	-3.71	CaSO4:0.5H2O
Birnessite	-11.27	-96.82	-85.55	Mn8O14:5H2O
Bischofite	-14.17	-9.78	4.39	MgCl2:6H2O
Bixbyite	-5.58	-6.55	-0.96	Mn2O3
Bloedite	-12.19	-14.67	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-2.25	5.30	7.55	AlO2H
Bornite	-498.78	-601.31	-102.53	Cu5FeS4
Brochantite	-14.94	0.48	15.42	Cu4(SO4)(OH)6
Brucite	-13.42	2.87	16.28	Mg(OH)2
Ca	-133.36	6.47	139.83	Ca
Ca(g)	-158.60	6.47	165.07	Ca
Ca2Al2O5:8H2O	-41.92	17.65	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-31.88	-5.59	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-24.46	-6.66	17.80	Ca3(AsO4)2
Ca3Al2O6	-91.85	21.18	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-105.11	35.37	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-82.55	24.70	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-78.98	24.70	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-66.87	1.46	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-32.78	14.12	46.91	CaAl2O4
CaAl2O4:10H2O	-23.87	14.12	37.99	CaAl2O4:10H2O
CaAl4O7	-43.87	24.72	68.59	CaAl4O7
Carnallite	-20.56	-16.28	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-2.03	-5.57	-3.54	CaSO4:0.5H2O
Chalcanthite	-4.07	-6.70	-2.63	CuSO4:5H2O
Chalcocite	-130.66	-165.40	-34.74	Cu2S
Chalcocyanite	-9.61	-6.70	2.91	CuSO4
Chalcopyrite	-237.90	-270.51	-32.60	CuFeS2
Chloromagnesite	-31.60	-9.78	21.82	MgCl2
Cl2(g)	-18.58	-15.59	2.99	Cl2
Claudetite	-52.63	-72.42	-19.80	As2O3
Corundum	-7.69	10.60	18.29	Al2O3
Covellite	-110.36	-133.22	-22.86	CuS
Cu	-26.16	5.34	31.50	Cu
Cu(g)	-78.32	5.34	83.66	Cu
CuCl2	-13.97	-10.25	3.72	CuCl2
CuF	-67.97	-60.89	7.08	CuF
CuF2	-88.98	-89.60	-0.62	CuF2

CuF2:2H2O	-85.05	-89.60	-4.55	CuF2:2H2O
Cuprite	-27.88	-29.79	-1.91	Cu2O
Delafossite	-3.13	-9.56	-6.44	CuFeO2
Diaspore	-1.85	5.30	7.15	AlHO2
Epsomite	-4.27	-6.23	-1.96	MgSO4:7H2O
Ettringite	-57.99	4.47	62.46	Ca6Al2(SO4)3(OH)12:26H2O
F2(g)	-150.65	-94.94	55.71	F2
Fe	-57.75	1.27	59.02	Fe
Fe(OH)2	-15.57	-1.68	13.89	Fe(OH)2
Fe(OH)3	-0.31	5.33	5.64	Fe(OH)3
Fe2(SO4)3	-19.67	-16.62	3.05	Fe2(SO4)3
FeF2	-91.25	-93.67	-2.42	FeF2
FeF3	-113.40	-132.66	-19.26	FeF3
FeO	-15.20	-1.68	13.52	FeO
Ferrite-Ca	-7.30	14.19	21.50	CaFe2O4
Ferrite-Cu	2.78	13.06	10.28	CuFe2O4
Ferrite-Dicalcium	-39.08	17.72	56.80	Ca2Fe2O5
Ferrite-Mg	-7.49	13.53	21.02	MgFe2O4
Ferrite-Zn	0.76	12.46	11.70	ZnFe2O4
FeSO4	-13.38	-10.77	2.61	FeSO4
Fluorite	-78.40	-88.47	-10.07	CaF2
Gibbsite	-2.44	5.30	7.74	Al(OH)3
Glauberite	-8.54	-14.01	-5.47	Na2Ca(SO4)2
Goethite	4.80	5.33	0.53	FeOOH
Gypsum	-1.04	-5.57	-4.53	CaSO4:2H2O
H2(g)	-40.06	-43.16	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-127.62	-135.61	-7.99	H2S
Halite	-7.56	-5.99	1.56	NaCl
Hausmannite	-14.42	-4.27	10.14	Mn3O4
HCl(g)	-12.63	-6.32	6.30	HCl
Hematite	10.59	10.67	0.08	Fe2O3
Hercynite	-19.88	8.92	28.80	FeAl2O4
Hexahydrite	-4.50	-6.23	-1.73	MgSO4:6H2O
Hydrophilite	-20.87	-9.12	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	7.04	-2.37	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	3.59	-1.86	-5.45	NaFe3(SO4)2(OH)6
K	-69.68	1.29	70.98	K
K(g)	-80.29	1.29	81.58	K
K2O	-84.39	-0.35	84.04	K2O
K3H(SO4)2	-15.10	-18.72	-3.62	K3H(SO4)2
Kainite	-12.42	-12.73	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-16.34	-13.07	3.27	KAl(SO4)2
Katoite	-57.77	21.18	78.94	Ca3Al2H12O12
Kieserite	-5.96	-6.23	-0.27	MgSO4:H2O
KMgCl3	-37.53	-16.28	21.25	KMgCl3
KMgCl3:2H2O	-30.24	-16.28	13.96	KMgCl3:2H2O
Lammerite	-11.61	-10.06	1.55	Cu3(AsO4)2
Lawrencite	-23.38	-14.32	9.05	FeCl2
Leonite	-11.57	-15.68	-4.11	K2Mg(SO4)2:4H2O
Lime	-29.04	3.53	32.57	CaO
Magnetite	-1.43	8.99	10.42	Fe3O4
Manganite	-3.11	-3.27	-0.16	MnO(OH)
Manganosite	-15.64	2.27	17.92	MnO
Mayenite	-377.65	116.50	494.15	Ca12Al14O33
Melanterite	-8.37	-10.77	-2.40	FeSO4:7H2O
Mercallite	-7.83	-9.27	-1.44	KHSO4
Mg	-116.71	5.81	122.52	Mg
Mg(g)	-136.44	5.81	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.71	-5.51	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-14.01	-4.80	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.51	-9.78	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.08	-9.78	7.30	MgCl2:4H2O
MgCl2:H2O	-25.85	-9.78	16.07	MgCl2:H2O
MgOHCl	-19.35	-3.46	15.89	MgOHCl
MgSO4	-11.06	-6.23	4.83	MgSO4

Mirabilite	-7.28	-8.44	-1.15	Na2SO4:10H2O
Misenite	-54.02	-65.09	-11.08	K8H6(SO4)7
Mn	-77.72	5.21	82.93	Mn
Mn(OH)2(am)	-13.04	2.27	15.31	Mn(OH)2
Mn(OH)3	-9.61	-3.27	6.34	Mn(OH)3
MnCl2:2H2O	-14.37	-10.37	4.00	MnCl2:2H2O
MnCl2:4H2O	-13.13	-10.38	2.75	MnCl2:4H2O
MnCl2:H2O	-15.92	-10.37	5.54	MnCl2:H2O
MnO2(gamma)	-0.77	-16.89	-16.13	MnO2
MnSO4	-9.43	-6.82	2.61	MnSO4
Molysite	-27.11	-13.64	13.47	FeCl3
N2(g)	-4.41	-7.59	-3.18	N2
Na	-65.57	1.80	67.37	Na
Na(g)	-79.06	1.80	80.86	Na
Na2O	-66.76	0.66	67.42	Na2O
Na3H(SO4)2	-16.31	-17.20	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.55	-22.44	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-14.22	5.66	19.88	NaFeO2
Nantokite	-14.45	-21.22	-6.77	CuCl
NH3(g)	-59.41	-57.61	1.80	NH3
Niter	-7.26	-7.49	-0.22	KNO3
NO(g)	-18.87	-18.13	0.74	NO
NO2(g)	-14.19	-5.84	8.35	NO2
O2(g)	-2.99	-5.88	-2.89	O2
Orpiment	-399.78	-479.26	-79.49	As2S3
Oxychloride-Mg	-26.42	-0.59	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.84	-6.23	-1.39	MgSO4:5H2O
Periclase	-18.46	2.87	21.33	MgO
Picromerite	-11.24	-15.68	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-12.51	-26.82	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-19.02	3.53	22.55	Ca(OH)2
Pyrite	-216.57	-241.27	-24.70	FeS2
Pyrolusite	0.77	-16.89	-17.66	MnO2
Pyrrhotite	-133.55	-137.29	-3.74	FeS
Realgar	-155.66	-215.94	-60.28	AsS
S	-93.44	-138.55	-45.11	S
S2(g)	-200.78	-207.97	-7.19	S2
Scacchite	-19.12	-10.37	8.74	MnCl2
Sellaite	-79.69	-89.13	-9.44	MgF2
SO2(g)	-43.83	-43.66	0.18	SO2
Sphalerite	-122.35	-133.82	-11.47	ZnS
Spinel	-24.14	13.46	37.61	Al2MgO4
Starkeyite	-5.23	-6.23	-1.00	MgSO4:4H2O
Sylvite	-7.33	-6.50	0.83	KCl
Syngenite	-7.42	-15.02	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-45.83	-28.68	17.14	Mg2CaCl6:12H2O
Tenorite	-5.25	2.39	7.65	CuO
Thenardite	-8.08	-8.44	-0.36	Na2SO4
Todorokite	-9.87	-55.70	-45.82	Mn7O12:3H2O
Troilite	-133.45	-137.29	-3.84	FeS
Wurtzite	-124.65	-133.82	-9.17	ZnS
Wustite	-13.25	-0.84	12.40	Fe.9470
Zincite	-9.41	1.79	11.20	ZnO
Zn	-64.05	4.74	68.79	Zn
Zn(ClO4)2:6H2O	-71.47	-65.84	5.63	Zn(ClO4)2:6H2O
Zn(g)	-80.67	4.74	85.41	Zn
Zn(NO3)2:6H2O	-16.23	-12.83	3.40	Zn(NO3)2:6H2O
Zn(OH)2(beta)	-10.14	1.79	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-9.87	1.79	11.66	Zn(OH)2
Zn(OH)2(gamma)	-10.09	1.79	11.88	Zn(OH)2
Zn2(OH)3Cl	-18.03	-2.74	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-13.09	-5.51	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-21.17	-11.86	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-31.90	-12.81	19.09	Zn3O(SO4)2
Zn5(NO3)2(OH)8	-48.32	-5.65	42.67	Zn5(NO3)2(OH)8
ZnCl2	-17.93	-10.85	7.08	ZnCl2
ZnCl2(NH3)2	-119.07	-126.08	-7.01	ZnCl2(NH3)2

ZnCl2(NH3)4	-234.59	-241.30	-6.71	ZnCl2(NH3)4
ZnCl2(NH3)6	-351.78	-356.52	-4.74	ZnCl2(NH3)6
ZnF2	-89.71	-90.20	-0.49	ZnF2
ZnSO4	-10.84	-7.30	3.53	ZnSO4
ZnSO4:6H2O	-5.60	-7.30	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.43	-7.30	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.75	-7.30	-0.55	ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
