
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 Inter 3
temp 25
units mg/l
pe 12
pH 2.29
Cl 39.1
S(6) 1113.00
Al 34.60
As 0.01
Ca 305.00
Cu 0.13
Fe 12.16
K 8.67
Mg 29.67
Mn 13.97
Na 65.26
Zn 0.02
C(4) 0
MIX 1
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.9470
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. Inter 3

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

Elements	Molality	Moles
Al	1.284e-003	1.284e-003
As	1.337e-007	1.337e-007

Ca	7.623e-003	7.623e-003
Cl	1.105e-003	1.105e-003
Cu	2.049e-006	2.049e-006
Fe	2.181e-004	2.181e-004
K	2.221e-004	2.221e-004
Mg	1.223e-003	1.223e-003
Mn	2.547e-004	2.547e-004
Na	2.843e-003	2.843e-003
S(6)	1.161e-002	1.161e-002
Zn	3.064e-007	3.064e-007

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

pH	=	2.290
pe	=	12.000
Activity of water	=	1.000
Ionic strength	=	3.680e-002
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	-7.977e-003
Total carbon (mol/kg)	=	0.000e+000
Total CO2 (mol/kg)	=	0.000e+000
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	9.172e-003
Percent error, 100*(Cat- An)/(Cat+ An)	=	21.65
Iterations	=	8
Total H	=	1.110586e+002
Total O	=	5.557178e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	5.903e-003	5.129e-003	-2.229	-2.290	-0.061
OH-	2.252e-012	1.878e-012	-11.648	-11.726	-0.079
H2O	5.553e+001	9.995e-001	1.744	-0.000	0.000
Al	1.284e-003				
AlSO4+	5.907e-004	4.949e-004	-3.229	-3.305	-0.077
Al+3	5.446e-004	1.494e-004	-3.264	-3.826	-0.562
Al(SO4)2-	1.484e-004	1.244e-004	-3.828	-3.905	-0.077
AlOH+2	6.571e-007	3.262e-007	-6.182	-6.487	-0.304
Al2(OH)2+4	2.524e-010	1.730e-011	-9.598	-10.762	-1.164
Al(OH)2+	1.762e-010	1.476e-010	-9.754	-9.831	-0.077
HALO2	4.189e-014	4.189e-014	-13.378	-13.378	0.000
Al3(OH)4+5	3.800e-015	6.338e-017	-14.420	-16.198	-1.778
AlO2-	3.339e-018	2.798e-018	-17.476	-17.553	-0.077
NaAlO2	1.245e-021	1.245e-021	-20.905	-20.905	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-71.703	-75.189	-3.486
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-107.015	-107.015	0.000
As(3)	8.809e-017				
HAsO2	4.701e-017	4.701e-017	-16.328	-16.328	0.000
As(OH)3	4.108e-017	4.108e-017	-16.386	-16.386	0.000
H2AsO3-	5.847e-024	4.899e-024	-23.233	-23.310	-0.077
AsO2-	5.592e-024	4.686e-024	-23.252	-23.329	-0.077
AsO2OH-2	1.914e-032	9.333e-033	-31.718	-32.030	-0.312
As(5)	1.337e-007				
H2AsO4-	7.609e-008	6.375e-008	-7.119	-7.195	-0.077
H3AsO4	5.759e-008	5.759e-008	-7.240	-7.240	0.000
HAsO4-2	4.231e-012	2.064e-012	-11.374	-11.685	-0.312
AsO4-3	5.216e-021	1.032e-021	-20.283	-20.986	-0.704
Ca	7.623e-003				
Ca+2	6.115e-003	3.186e-003	-2.214	-2.497	-0.283
CaSO4	1.507e-003	1.507e-003	-2.822	-2.822	0.000
CaCl+	7.369e-007	6.174e-007	-6.133	-6.209	-0.077
CaCl2	6.641e-010	6.641e-010	-9.178	-9.178	0.000
CaOH+	1.047e-013	8.770e-014	-12.980	-13.057	-0.077

Cl(-1)	1.105e-003					
Cl-	1.102e-003	9.144e-004	-2.958	-3.039	-0.081	
HCl	1.053e-006	1.053e-006	-5.977	-5.977	0.000	
CaCl+	7.369e-007	6.174e-007	-6.133	-6.209	-0.077	
MgCl+	3.884e-007	3.254e-007	-6.411	-6.488	-0.077	
NaCl	3.748e-007	3.748e-007	-6.426	-6.426	0.000	
MnCl+	2.176e-007	1.823e-007	-6.662	-6.739	-0.077	
FeCl+	5.641e-008	4.726e-008	-7.249	-7.325	-0.077	
KCl	5.516e-009	5.516e-009	-8.258	-8.258	0.000	
CuCl+	2.296e-009	1.924e-009	-8.639	-8.716	-0.077	
FeCl+2	2.088e-009	1.036e-009	-8.680	-8.984	-0.304	
FeCl2+	9.157e-010	7.673e-010	-9.038	-9.115	-0.077	
CaCl2	6.641e-010	6.641e-010	-9.178	-9.178	0.000	
ZnCl+	2.159e-010	1.809e-010	-9.666	-9.743	-0.077	
CuCl2	9.263e-013	9.263e-013	-12.033	-12.033	0.000	
FeCl2	2.319e-013	2.319e-013	-12.635	-12.635	0.000	
ZnCl2	1.932e-013	1.932e-013	-12.714	-12.714	0.000	
MnCl3-	3.974e-014	3.329e-014	-13.401	-13.478	-0.077	
Zn(OH)Cl	6.029e-016	6.029e-016	-15.220	-15.220	0.000	
ZnCl3-	1.165e-016	9.758e-017	-15.934	-16.011	-0.077	
CuCl2-	2.784e-017	2.332e-017	-16.555	-16.632	-0.077	
ZnCl4-2	1.387e-018	6.763e-019	-17.858	-18.170	-0.312	
FeCl4-2	1.149e-018	5.603e-019	-17.940	-18.252	-0.312	
FeCl4-	9.205e-019	7.713e-019	-18.036	-18.113	-0.077	
CuCl3-2	2.809e-019	1.370e-019	-18.552	-18.863	-0.312	
CuCl4-2	2.980e-023	1.454e-023	-22.526	-22.838	-0.312	
Cl(1)	5.148e-028					
HClO	5.148e-028	5.148e-028	-27.288	-27.288	0.000	
ClO-	3.230e-033	2.707e-033	-32.491	-32.568	-0.077	
Cl(3)	0.000e+000					
HClO2	0.000e+000	0.000e+000	-54.111	-54.111	0.000	
ClO2-	0.000e+000	0.000e+000	-54.914	-54.991	-0.077	
Cl(5)	0.000e+000					
ClO3-	0.000e+000	0.000e+000	-63.483	-63.562	-0.079	
Cl(7)	0.000e+000					
ClO4-	0.000e+000	0.000e+000	-76.356	-76.435	-0.079	
ZnClO4+	0.000e+000	0.000e+000	-82.010	-82.087	-0.077	
Cu(1)	5.307e-016					
Cu+	5.025e-016	4.211e-016	-15.299	-15.376	-0.077	
CuCl2-	2.784e-017	2.332e-017	-16.555	-16.632	-0.077	
CuCl3-2	2.809e-019	1.370e-019	-18.552	-18.863	-0.312	
Cu(2)	2.049e-006					
Cu+2	1.476e-006	7.692e-007	-5.831	-6.114	-0.283	
CuSO4	5.704e-007	5.704e-007	-6.244	-6.244	0.000	
CuCl+	2.296e-009	1.924e-009	-8.639	-8.716	-0.077	
CuOH+	9.229e-012	7.732e-012	-11.035	-11.112	-0.077	
CuCl2	9.263e-013	9.263e-013	-12.033	-12.033	0.000	
CuCl4-2	2.980e-023	1.454e-023	-22.526	-22.838	-0.312	
CuO2-2	8.086e-037	3.944e-037	-36.092	-36.404	-0.312	
Fe(2)	1.726e-004					
Fe+2	1.362e-004	7.095e-005	-3.866	-4.149	-0.283	
FeSO4	3.640e-005	3.640e-005	-4.439	-4.439	0.000	
FeCl+	5.641e-008	4.726e-008	-7.249	-7.325	-0.077	
FeOH+	5.219e-012	4.373e-012	-11.282	-11.359	-0.077	
FeCl2	2.319e-013	2.319e-013	-12.635	-12.635	0.000	
FeCl4-2	1.149e-018	5.603e-019	-17.940	-18.252	-0.312	
Fe(OH)2	6.769e-021	6.769e-021	-20.169	-20.169	0.000	
Fe(OH)3-	6.268e-029	5.252e-029	-28.203	-28.280	-0.077	
Fe(OH)4-2	0.000e+000	0.000e+000	-40.678	-40.990	-0.312	
Fe(3)	4.544e-005					
Fe+3	2.480e-005	6.803e-006	-4.606	-5.167	-0.562	
FeOH+2	1.724e-005	8.560e-006	-4.763	-5.068	-0.304	
FeSO4+	2.543e-006	2.131e-006	-5.595	-5.671	-0.077	
Fe(OH)2+	6.593e-007	5.524e-007	-6.181	-6.258	-0.077	
Fe(SO4)2-	1.392e-007	1.166e-007	-6.856	-6.933	-0.077	
Fe2(OH)2+4	2.876e-008	1.972e-009	-7.541	-8.705	-1.164	
FeCl+2	2.088e-009	1.036e-009	-8.680	-8.984	-0.304	

	FeCl ₂ +	9.157e-010	7.673e-010	-9.038	-9.115	-0.077
	Fe(OH) ₃	5.035e-011	5.035e-011	-10.298	-10.298	0.000
	Fe ₃ (OH) ₄₊₅	1.365e-011	2.276e-013	-10.865	-12.643	-1.778
	Fe(OH) ₄₋	2.942e-018	2.465e-018	-17.531	-17.608	-0.077
	FeCl ₄₋	9.205e-019	7.713e-019	-18.036	-18.113	-0.077
H(0)		4.137e-032				
	H ₂	2.069e-032	2.087e-032	-31.684	-31.680	0.004
K		2.221e-004				
	K+	2.165e-004	1.797e-004	-3.665	-3.746	-0.081
	KSO ₄₋	5.603e-006	4.694e-006	-5.252	-5.328	-0.077
	KHSO ₄	2.124e-008	2.124e-008	-7.673	-7.673	0.000
	KCl	5.516e-009	5.516e-009	-8.258	-8.258	0.000
	KOH	1.214e-016	1.214e-016	-15.916	-15.916	0.000
Mg		1.223e-003				
	Mg+2	8.282e-004	4.559e-004	-3.082	-3.341	-0.259
	MgSO ₄	3.941e-004	3.941e-004	-3.404	-3.404	0.000
	MgCl+	3.884e-007	3.254e-007	-6.411	-6.488	-0.077
	Mg ₄ (OH) ₄₊₄	0.000e+000	0.000e+000	-42.792	-43.955	-1.164
Mn(2)		2.547e-004				
	Mn+2	1.797e-004	9.362e-005	-3.745	-4.029	-0.283
	MnSO ₄	7.478e-005	7.478e-005	-4.126	-4.126	0.000
	MnCl+	2.176e-007	1.823e-007	-6.662	-6.739	-0.077
	MnOH+	5.598e-013	4.690e-013	-12.252	-12.329	-0.077
	MnCl ₃₋	3.974e-014	3.329e-014	-13.401	-13.478	-0.077
	Mn ₂ OH+3	2.199e-016	4.705e-017	-15.658	-16.327	-0.670
	Mn(OH) ₂	2.244e-022	2.244e-022	-21.649	-21.649	0.000
	Mn ₂ (OH) ₃₊	9.749e-026	8.168e-026	-25.011	-25.088	-0.077
	Mn(OH) ₃₋	4.895e-032	4.101e-032	-31.310	-31.387	-0.077
	Mn(OH) ₄₋₂	0.000e+000	0.000e+000	-42.858	-43.169	-0.312
Mn(3)		1.167e-017				
	Mn+3	1.167e-017	2.497e-018	-16.933	-17.603	-0.670
Mn(6)		0.000e+000				
	MnO ₄₋₂	0.000e+000	0.000e+000	-55.845	-56.156	-0.312
Mn(7)		0.000e+000				
	MnO ₄₋	0.000e+000	0.000e+000	-53.434	-53.513	-0.079
Na		2.843e-003				
	Na+	2.783e-003	2.332e-003	-2.555	-2.632	-0.077
	NaSO ₄₋	5.953e-005	4.988e-005	-4.225	-4.302	-0.077
	NaCl	3.748e-007	3.748e-007	-6.426	-6.426	0.000
	NaOH	7.555e-016	7.555e-016	-15.122	-15.122	0.000
	NaAlO ₂	1.245e-021	1.245e-021	-20.905	-20.905	0.000
O(0)		2.895e-029				
	O ₂	1.448e-029	1.460e-029	-28.839	-28.836	0.004
S(6)		1.161e-002				
	SO ₄₋₂	6.638e-003	3.237e-003	-2.178	-2.490	-0.312
	HSO ₄₋	2.002e-003	1.677e-003	-2.699	-2.775	-0.077
	CaSO ₄	1.507e-003	1.507e-003	-2.822	-2.822	0.000
	AlSO ₄₊	5.907e-004	4.949e-004	-3.229	-3.305	-0.077
	MgSO ₄	3.941e-004	3.941e-004	-3.404	-3.404	0.000
	Al(SO ₄) ₂₋	1.484e-004	1.244e-004	-3.828	-3.905	-0.077
	MnSO ₄	7.478e-005	7.478e-005	-4.126	-4.126	0.000
	NaSO ₄₋	5.953e-005	4.988e-005	-4.225	-4.302	-0.077
	FeSO ₄	3.640e-005	3.640e-005	-4.439	-4.439	0.000
	KSO ₄₋	5.603e-006	4.694e-006	-5.252	-5.328	-0.077
	FeSO ₄₊	2.543e-006	2.131e-006	-5.595	-5.671	-0.077
	CuSO ₄	5.704e-007	5.704e-007	-6.244	-6.244	0.000
	Fe(SO ₄) ₂₋	1.392e-007	1.166e-007	-6.856	-6.933	-0.077
	ZnSO ₄	8.010e-008	8.010e-008	-7.096	-7.096	0.000
	KHSO ₄	2.124e-008	2.124e-008	-7.673	-7.673	0.000
	H ₂ SO ₄	8.115e-009	8.115e-009	-8.091	-8.091	0.000
Zn		3.064e-007				
	Zn+2	2.260e-007	1.178e-007	-6.646	-6.929	-0.283
	ZnSO ₄	8.010e-008	8.010e-008	-7.096	-7.096	0.000
	ZnCl+	2.159e-010	1.809e-010	-9.666	-9.743	-0.077
	ZnCl ₂	1.932e-013	1.932e-013	-12.714	-12.714	0.000
	ZnOH+	3.004e-014	2.517e-014	-13.522	-13.599	-0.077
	Zn(OH)Cl	6.029e-016	6.029e-016	-15.220	-15.220	0.000

ZnCl3-	1.165e-016	9.758e-017	-15.934	-16.011	-0.077
ZnCl4-2	1.387e-018	6.763e-019	-17.858	-18.170	-0.312
Zn(OH)2	2.101e-020	2.101e-020	-19.678	-19.678	0.000
Zn(OH)3-	1.515e-029	1.269e-029	-28.820	-28.897	-0.077
Zn(OH)4-2	8.646e-040	4.216e-040	-39.063	-39.375	-0.312
ZnClO4+	0.000e+000	0.000e+000	-82.010	-82.087	-0.077

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

Phase	SI	log IAP	log KT	
Al	-125.24	24.67	149.91	Al
Al(g)	-175.95	24.67	200.62	Al
Al2(SO4)3	-34.02	-15.12	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-16.68	-15.12	1.56	Al2(SO4)3:6H2O
Alum-K	-7.58	-12.55	-4.97	KAl(SO4)2:12H2O
Alunite	-5.99	-6.46	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.64	-4.99	-4.35	CaSO4
Antarcticite	-12.67	-8.58	4.09	CaCl2:6H2O
Antlerite	-20.40	-11.67	8.73	Cu3(SO4)(OH)4
Aphthitalite	-14.96	-18.85	-3.89	NaK3(SO4)2
Arcanite	-8.14	-9.98	-1.84	K2SO4
Arsenolite	-31.36	-51.20	-19.84	As2O3
As	-46.66	-3.97	42.68	As
As2O5	-21.11	-18.97	2.14	As2O5
As4O6(cubi)	-62.57	-102.40	-39.82	As4O6
As4O6(mono)	-62.35	-102.40	-40.05	As4O6
Atacamite	-31.06	-16.79	14.26	Cu4Cl2(OH)6
Bassanite	-1.28	-4.99	-3.71	CaSO4:0.5H2O
Birnessite	-93.91	-179.45	-85.55	Mn8O14:5H2O
Bischofite	-13.81	-9.42	4.39	MgCl2:6H2O
Bixbyite	-20.50	-21.47	-0.96	Mn2O3
Bloedite	-11.11	-13.59	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-4.51	3.04	7.55	AlO2H
Brochantite	-28.63	-13.21	15.42	Cu4(SO4)(OH)6
Brucite	-15.04	1.24	16.28	Mg(OH)2
Ca	-123.33	16.50	139.83	Ca
Ca(g)	-148.57	16.50	165.07	Ca
Ca2Al2O5:8H2O	-49.32	10.25	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-32.78	-6.49	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-30.52	-12.72	17.80	Ca3(AsO4)2
Ca3Al2O6	-100.69	12.34	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-122.66	17.82	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-92.84	14.42	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-89.27	14.42	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-70.66	-2.33	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-38.74	8.17	46.91	CaAl2O4
CaAl2O4:10H2O	-29.83	8.17	37.99	CaAl2O4:10H2O
CaAl4O7	-54.33	14.26	68.59	CaAl4O7
Carnallite	-20.48	-16.20	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.45	-4.99	-3.54	CaSO4:0.5H2O
Chalcanthite	-5.98	-8.60	-2.63	CuSO4:5H2O
Chalcocyanite	-11.52	-8.60	2.91	CuSO4
Chloromagnesite	-31.23	-9.42	21.82	MgCl2
Cl2(g)	-28.07	-25.08	2.99	Cl2
Claudetite	-31.40	-51.20	-19.80	As2O3
Corundum	-12.20	6.09	18.29	Al2O3
Cu	-18.61	12.88	31.50	Cu
Cu(g)	-70.77	12.88	83.66	Cu
CuCl2	-15.91	-12.19	3.72	CuCl2
Cuprite	-24.26	-26.17	-1.91	Cu2O
Delafossite	-4.95	-11.38	-6.44	CuFeO2
Diaspore	-4.10	3.04	7.15	AlHO2
Epsomite	-3.87	-5.83	-1.96	MgSO4:7H2O
Ettringite	-65.09	-2.63	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-44.17	14.85	59.02	Fe
Fe(OH)2	-13.46	0.43	13.89	Fe(OH)2

Fe(OH)3	-3.94	1.70	5.64	Fe(OH)3
Fe2(SO4)3	-20.85	-17.80	3.05	Fe2(SO4)3
FeO	-13.09	0.43	13.52	FeO
Ferrite-Ca	-16.01	5.49	21.50	CaFe2O4
Ferrite-Cu	-8.41	1.87	10.28	CuFe2O4
Ferrite-Dicalcium	-49.23	7.57	56.80	Ca2Fe2O5
Ferrite-Mg	-16.38	4.64	21.02	MgFe2O4
Ferrite-Zn	-10.64	1.06	11.70	ZnFe2O4
FeSO4	-9.25	-6.64	2.61	FeSO4
Gibbsite	-4.70	3.04	7.74	Al(OH)3
Glauberite	-7.27	-12.74	-5.47	Na2Ca(SO4)2
Goethite	1.17	1.70	0.53	FeOOH
Gypsum	-0.46	-4.99	-4.53	CaSO4:2H2O
H2(g)	-28.58	-31.68	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.23	-5.67	1.56	NaCl
Hausmannite	-31.06	-20.91	10.14	Mn3O4
HCl(g)	-11.63	-5.33	6.30	HCl
Hematite	3.33	3.40	0.08	Fe2O3
Hercynite	-22.28	6.52	28.80	FeAl2O4
Hexahydrite	-4.11	-5.83	-1.73	MgSO4:6H2O
Hydrophilite	-20.32	-8.57	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	-1.08	-10.49	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	-3.93	-9.38	-5.45	NaFe3(SO4)2(OH)6
K	-65.22	5.75	70.98	K
K(g)	-75.83	5.75	81.58	K
K2O	-86.95	-2.91	84.04	K2O
K3H(SO4)2	-14.88	-18.51	-3.62	K3H(SO4)2
Kainite	-12.30	-12.62	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-15.82	-12.55	3.27	KAl(SO4)2
Katoite	-66.61	12.34	78.94	Ca3Al2H12O12
Kieserite	-5.56	-5.83	-0.27	MgSO4:H2O
KMgCl3	-37.45	-16.20	21.25	KMgCl3
KMgCl3:2H2O	-30.17	-16.20	13.96	KMgCl3:2H2O
Lammerite	-25.13	-23.57	1.55	Cu3(AsO4)2
Lawrencite	-19.28	-10.23	9.05	FeCl2
Leonite	-11.70	-15.81	-4.11	K2Mg(SO4)2:4H2O
Lime	-30.49	2.08	32.57	CaO
Magnetite	-6.58	3.84	10.42	Fe3O4
Manganite	-10.57	-10.73	-0.16	MnO(OH)
Manganosite	-17.36	0.55	17.92	MnO
Mayenite	-426.54	67.61	494.15	Ca12Al14O33
Melanterite	-4.24	-6.64	-2.40	FeSO4:7H2O
Mercallite	-7.09	-8.53	-1.44	KHSO4
Mg	-106.86	15.66	122.52	Mg
Mg(g)	-126.59	15.66	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.72	-5.52	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-14.42	-5.21	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.15	-9.42	12.73	MgCl2:2H2O
MgCl2:4H2O	-16.72	-9.42	7.30	MgCl2:4H2O
MgCl2:H2O	-25.49	-9.42	16.07	MgCl2:H2O
MgOHCl	-19.98	-4.09	15.89	MgOHCl
MgSO4	-10.66	-5.83	4.83	MgSO4
Mirabilite	-6.60	-7.76	-1.15	Na2SO4:10H2O
Misenite	-50.06	-61.13	-11.08	K8H6(SO4)7
Mn	-67.96	14.97	82.93	Mn
Mn(OH)2(am)	-14.76	0.55	15.31	Mn(OH)2
Mn(OH)3	-17.07	-10.73	6.34	Mn(OH)3
MnCl2:2H2O	-14.10	-10.11	4.00	MnCl2:2H2O
MnCl2:4H2O	-12.86	-10.11	2.75	MnCl2:4H2O
MnCl2:H2O	-15.65	-10.11	5.54	MnCl2:H2O
MnO2(gamma)	-13.97	-30.09	-16.13	MnO2
MnSO4	-9.13	-6.52	2.61	MnSO4
Molysite	-27.75	-14.28	13.47	FeCl3
Na	-60.50	6.87	67.37	Na
Na(g)	-73.99	6.87	80.86	Na

Na2O	-68.10	-0.68	67.42	Na2O
Na3H(SO4)2	-14.28	-15.17	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-14.60	-20.50	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-18.52	1.36	19.88	NaFeO2
Nantokite	-11.65	-18.41	-6.77	CuCl
O2(g)	-25.94	-28.84	-2.89	O2
Oxychloride-Mg	-28.68	-2.85	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.44	-5.83	-1.39	MgSO4:5H2O
Periclase	-20.09	1.24	21.33	MgO
Picromerite	-11.37	-15.81	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-11.47	-25.79	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-20.46	2.08	22.55	Ca(OH)2
Pyrolusite	-12.43	-30.09	-17.66	MnO2
Scacchite	-18.85	-10.11	8.74	MnCl2
Spinel	-30.28	7.33	37.61	Al2MgO4
Starkeyite	-4.83	-5.83	-1.00	MgSO4:4H2O
Sylvite	-7.61	-6.78	0.83	KCl
Syngenite	-7.37	-14.97	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-44.56	-27.41	17.14	Mg2CaCl6:12H2O
Tenorite	-9.18	-1.53	7.65	CuO
Thenardite	-7.40	-7.75	-0.36	Na2SO4
Todorokite	-79.31	-125.13	-45.82	Mn7O12:3H2O
Wustite	-11.86	0.54	12.40	Fe.9470
Zincite	-13.55	-2.35	11.20	ZnO
Zn	-56.72	12.07	68.79	Zn
Zn(ClO4)2:6H2O	-165.43	-159.80	5.63	Zn(ClO4)2:6H2O
Zn(g)	-73.34	12.07	85.41	Zn
Zn(OH)2(beta)	-14.28	-2.35	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-14.01	-2.35	11.66	Zn(OH)2
Zn(OH)2(gamma)	-14.23	-2.35	11.88	Zn(OH)2
Zn2(OH)3Cl	-25.32	-10.03	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-19.35	-11.77	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-35.33	-26.02	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-40.28	-21.19	19.09	Zn3O(SO4)2
ZnCl2	-20.09	-13.01	7.08	ZnCl2
ZnSO4	-12.95	-9.42	3.53	ZnSO4
ZnSO4:6H2O	-7.72	-9.42	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-7.54	-9.42	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-8.87	-9.42	-0.55	ZnSO4:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using mix 1.

Mixture 1.

1.000e+000 Solution 1 Flujo 1
1.000e+000 Solution 2 Inter 3

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

Elements	Molality	Moles
Al	8.574e-004	1.715e-003
As	1.143e-005	2.285e-005
Ca	4.791e-003	9.581e-003
Cl	1.208e-003	2.415e-003
Cu	1.688e-004	3.376e-004
Fe	1.306e-003	2.611e-003
K	4.990e-004	9.980e-004
Mg	7.885e-004	1.577e-003
Mn	2.558e-004	5.117e-004
Na	1.846e-003	3.692e-003

S 1.013e-002 2.026e-002
Zn 3.996e-005 7.992e-005

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

pH = 2.578 Charge balance
pe = 13.598 Adjusted to redox equilibrium
Activity of water = 1.000
Ionic strength = 3.218e-002
Mass of water (kg) = 2.000e+000
Total alkalinity (eq/kg) = -5.793e-003
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = 5.413e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 7.73
Iterations = 9
Total H = 2.221130e+002
Total O = 1.111343e+002

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	3.023e-003	2.642e-003	-2.520	-2.578	-0.059
OH-	4.330e-012	3.646e-012	-11.363	-11.438	-0.075
H2O	5.553e+001	9.996e-001	1.744	-0.000	0.000
Al	8.574e-004				
AlSO4+	4.094e-004	3.461e-004	-3.388	-3.461	-0.073
Al+3	3.371e-004	9.767e-005	-3.472	-4.010	-0.538
Al(SO4)2-	1.101e-004	9.306e-005	-3.958	-4.031	-0.073
AlOH+2	8.049e-007	4.140e-007	-6.094	-6.383	-0.289
Al(OH)2+	4.303e-010	3.638e-010	-9.366	-9.439	-0.073
Al2(OH)2+4	3.566e-010	2.788e-011	-9.448	-10.555	-1.107
HA1O2	2.004e-013	2.004e-013	-12.698	-12.698	0.000
Al3(OH)4+5	1.240e-014	2.516e-016	-13.906	-15.599	-1.693
AlO2-	3.074e-017	2.599e-017	-16.512	-16.585	-0.073
NaAlO2	7.564e-021	7.564e-021	-20.121	-20.121	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-65.049	-68.368	-3.319
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-120.359	-120.359	0.000
As(3)	8.318e-019				
HAsO2	4.439e-019	4.439e-019	-18.353	-18.353	0.000
As(OH)3	3.880e-019	3.880e-019	-18.411	-18.411	0.000
H2AsO3-	1.062e-025	8.981e-026	-24.974	-25.047	-0.073
AsO2-	1.016e-025	8.589e-026	-24.993	-25.066	-0.073
AsO2OH-2	6.561e-034	3.322e-034	-33.183	-33.479	-0.296
HAsS2	0.000e+000	0.000e+000	-203.785	-203.785	0.000
As(5)	1.143e-005				
H2AsO4-	8.199e-006	6.932e-006	-5.086	-5.159	-0.073
H3AsO4	3.226e-006	3.226e-006	-5.491	-5.491	0.000
HAsO4-2	8.603e-010	4.356e-010	-9.065	-9.361	-0.296
AsO4-3	1.964e-018	4.230e-019	-17.707	-18.374	-0.667
Ca	4.791e-003				
Ca+2	3.766e-003	2.024e-003	-2.424	-2.694	-0.270
CaSO4	1.024e-003	1.024e-003	-2.990	-2.990	0.000
CaCl+	5.126e-007	4.334e-007	-6.290	-6.363	-0.073
CaCl2	5.150e-010	5.150e-010	-9.288	-9.288	0.000
CaOH+	1.279e-013	1.082e-013	-12.893	-12.966	-0.073
Cl(-1)	1.208e-003				
Cl-	1.205e-003	1.010e-003	-2.919	-2.996	-0.077
HCl	5.994e-007	5.994e-007	-6.222	-6.222	0.000
CaCl+	5.126e-007	4.334e-007	-6.290	-6.363	-0.073
MgCl+	2.728e-007	2.307e-007	-6.564	-6.637	-0.073
NaCl	2.709e-007	2.709e-007	-6.567	-6.567	0.000
MnCl+	2.395e-007	2.025e-007	-6.621	-6.694	-0.073

CuCl+	2.076e-007	1.755e-007	-6.683	-6.756	-0.073
FeCl+2	4.201e-008	2.161e-008	-7.377	-7.665	-0.289
ZnCl+	3.097e-008	2.618e-008	-7.509	-7.582	-0.073
FeCl+	2.939e-008	2.485e-008	-7.532	-7.605	-0.073
FeCl2+	2.091e-008	1.768e-008	-7.680	-7.753	-0.073
KCl	1.381e-008	1.381e-008	-7.860	-7.860	0.000
CaCl2	5.150e-010	5.150e-010	-9.288	-9.288	0.000
CuCl2	9.339e-011	9.339e-011	-10.030	-10.030	0.000
ZnCl2	3.090e-011	3.090e-011	-10.510	-10.510	0.000
Zn(OH)Cl	1.694e-013	1.694e-013	-12.771	-12.771	0.000
FeCl2	1.347e-013	1.347e-013	-12.871	-12.871	0.000
MnCl3-	5.340e-014	4.515e-014	-13.272	-13.345	-0.073
ZnCl3-	2.039e-014	1.724e-014	-13.691	-13.763	-0.073
ZnCl4-2	2.608e-016	1.320e-016	-15.584	-15.879	-0.296
CuCl2-	7.012e-017	5.928e-017	-16.154	-16.227	-0.073
FeCl4-	2.566e-017	2.169e-017	-16.591	-16.664	-0.073
FeCl4-2	7.847e-019	3.973e-019	-18.105	-18.401	-0.296
CuCl3-2	7.598e-019	3.847e-019	-18.119	-18.415	-0.296
CuCl4-2	3.534e-021	1.789e-021	-20.452	-20.747	-0.296
Cl(1)	1.738e-024				
HClO	1.738e-024	1.738e-024	-23.760	-23.760	0.000
ClO-	2.098e-029	1.774e-029	-28.678	-28.751	-0.073
Cl(3)	0.000e+000				
HClO2	0.000e+000	0.000e+000	-46.810	-46.810	0.000
ClO2-	0.000e+000	0.000e+000	-47.328	-47.401	-0.073
Cl(5)	0.000e+000				
ClO3-	0.000e+000	0.000e+000	-52.125	-52.199	-0.075
Cl(7)	0.000e+000				
ClO4-	0.000e+000	0.000e+000	-61.224	-61.299	-0.075
ZnClO4+	0.000e+000	0.000e+000	-64.761	-64.834	-0.073
Cu(1)	1.108e-015				
Cu+	1.037e-015	8.767e-016	-14.984	-15.057	-0.073
CuCl2-	7.012e-017	5.928e-017	-16.154	-16.227	-0.073
CuCl3-2	7.598e-019	3.847e-019	-18.119	-18.415	-0.296
Cu(2)	1.688e-004				
Cu+2	1.182e-004	6.352e-005	-3.927	-4.197	-0.270
CuSO4	5.040e-005	5.040e-005	-4.298	-4.298	0.000
CuCl+	2.076e-007	1.755e-007	-6.683	-6.756	-0.073
CuOH+	1.467e-009	1.240e-009	-8.834	-8.907	-0.073
CuCl2	9.339e-011	9.339e-011	-10.030	-10.030	0.000
CuCl4-2	3.534e-021	1.789e-021	-20.452	-20.747	-0.296
CuO2-2	9.140e-034	4.628e-034	-33.039	-33.335	-0.296
Fe(2)	8.138e-005				
Fe+2	6.282e-005	3.376e-005	-4.202	-4.472	-0.270
FeSO4	1.853e-005	1.853e-005	-4.732	-4.732	0.000
FeCl+	2.939e-008	2.485e-008	-7.532	-7.605	-0.073
FeOH+	4.778e-012	4.040e-012	-11.321	-11.394	-0.073
FeCl2	1.347e-013	1.347e-013	-12.871	-12.871	0.000
FeCl4-2	7.847e-019	3.973e-019	-18.105	-18.401	-0.296
Fe(OH)2	1.214e-020	1.214e-020	-19.916	-19.916	0.000
Fe(OH)3-	2.163e-028	1.829e-028	-27.665	-27.738	-0.073
Fe(OH)4-2	1.367e-040	0.000e+000	-39.864	-40.160	-0.296
Fe(3)	1.224e-003				
FeOH+2	6.098e-004	3.137e-004	-3.215	-3.504	-0.289
Fe+3	4.432e-004	1.284e-004	-3.353	-3.891	-0.538
FeSO4+	5.089e-005	4.302e-005	-4.293	-4.366	-0.073
Fe(OH)2+	4.649e-005	3.930e-005	-4.333	-4.406	-0.073
Fe2(OH)2+4	3.388e-005	2.648e-006	-4.470	-5.577	-1.107
Fe(SO4)2-	2.979e-006	2.519e-006	-5.526	-5.599	-0.073
Fe3(OH)4+5	1.072e-006	2.175e-008	-5.970	-7.663	-1.693
FeCl+2	4.201e-008	2.161e-008	-7.377	-7.665	-0.289
FeCl2+	2.091e-008	1.768e-008	-7.680	-7.753	-0.073
Fe(OH)3	6.956e-009	6.956e-009	-8.158	-8.158	0.000
Fe(OH)4-	7.820e-016	6.612e-016	-15.107	-15.180	-0.073
FeCl4-	2.566e-017	2.169e-017	-16.591	-16.664	-0.073
H(0)	6.984e-036				
H2	3.492e-036	3.520e-036	-35.457	-35.454	0.003

K	4.990e-004					
K+	4.855e-004	4.070e-004	-3.314	-3.390	-0.077	
KSO4-	1.346e-005	1.138e-005	-4.871	-4.944	-0.073	
KHSO4	2.652e-008	2.652e-008	-7.576	-7.576	0.000	
KCl	1.381e-008	1.381e-008	-7.860	-7.860	0.000	
KOH	5.340e-016	5.340e-016	-15.272	-15.272	0.000	
Mg	7.885e-004					
Mg+2	5.177e-004	2.925e-004	-3.286	-3.534	-0.248	
MgSO4	2.705e-004	2.705e-004	-3.568	-3.568	0.000	
MgCl+	2.728e-007	2.307e-007	-6.564	-6.637	-0.073	
Mg4(OH)4+4	0.000e+000	0.000e+000	-42.467	-43.574	-1.107	
Mn(2)	2.558e-004					
Mn+2	1.752e-004	9.412e-005	-3.757	-4.026	-0.270	
MnSO4	8.043e-005	8.043e-005	-4.095	-4.095	0.000	
MnCl+	2.395e-007	2.025e-007	-6.621	-6.694	-0.073	
MnOH+	1.083e-012	9.155e-013	-11.965	-12.038	-0.073	
MnCl3-	5.340e-014	4.515e-014	-13.272	-13.345	-0.073	
Mn2OH+3	3.996e-016	9.233e-017	-15.398	-16.035	-0.636	
Mn(OH)2	8.503e-022	8.503e-022	-21.070	-21.070	0.000	
Mn2(OH)3+	7.147e-025	6.043e-025	-24.146	-24.219	-0.073	
Mn(OH)3-	3.570e-031	3.018e-031	-30.447	-30.520	-0.073	
Mn(OH)4-2	0.000e+000	0.000e+000	-41.719	-42.015	-0.296	
Mn(3)	4.310e-016					
Mn+3	4.310e-016	9.958e-017	-15.365	-16.002	-0.636	
Mn(6)	0.000e+000					
MnO4-2	0.000e+000	0.000e+000	-47.160	-47.455	-0.296	
Mn(7)	0.000e+000					
MnO4-	0.000e+000	0.000e+000	-43.138	-43.213	-0.075	
Na	1.846e-003					
Na+	1.805e-003	1.526e-003	-2.744	-2.817	-0.073	
NaSO4-	4.129e-005	3.491e-005	-4.384	-4.457	-0.073	
NaCl	2.709e-007	2.709e-007	-6.567	-6.567	0.000	
NaOH	9.597e-016	9.597e-016	-15.018	-15.018	0.000	
NaAlO2	7.564e-021	7.564e-021	-20.121	-20.121	0.000	
O(0)	1.019e-021					
O2	5.097e-022	5.137e-022	-21.293	-21.289	0.003	
S(-2)	0.000e+000					
H2S	0.000e+000	0.000e+000	-96.311	-96.311	0.000	
HS-	0.000e+000	0.000e+000	-100.668	-100.743	-0.075	
S-2	0.000e+000	0.000e+000	-110.808	-111.090	-0.282	
S2-2	0.000e+000	0.000e+000	-178.577	-178.872	-0.296	
HAsS2	0.000e+000	0.000e+000	-203.785	-203.785	0.000	
S3-2	0.000e+000	0.000e+000	-246.399	-246.695	-0.296	
S4-2	0.000e+000	0.000e+000	-314.450	-314.745	-0.296	
S5-2	0.000e+000	0.000e+000	-382.716	-383.012	-0.296	
S(2)	0.000e+000					
S2O3-2	0.000e+000	0.000e+000	-100.677	-100.972	-0.296	
HS2O3-	0.000e+000	0.000e+000	-102.464	-102.536	-0.073	
S(3)	0.000e+000					
S2O4-2	0.000e+000	0.000e+000	-96.263	-96.545	-0.282	
S(4)	2.716e-034					
HSO3-	1.962e-034	1.659e-034	-33.707	-33.780	-0.073	
H2SO3	4.200e-035	4.200e-035	-34.377	-34.377	0.000	
SO2	3.336e-035	3.336e-035	-34.477	-34.477	0.000	
SO3-2	7.161e-039	3.684e-039	-38.145	-38.434	-0.289	
S2O6-2	0.000e+000	0.000e+000	-50.506	-50.801	-0.296	
S3O6-2	0.000e+000	0.000e+000	-120.811	-121.107	-0.296	
S4O6-2	0.000e+000	0.000e+000	-175.211	-175.507	-0.296	
S5O6-2	0.000e+000	0.000e+000	-258.491	-258.786	-0.296	
S(5)	0.000e+000					
S2O5-2	0.000e+000	0.000e+000	-72.095	-72.390	-0.296	
S(6)	1.013e-002					
SO4-2	6.841e-003	3.463e-003	-2.165	-2.461	-0.296	
HSO4-	1.093e-003	9.242e-004	-2.961	-3.034	-0.073	
CaSO4	1.024e-003	1.024e-003	-2.990	-2.990	0.000	
AlSO4+	4.094e-004	3.461e-004	-3.388	-3.461	-0.073	
MgSO4	2.705e-004	2.705e-004	-3.568	-3.568	0.000	

Al(SO4)2-	1.101e-004	9.306e-005	-3.958	-4.031	-0.073
MnSO4	8.043e-005	8.043e-005	-4.095	-4.095	0.000
FeSO4+	5.089e-005	4.302e-005	-4.293	-4.366	-0.073
CuSO4	5.040e-005	5.040e-005	-4.298	-4.298	0.000
NaSO4-	4.129e-005	3.491e-005	-4.384	-4.457	-0.073
FeSO4	1.853e-005	1.853e-005	-4.732	-4.732	0.000
KSO4-	1.346e-005	1.138e-005	-4.871	-4.944	-0.073
ZnSO4	1.123e-005	1.123e-005	-4.950	-4.950	0.000
Fe(SO4)2-	2.979e-006	2.519e-006	-5.526	-5.599	-0.073
KHSO4	2.652e-008	2.652e-008	-7.576	-7.576	0.000
H2SO4	2.303e-009	2.303e-009	-8.638	-8.638	0.000
S(7)	0.000e+000				
S2O8-2	0.000e+000	0.000e+000	-42.881	-43.177	-0.296
S(8)	1.346e-033				
HSO5-	1.346e-033	1.138e-033	-32.871	-32.944	-0.073
Zn	3.996e-005				
Zn+2	2.871e-005	1.543e-005	-4.542	-4.812	-0.270
ZnSO4	1.123e-005	1.123e-005	-4.950	-4.950	0.000
ZnCl+	3.097e-008	2.618e-008	-7.509	-7.582	-0.073
ZnCl2	3.090e-011	3.090e-011	-10.510	-10.510	0.000
ZnOH+	7.571e-012	6.401e-012	-11.121	-11.194	-0.073
Zn(OH)Cl	1.694e-013	1.694e-013	-12.771	-12.771	0.000
ZnCl3-	2.039e-014	1.724e-014	-13.691	-13.763	-0.073
ZnCl4-2	2.608e-016	1.320e-016	-15.584	-15.879	-0.296
Zn(OH)2	1.037e-017	1.037e-017	-16.984	-16.984	0.000
Zn(OH)3-	1.439e-026	1.217e-026	-25.842	-25.915	-0.073
Zn(OH)4-2	1.550e-036	7.849e-037	-35.810	-36.105	-0.296
ZnClO4+	0.000e+000	0.000e+000	-64.761	-64.834	-0.073

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

Phase	SI	log IAP	log KT	
Al	-130.22	19.69	149.91	Al
Al(g)	-180.93	19.69	200.62	Al
Al2(SO4)3	-34.30	-15.40	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-16.96	-15.40	1.56	Al2(SO4)3:6H2O
Alabandite	-101.77	-102.19	-0.42	MnS
Alum-K	-7.35	-12.32	-4.97	KAl(SO4)2:12H2O
Alunite	-4.40	-4.87	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.80	-5.15	-4.35	CaSO4
Antarcticite	-12.78	-8.69	4.09	CaCl2:6H2O
Antlerite	-13.47	-4.74	8.73	Cu3(SO4)(OH)4
Aphthitalite	-14.02	-17.91	-3.89	NaK3(SO4)2
Arcanite	-7.40	-9.24	-1.84	K2SO4
Arsenolite	-35.41	-55.25	-19.84	As2O3
Arsenopyrite	-162.18	-176.63	-14.45	FeAsS
As	-54.34	-11.66	42.68	As
As2O5	-17.61	-15.47	2.14	As2O5
As4O6(cubi)	-70.67	-110.50	-39.82	As4O6
As4O6(mono)	-70.45	-110.50	-40.05	As4O6
Atacamite	-21.58	-7.31	14.26	Cu4Cl2(OH)6
Bassanite	-1.45	-5.15	-3.71	CaSO4:0.5H2O
Birnessite	-66.64	-152.19	-85.55	Mn8O14:5H2O
Bischofite	-13.92	-9.53	4.39	MgCl2:6H2O
Bixbyite	-15.57	-16.54	-0.96	Mn2O3
Bloedite	-11.61	-14.09	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-3.83	3.72	7.55	AlO2H
Bornite	-359.02	-461.56	-102.53	Cu5FeS4
Brochantite	-19.20	-3.78	15.42	Cu4(SO4)(OH)6
Brucite	-14.66	1.62	16.28	Mg(OH)2
Ca	-126.73	13.11	139.83	Ca
Ca(g)	-151.96	13.11	165.07	Ca
Ca2Al2O5:8H2O	-47.20	12.37	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-32.51	-6.22	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-25.89	-8.09	17.80	Ca3(AsO4)2
Ca3Al2O6	-98.20	14.83	113.03	Ca3Al2O6

Ca4Al2Fe2O10	-115.50	24.98	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-89.96	17.29	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-86.39	17.29	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-69.63	-1.30	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-37.00	9.91	46.91	CaAl2O4
CaAl2O4:10H2O	-28.09	9.91	37.99	CaAl2O4:10H2O
CaAl4O7	-51.23	17.36	68.59	CaAl4O7
Carnallite	-20.18	-15.91	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.62	-5.15	-3.54	CaSO4:0.5H2O
Chalcanthite	-4.03	-6.66	-2.63	CuSO4:5H2O
Chalcocite	-93.54	-128.28	-34.74	Cu2S
Chalcocyanite	-9.57	-6.66	2.91	CuSO4
Chalcopyrite	-172.39	-205.00	-32.60	CuFeS2
Chloromagnesite	-31.34	-9.53	21.82	MgCl2
Cl2(g)	-24.79	-21.79	2.99	Cl2
Claudetite	-35.45	-55.25	-19.80	As2O3
Corundum	-10.84	7.45	18.29	Al2O3
Covellite	-79.50	-102.36	-22.86	CuS
Cu	-19.89	11.60	31.50	Cu
Cu(g)	-72.05	11.60	83.66	Cu
CuCl2	-13.91	-10.19	3.72	CuCl2
Cuprite	-23.05	-24.96	-1.91	Cu2O
Delafossite	-2.20	-8.64	-6.44	CuFeO2
Diaspore	-3.42	3.72	7.15	AlHO2
Epsomite	-4.03	-6.00	-1.96	MgSO4:7H2O
Ettringite	-63.10	-0.63	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-47.69	11.33	59.02	Fe
Fe(OH)2	-13.21	0.68	13.89	Fe(OH)2
Fe(OH)3	-1.80	3.84	5.64	Fe(OH)3
Fe2(SO4)3	-18.21	-15.16	3.05	Fe2(SO4)3
FeO	-12.84	0.68	13.52	FeO
Ferrite-Ca	-11.35	10.15	21.50	CaFe2O4
Ferrite-Cu	-1.64	8.64	10.28	CuFe2O4
Ferrite-Dicalcium	-44.19	12.61	56.80	Ca2Fe2O5
Ferrite-Mg	-11.71	9.31	21.02	MgFe2O4
Ferrite-Zn	-3.67	8.03	11.70	ZnFe2O4
FeSO4	-9.54	-6.93	2.61	FeSO4
Gibbsite	-4.02	3.72	7.74	Al(OH)3
Glauberite	-7.78	-13.25	-5.47	Na2Ca(SO4)2
Goethite	3.31	3.84	0.53	FeOOH
Gypsum	-0.62	-5.15	-4.53	CaSO4:2H2O
H2(g)	-32.35	-35.45	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-95.33	-103.32	-7.99	H2S
Halite	-7.38	-5.81	1.56	NaCl
Hausmannite	-25.55	-15.41	10.14	Mn3O4
HCl(g)	-11.88	-5.57	6.30	HCl
Hematite	7.61	7.69	0.08	Fe2O3
Hercynite	-20.67	8.13	28.80	FeAl2O4
Hexahydrite	-4.27	-6.00	-1.73	MgSO4:6H2O
Hydrophilite	-20.43	-8.68	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	4.89	-4.52	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	1.50	-3.94	-5.45	NaFe3(SO4)2(OH)6
K	-66.47	4.51	70.98	K
K(g)	-77.07	4.51	81.58	K
K2O	-85.66	-1.62	84.04	K2O
K3H(SO4)2	-14.05	-17.67	-3.62	K3H(SO4)2
Kainite	-12.07	-12.38	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-15.59	-12.32	3.27	KAl(SO4)2
Katoite	-64.11	14.83	78.94	Ca3Al2H12O12
Kieserite	-5.73	-5.99	-0.27	MgSO4:H2O
KMgCl3	-37.16	-15.91	21.25	KMgCl3
KMgCl3:2H2O	-29.87	-15.91	13.96	KMgCl3:2H2O
Lammerite	-14.15	-12.60	1.55	Cu3(AsO4)2
Lawrencite	-19.52	-10.46	9.05	FeCl2
Leonite	-11.12	-15.24	-4.11	K2Mg(SO4)2:4H2O

Lime	-30.11	2.46	32.57	CaO
Magnetite	-2.05	8.37	10.42	Fe ₃ O ₄
Manganite	-8.10	-8.27	-0.16	MnO(OH)
Manganosite	-16.79	1.13	17.92	MnO
Mayenite	-412.47	81.68	494.15	Ca ₁₂ Al ₁₄ O ₃₃
Melanterite	-4.54	-6.93	-2.40	FeSO ₄ ·7H ₂ O
Mercallite	-6.99	-8.43	-1.44	KHSO ₄
Mg	-110.25	12.27	122.52	Mg
Mg(g)	-129.98	12.27	142.25	Mg
Mg1.25SO ₄ (OH)0.5:0.5H ₂ O	-10.78	-5.59	5.20	Mg1.25SO ₄ (OH)0.5:0.5H ₂ O
Mg1.5SO ₄ (OH)	-14.39	-5.18	9.21	Mg1.5SO ₄ (OH)
MgCl ₂ :2H ₂ O	-22.26	-9.53	12.73	MgCl ₂ :2H ₂ O
MgCl ₂ :4H ₂ O	-16.83	-9.53	7.30	MgCl ₂ :4H ₂ O
MgCl ₂ :H ₂ O	-25.60	-9.53	16.07	MgCl ₂ :H ₂ O
MgOHCl	-19.84	-3.95	15.89	MgOHCl
MgSO ₄	-10.82	-5.99	4.83	MgSO ₄
Mirabilite	-6.94	-8.10	-1.15	Na ₂ SO ₄ ·10H ₂ O
Misenite	-48.74	-59.82	-11.08	K ₈ H ₆ (SO ₄) ₇
Mn	-71.16	11.77	82.93	Mn
Mn(OH) ₂ (am)	-14.18	1.13	15.31	Mn(OH) ₂
Mn(OH) ₃	-14.61	-8.27	6.34	Mn(OH) ₃
MnCl ₂ :2H ₂ O	-14.02	-10.02	4.00	MnCl ₂ :2H ₂ O
MnCl ₂ :4H ₂ O	-12.77	-10.02	2.75	MnCl ₂ :4H ₂ O
MnCl ₂ :H ₂ O	-15.56	-10.02	5.54	MnCl ₂ :H ₂ O
MnO ₂ (gamma)	-9.61	-25.74	-16.13	MnO ₂
MnSO ₄	-9.10	-6.49	2.61	MnSO ₄
Molysite	-26.35	-12.88	13.47	FeCl ₃
Na	-62.29	5.08	67.37	Na
Na(g)	-75.78	5.08	80.86	Na
Na ₂ O	-67.89	-0.48	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-15.06	-15.95	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-15.45	-21.34	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
NaFeO ₂	-16.28	3.60	19.88	NaFeO ₂
Nantokite	-11.29	-18.05	-6.77	CuCl
O ₂ (g)	-18.40	-21.29	-2.89	O ₂
Orpiment	-285.73	-365.21	-79.49	As ₂ S ₃
Oxychloride-Mg	-28.16	-2.33	25.83	Mg ₂ Cl(OH) ₃ :4H ₂ O
Pentahydrite	-4.61	-6.00	-1.39	MgSO ₄ :5H ₂ O
Periclase	-19.70	1.62	21.33	MgO
Picromerite	-10.80	-15.24	-4.44	K ₂ Mg(SO ₄) ₂ :6H ₂ O
Polyhalite	-11.23	-25.54	-14.31	K ₂ MgCa ₂ (SO ₄) ₄ :2H ₂ O
Portlandite	-20.08	2.46	22.55	Ca(OH) ₂
Pyrite	-157.33	-182.03	-24.70	FeS ₂
Pyrolusite	-8.08	-25.74	-17.66	MnO ₂
Pyrrhotite	-98.90	-102.64	-3.74	FeS
Realgar	-110.93	-171.21	-60.28	AsS
S	-68.85	-113.97	-45.11	S
S ₂ (g)	-151.60	-158.79	-7.19	S ₂
Scacchite	-18.76	-10.02	8.74	MnCl ₂
SO ₂ (g)	-34.65	-34.48	0.18	SO ₂
Sphalerite	-91.51	-102.98	-11.47	ZnS
Spinel	-28.54	9.07	37.61	Al ₂ MgO ₄
Starkeyite	-5.00	-6.00	-1.00	MgSO ₄ :4H ₂ O
Sylvite	-7.21	-6.39	0.83	KCl
Syngenite	-6.80	-14.40	-7.60	K ₂ Ca(SO ₄) ₂ :H ₂ O
Tachyhydrite	-44.88	-27.74	17.14	Mg ₂ CaCl ₆ :12H ₂ O
Tenorite	-6.69	0.96	7.65	CuO
Thenardite	-7.74	-8.09	-0.36	Na ₂ SO ₄
Todorokite	-56.39	-102.22	-45.82	Mn ₇ O ₁₂ :3H ₂ O
Troilite	-98.79	-102.64	-3.84	FeS
Wurtzite	-93.81	-102.98	-9.17	ZnS
Wustite	-11.42	0.98	12.40	Fe ₉₄ 7O
Zincite	-10.85	0.34	11.20	ZnO
Zn	-57.80	10.99	68.79	Zn
Zn(ClO ₄) ₂ :6H ₂ O	-133.04	-127.41	5.63	Zn(ClO ₄) ₂ :6H ₂ O
Zn(g)	-74.42	10.99	85.41	Zn
Zn(OH) ₂ (beta)	-11.59	0.34	11.93	Zn(OH) ₂

Zn(OH)2(epsilon)	-11.32	0.34	11.66	Zn(OH)2
Zn(OH)2(gamma)	-11.54	0.34	11.88	Zn(OH)2
Zn2(OH)3Cl	-20.18	-4.89	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-14.51	-6.93	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-23.75	-14.44	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-33.29	-14.20	19.09	Zn3O(SO4)2
ZnCl2	-17.88	-10.80	7.08	ZnCl2
ZnSO4	-10.81	-7.27	3.53	ZnSO4
ZnSO4:6H2O	-5.57	-7.27	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.40	-7.27	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.72	-7.27	-0.55	ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
