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

```

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

```

Beginning of initial solution calculations.

Initial solution 1. Flujo 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
Tachyhydrate	-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 4. AS3

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Beginning of batch-reaction calculations.

Reaction step 1.

Using mix 4.

Mixture 4.

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

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

Elements	Molality	Moles
Al	1.076e-004	4.304e-004
As	6.647e-006	2.659e-005
C	1.426e-003	5.703e-003
Ca	2.115e-003	8.461e-003
Cl	8.398e-004	3.359e-003
Cu	8.523e-005	3.409e-004
Fe	5.983e-004	2.393e-003
K	2.529e-004	1.012e-003
Mg	5.878e-004	2.351e-003
Mn	6.671e-005	2.669e-004
Na	1.616e-003	6.465e-003
S	4.062e-003	1.625e-002
Zn	2.214e-005	8.857e-005

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

pH	=	5.467	Charge balance
pe	=	14.480	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	1.350e-002	
Mass of water (kg)	=	4.000e+000	
Total alkalinity (eq/kg)	=	4.925e-004	
Total CO2 (mol/kg)	=	1.426e-003	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	-3.672e-003	
Percent error, 100*(Cat- An)/(Cat+ An)	=	-6.09	
Iterations	=	9	
Total H	=	4.442118e+002	
Total O	=	2.221858e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	3.771e-006	3.411e-006	-5.424	-5.467	-0.044
OH-	3.183e-009	2.824e-009	-8.497	-8.549	-0.052
H2O	5.553e+001	9.998e-001	1.744	-0.000	0.000
Al	1.076e-004				
Al13O4(OH)24+7	7.878e-006	3.375e-008	-5.104	-7.472	-2.368
AlOH+2	1.910e-006	1.199e-006	-5.719	-5.921	-0.202

Al(OH)2+	9.178e-007	8.161e-007	-6.037	-6.088	-0.051
Al+3	9.115e-007	3.651e-007	-6.040	-6.438	-0.397
AlSO4+	9.087e-007	8.080e-007	-6.042	-6.093	-0.051
HALO2	3.483e-007	3.483e-007	-6.458	-6.458	0.000
Al(SO4)2-	1.526e-007	1.357e-007	-6.817	-6.868	-0.051
ALO2-	3.934e-008	3.498e-008	-7.405	-7.456	-0.051
Al2(OH)2+4	1.425e-009	2.337e-010	-8.846	-9.631	-0.785
Al3(OH)4+5	7.641e-011	4.734e-012	-10.117	-11.325	-1.208
NaALO2	9.452e-012	9.452e-012	-11.024	-11.024	0.000
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-153.510	-153.510	0.000
As(3)	2.464e-029				
HAsO2	1.314e-029	1.314e-029	-28.881	-28.881	0.000
As(OH)3	1.149e-029	1.149e-029	-28.940	-28.940	0.000
H2AsO3-	2.317e-033	2.060e-033	-32.635	-32.686	-0.051
AsO2-	2.215e-033	1.970e-033	-32.655	-32.706	-0.051
AsO2OH-2	9.477e-039	5.902e-039	-38.023	-38.229	-0.206
HAsS2	0.000e+000	0.000e+000	-286.605	-286.605	0.000
As(5)	6.647e-006				
H2AsO4-	6.212e-006	5.524e-006	-5.207	-5.258	-0.051
HAsO4-2	4.317e-007	2.689e-007	-6.365	-6.570	-0.206
H3AsO4	3.318e-009	3.318e-009	-8.479	-8.479	0.000
AsO4-3	5.877e-013	2.022e-013	-12.231	-12.694	-0.463
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-254.332	-254.332	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-225.339	-225.339	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-140.945	-140.945	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-47.839	-47.839	0.000
C(4)	1.426e-003				
CO2	1.244e-003	1.248e-003	-2.905	-2.904	0.001
HCO3-	1.774e-004	1.578e-004	-3.751	-3.802	-0.051
CaHCO3+	2.369e-006	2.107e-006	-5.625	-5.676	-0.051
CuCO3	7.970e-007	7.970e-007	-6.099	-6.099	0.000
MgHCO3+	5.770e-007	5.131e-007	-6.239	-6.290	-0.051
NaHCO3	3.196e-007	3.196e-007	-6.495	-6.495	0.000
ZnHCO3+	5.013e-008	4.458e-008	-7.300	-7.351	-0.051
MnHCO3+	4.300e-008	3.823e-008	-7.367	-7.418	-0.051
FeCO3+	3.396e-008	3.019e-008	-7.469	-7.520	-0.051
CaCO3	5.359e-009	5.359e-009	-8.271	-8.271	0.000
CO3-2	3.269e-009	2.052e-009	-8.486	-8.688	-0.202
MnCO3	2.287e-009	2.287e-009	-8.641	-8.641	0.000
MgCO3	6.079e-010	6.079e-010	-9.216	-9.216	0.000
ZnCO3	1.889e-010	1.889e-010	-9.724	-9.724	0.000
NaCO3-	1.144e-011	1.017e-011	-10.942	-10.993	-0.051
FeHCO3+	8.198e-012	7.290e-012	-11.086	-11.137	-0.051
Cu(CO3)2-2	4.678e-012	2.914e-012	-11.330	-11.536	-0.206
FeCO3	1.026e-014	1.026e-014	-13.989	-13.989	0.000
CuCO3(OH)2-2	9.349e-016	5.823e-016	-15.029	-15.235	-0.206
Ca	2.115e-003				
Ca+2	1.757e-003	1.127e-003	-2.755	-2.948	-0.193
CaSO4	3.560e-004	3.560e-004	-3.449	-3.449	0.000
CaHCO3+	2.369e-006	2.107e-006	-5.625	-5.676	-0.051
CaCl+	1.996e-007	1.775e-007	-6.700	-6.751	-0.051
CaCO3	5.359e-009	5.359e-009	-8.271	-8.271	0.000
CaCl2	1.551e-010	1.551e-010	-9.809	-9.809	0.000
CaOH+	5.248e-011	4.666e-011	-10.280	-10.331	-0.051
Cl(-1)	8.398e-004				
Cl-	8.391e-004	7.431e-004	-3.076	-3.129	-0.053
CaCl+	1.996e-007	1.775e-007	-6.700	-6.751	-0.051
NaCl	1.850e-007	1.850e-007	-6.733	-6.733	0.000
MgCl+	1.827e-007	1.625e-007	-6.738	-6.789	-0.051
CuCl+	9.307e-008	8.276e-008	-7.031	-7.082	-0.051
MnCl+	5.664e-008	5.037e-008	-7.247	-7.298	-0.051
ZnCl+	1.539e-008	1.369e-008	-7.813	-7.864	-0.051

KCl	5.493e-009	5.493e-009	-8.260	-8.260	0.000
HCl	5.692e-010	5.692e-010	-9.245	-9.245	0.000
CaCl2	1.551e-010	1.551e-010	-9.809	-9.809	0.000
Zn(OH)Cl	6.861e-011	6.861e-011	-10.164	-10.164	0.000
CuCl2	3.239e-011	3.239e-011	-10.490	-10.490	0.000
ZnCl2	1.188e-011	1.188e-011	-10.925	-10.925	0.000
FeCl+2	5.026e-013	3.154e-013	-12.299	-12.501	-0.202
FeCl2+	2.134e-013	1.898e-013	-12.671	-12.722	-0.051
FeCl+	5.360e-014	4.766e-014	-13.271	-13.322	-0.051
MnCl3-	6.832e-015	6.076e-015	-14.165	-14.216	-0.051
ZnCl3-	5.483e-015	4.876e-015	-14.261	-14.312	-0.051
ZnCl4-2	4.409e-017	2.746e-017	-16.356	-16.561	-0.206
CuCl2-	3.039e-018	2.702e-018	-17.517	-17.568	-0.051
FeCl2	1.901e-019	1.901e-019	-18.721	-18.721	0.000
CuCl3-2	2.070e-020	1.290e-020	-19.684	-19.890	-0.206
CuCl4-2	5.389e-022	3.356e-022	-21.269	-21.474	-0.206
FeCl4-	1.417e-022	1.260e-022	-21.849	-21.900	-0.051
FeCl4-2	4.869e-025	3.033e-025	-24.313	-24.518	-0.206
Cl(1)	5.782e-020				
HClO	5.731e-020	5.731e-020	-19.242	-19.242	0.000
ClO-	5.096e-022	4.531e-022	-21.293	-21.344	-0.051
Cl(3)	3.978e-033				
ClO2-	3.961e-033	3.522e-033	-32.402	-32.453	-0.051
HClO2	1.776e-035	1.776e-035	-34.751	-34.751	0.000
Cl(5)	2.195e-030				
ClO3-	2.195e-030	1.948e-030	-29.659	-29.710	-0.052
Cl(7)	6.061e-032				
ClO4-	6.060e-032	5.378e-032	-31.218	-31.269	-0.052
ZnClO4+	1.254e-035	1.115e-035	-34.902	-34.953	-0.051
Cu(1)	8.612e-017				
Cu+	8.306e-017	7.386e-017	-16.081	-16.132	-0.051
CuCl2-	3.039e-018	2.702e-018	-17.517	-17.568	-0.051
CuCl3-2	2.070e-020	1.290e-020	-19.684	-19.890	-0.206
Cu(2)	8.523e-005				
Cu+2	6.347e-005	4.072e-005	-4.197	-4.390	-0.193
CuSO4	2.018e-005	2.018e-005	-4.695	-4.695	0.000
CuCO3	7.970e-007	7.970e-007	-6.099	-6.099	0.000
CuOH+	6.924e-007	6.157e-007	-6.160	-6.211	-0.051
CuCl+	9.307e-008	8.276e-008	-7.031	-7.082	-0.051
CuCl2	3.239e-011	3.239e-011	-10.490	-10.490	0.000
Cu(CO3)2-2	4.678e-012	2.914e-012	-11.330	-11.536	-0.206
CuCO3(OH)2-2	9.349e-016	5.823e-016	-15.029	-15.235	-0.206
CuCl4-2	5.389e-022	3.356e-022	-21.269	-21.474	-0.206
CuO2-2	1.715e-022	1.068e-022	-21.766	-21.971	-0.206
Fe(2)	1.757e-010				
Fe+2	1.373e-010	8.805e-011	-9.862	-10.055	-0.193
FeSO4	3.018e-011	3.018e-011	-10.520	-10.520	0.000
FeHCO3+	8.198e-012	7.290e-012	-11.086	-11.137	-0.051
FeCl+	5.360e-014	4.766e-014	-13.271	-13.322	-0.051
FeCO3	1.026e-014	1.026e-014	-13.989	-13.989	0.000
FeOH+	9.179e-015	8.162e-015	-14.037	-14.088	-0.051
FeCl2	1.901e-019	1.901e-019	-18.721	-18.721	0.000
Fe(OH)2	1.901e-020	1.901e-020	-19.721	-19.721	0.000
FeCl4-2	4.869e-025	3.033e-025	-24.313	-24.518	-0.206
Fe(OH)3-	2.495e-025	2.218e-025	-24.603	-24.654	-0.051
Fe(OH)4-2	1.044e-034	6.503e-035	-33.981	-34.187	-0.206
Fe(3)	5.983e-004				
Fe(OH)2+	5.264e-004	4.681e-004	-3.279	-3.330	-0.051
Fe(OH)3	6.418e-005	6.418e-005	-4.193	-4.193	0.000
FeOH+2	7.682e-006	4.822e-006	-5.115	-5.317	-0.202
FeCO3+	3.396e-008	3.019e-008	-7.469	-7.520	-0.051
Fe+3	6.361e-009	2.548e-009	-8.196	-8.594	-0.397
Fe(OH)4-	5.315e-009	4.726e-009	-8.274	-8.325	-0.051
Fe2(OH)2+4	3.816e-009	6.258e-010	-8.418	-9.204	-0.785
Fe3(OH)4+5	9.880e-010	6.121e-011	-9.005	-10.213	-1.208
FeSO4+	5.995e-010	5.331e-010	-9.222	-9.273	-0.051
Fe(SO4)2-	2.192e-011	1.949e-011	-10.659	-10.710	-0.051

FeCl+2	5.026e-013	3.154e-013	-12.299	-12.501	-0.202
FeCl2+	2.134e-013	1.898e-013	-12.671	-12.722	-0.051
FeCl4-	1.417e-022	1.260e-022	-21.849	-21.900	-0.051
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-42.996	-42.994	0.001
K	2.529e-004				
K+	2.486e-004	2.201e-004	-3.605	-3.657	-0.053
KSO4-	4.322e-006	3.843e-006	-5.364	-5.415	-0.051
KCl	5.493e-009	5.493e-009	-8.260	-8.260	0.000
KHSO4	1.156e-011	1.156e-011	-10.937	-10.937	0.000
KOH	2.238e-013	2.238e-013	-12.650	-12.650	0.000
Mg	5.878e-004				
Mg+2	4.253e-004	2.800e-004	-3.371	-3.553	-0.181
MgSO4	1.617e-004	1.617e-004	-3.791	-3.791	0.000
MgHCO3+	5.770e-007	5.131e-007	-6.239	-6.290	-0.051
MgCl+	1.827e-007	1.625e-007	-6.738	-6.789	-0.051
MgCO3	6.079e-010	6.079e-010	-9.216	-9.216	0.000
Mg4(OH)4+4	4.924e-032	8.076e-033	-31.308	-32.093	-0.785
Mn(2)	6.671e-005				
Mn+2	4.962e-005	3.183e-005	-4.304	-4.497	-0.193
MnSO4	1.699e-005	1.699e-005	-4.770	-4.770	0.000
MnCl+	5.664e-008	5.037e-008	-7.247	-7.298	-0.051
MnHCO3+	4.300e-008	3.823e-008	-7.367	-7.418	-0.051
MnCO3	2.287e-009	2.287e-009	-8.641	-8.641	0.000
MnOH+	2.697e-010	2.399e-010	-9.569	-9.620	-0.051
Mn2OH+3	2.298e-014	8.182e-015	-13.639	-14.087	-0.448
MnCl3-	6.832e-015	6.076e-015	-14.165	-14.216	-0.051
Mn(OH)2	1.726e-016	1.726e-016	-15.763	-15.763	0.000
Mn2(OH)3+	3.614e-017	3.214e-017	-16.442	-16.493	-0.051
Mn(OH)3-	5.338e-023	4.746e-023	-22.273	-22.324	-0.051
Mn(OH)4-2	1.892e-031	1.178e-031	-30.723	-30.929	-0.206
Mn(3)	7.196e-016				
Mn+3	7.196e-016	2.562e-016	-15.143	-15.591	-0.448
Mn(6)	8.269e-022				
MnO4-2	8.269e-022	5.150e-022	-21.083	-21.288	-0.206
Mn(7)	7.712e-017				
MnO4-	7.712e-017	6.844e-017	-16.113	-16.165	-0.052
Na	1.616e-003				
Na+	1.593e-003	1.416e-003	-2.798	-2.849	-0.051
NaSO4-	2.276e-005	2.024e-005	-4.643	-4.694	-0.051
NaHCO3	3.196e-007	3.196e-007	-6.495	-6.495	0.000
NaCl	1.850e-007	1.850e-007	-6.733	-6.733	0.000
NaCO3-	1.144e-011	1.017e-011	-10.942	-10.993	-0.051
NaAlO2	9.452e-012	9.452e-012	-11.024	-11.024	0.000
NaOH	6.902e-013	6.902e-013	-12.161	-12.161	0.000
O(0)	1.236e-006				
O2	6.178e-007	6.198e-007	-6.209	-6.208	0.001
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-132.457	-132.457	0.000
HS-	0.000e+000	0.000e+000	-133.947	-133.999	-0.052
S-2	0.000e+000	0.000e+000	-141.259	-141.458	-0.199
S2-2	0.000e+000	0.000e+000	-237.639	-237.845	-0.206
HAsS2	0.000e+000	0.000e+000	-286.605	-286.605	0.000
S3-2	0.000e+000	0.000e+000	-334.067	-334.273	-0.206
S4-2	0.000e+000	0.000e+000	-430.722	-430.928	-0.206
S5-2	0.000e+000	0.000e+000	-527.594	-527.799	-0.206
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-137.117	-137.322	-0.206
HS2O3-	0.000e+000	0.000e+000	-141.725	-141.776	-0.051
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-125.156	-125.355	-0.199
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-44.364	-44.415	-0.051
SO3-2	0.000e+000	0.000e+000	-45.977	-46.179	-0.202
H2SO3	0.000e+000	0.000e+000	-47.900	-47.900	0.000
SO2	0.000e+000	0.000e+000	-48.000	-48.000	0.000
S2O6-2	0.000e+000	0.000e+000	-64.323	-64.529	-0.206

S3O6-2	0.000e+000	0.000e+000	-163.234	-163.440	-0.206
S4O6-2	0.000e+000	0.000e+000	-246.239	-246.445	-0.206
S5O6-2	0.000e+000	0.000e+000	-358.124	-358.329	-0.206
S(5)	0.000e+000				
S2O5-2	0.000e+000	0.000e+000	-93.454	-93.659	-0.206
S(6)	4.062e-003				
SO4-2	3.473e-003	2.163e-003	-2.459	-2.665	-0.206
CaSO4	3.560e-004	3.560e-004	-3.449	-3.449	0.000
MgSO4	1.617e-004	1.617e-004	-3.791	-3.791	0.000
NaSO4-	2.276e-005	2.024e-005	-4.643	-4.694	-0.051
CuSO4	2.018e-005	2.018e-005	-4.695	-4.695	0.000
MnSO4	1.699e-005	1.699e-005	-4.770	-4.770	0.000
ZnSO4	4.982e-006	4.982e-006	-5.303	-5.303	0.000
KSO4-	4.322e-006	3.843e-006	-5.364	-5.415	-0.051
AlSO4+	9.087e-007	8.080e-007	-6.042	-6.093	-0.051
HSO4-	8.380e-007	7.451e-007	-6.077	-6.128	-0.051
Al(SO4)2-	1.526e-007	1.357e-007	-6.817	-6.868	-0.051
FeSO4+	5.995e-010	5.331e-010	-9.222	-9.273	-0.051
FeSO4	3.018e-011	3.018e-011	-10.520	-10.520	0.000
Fe(SO4)2-	2.192e-011	1.949e-011	-10.659	-10.710	-0.051
KHSO4	1.156e-011	1.156e-011	-10.937	-10.937	0.000
H2SO4	2.398e-015	2.398e-015	-14.620	-14.620	0.000
S(7)	0.000e+000				
S2O8-2	0.000e+000	0.000e+000	-41.618	-41.823	-0.206
S(8)	3.584e-029				
HSO5-	3.584e-029	3.187e-029	-28.446	-28.497	-0.051
Zn	2.214e-005				
Zn+2	1.709e-005	1.096e-005	-4.767	-4.960	-0.193
ZnSO4	4.982e-006	4.982e-006	-5.303	-5.303	0.000
ZnHCO3+	5.013e-008	4.458e-008	-7.300	-7.351	-0.051
ZnCl+	1.539e-008	1.369e-008	-7.813	-7.864	-0.051
ZnOH+	3.964e-009	3.525e-009	-8.402	-8.453	-0.051
ZnCO3	1.889e-010	1.889e-010	-9.724	-9.724	0.000
Zn(OH)Cl	6.861e-011	6.861e-011	-10.164	-10.164	0.000
ZnCl2	1.188e-011	1.188e-011	-10.925	-10.925	0.000
Zn(OH)2	4.425e-012	4.425e-012	-11.354	-11.354	0.000
ZnCl3-	5.483e-015	4.876e-015	-14.261	-14.312	-0.051
ZnCl4-2	4.409e-017	2.746e-017	-16.356	-16.561	-0.206
Zn(OH)3-	4.522e-018	4.021e-018	-17.345	-17.396	-0.051
Zn(OH)4-2	3.227e-025	2.010e-025	-24.491	-24.697	-0.206
ZnClO4+	1.254e-035	1.115e-035	-34.902	-34.953	-0.051

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

Phase	SI	log IAP	log KT	
Al	-135.29	14.62	149.91	Al
Al(g)	-186.00	14.62	200.62	Al
Al2(SO4)3	-39.77	-20.87	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-22.43	-20.87	1.56	Al2(SO4)3:6H2O
Alabandite	-132.61	-133.03	-0.42	MnS
Alum-K	-10.46	-15.43	-4.97	KAl(SO4)2:12H2O
Alunite	4.97	4.50	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.26	-5.61	-4.35	CaSO4
Antarcticite	-13.30	-9.21	4.09	CaCl2:6H2O
Antlerite	-2.70	6.03	8.73	Cu3(SO4)(OH)4
Aphthitalite	-15.26	-19.15	-3.89	NaK3(SO4)2
Aragonite	-3.25	-1.28	1.97	CaCO3
Arcanite	-8.14	-9.98	-1.84	K2SO4
Arsenolite	-56.46	-76.31	-19.84	As2O3
Arsenopyrite	-219.97	-234.42	-14.45	FeAsS
Artinite	-14.13	5.49	19.63	Mg2CO3(OH)2:3H2O
As	-76.18	-33.50	42.68	As
As2O5	-23.59	-21.45	2.14	As2O5
As4O6(cubi)	-112.79	-152.61	-39.82	As4O6
As4O6(mono)	-112.56	-152.61	-40.05	As4O6
Atacamite	-5.28	8.98	14.26	Cu4Cl2(OH)6

Azurite	-8.02	1.09	9.12	$\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$
Bassanite	-1.91	-5.61	-3.71	$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$
Birnessite	21.06	-64.48	-85.55	$\text{Mn}_8\text{O}_{14} \cdot 5\text{H}_2\text{O}$
Bischofite	-14.20	-9.81	4.39	$\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$
Bixbyite	2.58	1.62	-0.96	Mn_2O_3
Bloedite	-12.10	-14.58	-2.48	$\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$
Boehmite	2.41	9.96	7.55	AlO_2H
Bornite	-490.57	-593.10	-102.53	Cu_5FeS_4
Brochantite	-2.85	12.58	15.42	$\text{Cu}_4(\text{SO}_4)(\text{OH})_6$
Brucite	-8.90	7.38	16.28	$\text{Mg}(\text{OH})_2$
Burkeite	-30.24	-20.76	9.49	$\text{Na}_6\text{CO}_3(\text{SO}_4)_2$
C	-67.21	-3.06	64.15	C
C(g)	-184.83	-3.06	181.77	C
Ca	-128.74	11.09	139.83	Ca
Ca(g)	-153.98	11.09	165.07	Ca
$\text{Ca}_2\text{Al}_2\text{O}_5 \cdot 8\text{H}_2\text{O}$	-23.67	35.90	59.57	$\text{Ca}_2\text{Al}_2\text{O}_5 \cdot 8\text{H}_2\text{O}$
$\text{Ca}_2\text{Cl}_2(\text{OH})_2 \cdot \text{H}_2\text{O}$	-27.51	-1.22	26.29	$\text{Ca}_2\text{Cl}_2(\text{OH})_2 \cdot \text{H}_2\text{O}$
$\text{Ca}_3(\text{AsO}_4)_2$	-15.29	2.51	17.80	$\text{Ca}_3(\text{AsO}_4)_2$
$\text{Ca}_3\text{Al}_2\text{O}_6$	-69.15	43.89	113.03	$\text{Ca}_3\text{Al}_2\text{O}_6$
$\text{Ca}_4\text{Al}_2\text{Fe}_2\text{O}_{10}$	-73.00	67.49	140.48	$\text{Ca}_4\text{Al}_2\text{Fe}_2\text{O}_{10}$
$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 13\text{H}_2\text{O}$	-55.38	51.87	107.25	$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 13\text{H}_2\text{O}$
$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 19\text{H}_2\text{O}$	-51.81	51.87	103.68	$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 19\text{H}_2\text{O}$
$\text{Ca}_4\text{Cl}_2(\text{OH})_6 \cdot 13\text{H}_2\text{O}$	-53.58	14.75	68.33	$\text{Ca}_4\text{Cl}_2(\text{OH})_6 \cdot 13\text{H}_2\text{O}$
CaAl_2O_4	-18.99	27.91	46.91	CaAl_2O_4
$\text{CaAl}_2\text{O}_4 \cdot 10\text{H}_2\text{O}$	-10.08	27.91	37.99	$\text{CaAl}_2\text{O}_4 \cdot 10\text{H}_2\text{O}$
CaAl_4O_7	-20.75	47.84	68.59	CaAl_4O_7
Calcite	-3.11	-1.28	1.82	CaCO_3
Carnallite	-20.87	-16.60	4.27	$\text{KMgCl}_3 \cdot 6\text{H}_2\text{O}$
$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}(\text{beta})$	-2.08	-5.61	-3.54	$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$
$\text{CH}_4(\text{g})$	-138.10	-140.95	-2.84	CH_4
Chalcanthite	-4.43	-7.06	-2.63	$\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$
Chalcocite	-126.05	-160.80	-34.74	Cu_2S
Chalcocyanite	-9.97	-7.06	2.91	CuSO_4
Chalcopyrite	-238.90	-271.51	-32.60	CuFeS_2
Chloromagnesite	-31.63	-9.81	21.82	MgCl_2
$\text{Cl}_2(\text{g})$	-23.29	-20.30	2.99	Cl_2
Claudetite	-56.51	-76.31	-19.80	As_2O_3
$\text{CO}(\text{g})$	-44.84	-47.84	-3.00	CO
$\text{CO}_2(\text{g})$	-1.44	-9.27	-7.83	CO_2
Corundum	1.64	19.93	18.29	Al_2O_3
Covellite	-110.06	-132.92	-22.86	CuS
Cu	-21.85	9.65	31.50	Cu
Cu(g)	-74.01	9.65	83.66	Cu
CuCl_2	-14.37	-10.65	3.72	CuCl_2
Cuprite	-19.42	-21.33	-1.91	Cu_2O
Dawsonite	-1.03	3.31	4.34	$\text{NaAlCO}_3(\text{OH})_2$
Delafossite	3.58	-2.86	-6.44	CuFeO_2
Diaspore	2.82	9.96	7.15	AlHO_2
Dolomite	-5.64	-3.17	2.47	$\text{CaMg}(\text{CO}_3)_2$
Dolomite-dis	-7.18	-3.17	4.01	$\text{CaMg}(\text{CO}_3)_2$
Dolomite-ord	-5.64	-3.17	2.46	$\text{CaMg}(\text{CO}_3)_2$
Epsomite	-4.26	-6.22	-1.96	$\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$
Ettringite	-35.42	27.04	62.46	$\text{Ca}_6\text{Al}_2(\text{SO}_4)_3(\text{OH})_{12} \cdot 26\text{H}_2\text{O}$
Fe	-55.03	3.98	59.02	Fe
$\text{Fe}(\text{OH})_2$	-13.02	0.88	13.89	$\text{Fe}(\text{OH})_2$
$\text{Fe}(\text{OH})_3$	2.17	7.81	5.64	$\text{Fe}(\text{OH})_3$
$\text{Fe}_2(\text{SO}_4)_3$	-28.23	-25.18	3.05	$\text{Fe}_2(\text{SO}_4)_3$
FeO	-12.64	0.88	13.52	FeO
Ferrite-Ca	2.11	23.60	21.50	CaFe_2O_4
Ferrite-Cu	11.88	22.16	10.28	CuFe_2O_4
Ferrite-Dicalcium	-25.21	31.59	56.80	$\text{Ca}_2\text{Fe}_2\text{O}_5$
Ferrite-Mg	1.98	23.00	21.02	MgFe_2O_4
Ferrite-Zn	9.89	21.59	11.70	ZnFe_2O_4
FeSO_4	-15.33	-12.72	2.61	FeSO_4
Gaylussite	-16.48	-5.32	11.16	$\text{CaNa}_2(\text{CO}_3)_2 \cdot 5\text{H}_2\text{O}$
Gibbsite	2.22	9.96	7.74	$\text{Al}(\text{OH})_3$
Glauberite	-8.51	-13.98	-5.47	$\text{Na}_2\text{Ca}(\text{SO}_4)_2$

Goethite	7.28	7.81	0.53	FeOOH
Gypsum	-1.08	-5.61	-4.53	CaSO4:2H2O
H2(g)	-39.89	-42.99	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-131.47	-139.47	-7.99	H2S
Halite	-7.54	-5.98	1.56	NaCl
Hausmannite	-2.09	8.06	10.14	Mn3O4
HCl(g)	-14.90	-8.60	6.30	HCl
Hematite	15.54	15.62	0.08	Fe2O3
Hercynite	-8.00	20.81	28.80	FeAl2O4
Hexahydrite	-4.49	-6.22	-1.73	MgSO4:6H2O
Huntite	-17.16	-6.95	10.22	CaMg3(CO3)4
Hydromagnesite	-30.91	-0.17	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-20.95	-9.21	11.75	CaCl2
Hydrozincite	-18.98	11.33	30.31	Zn5(OH)6(CO3)2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	7.44	-1.97	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	4.29	-1.16	-5.45	NaFe3(SO4)2(OH)6
K	-67.61	3.36	70.98	K
K(g)	-78.22	3.36	81.58	K
K2CO3:1.5H2O	-19.03	-5.65	13.38	K2CO3:1.5H2O
K2O	-80.42	3.62	84.04	K2O
K3H(SO4)2	-18.15	-21.77	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-68.85	-41.14	27.71	K8H4(CO3)6:3H2O
Kainite	-12.69	-13.00	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-18.70	-15.42	3.27	KAl(SO4)2
Kalinite	-7.74	-7.46	0.28	KHCO3
Katoite	-35.06	43.89	78.94	Ca3Al2H12O12
Kieserite	-5.95	-6.22	-0.27	MgSO4:H2O
KMgCl3	-37.84	-16.60	21.25	KMgCl3
KMgCl3:2H2O	-30.56	-16.60	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-15.10	-4.84	10.26	KNaCO3:6H2O
Lammerite	-3.37	-1.82	1.55	Cu3(AsO4)2
Lansfordite	-6.73	-1.89	4.84	MgCO3:5H2O
Lawrencite	-25.37	-16.31	9.05	FeCl2
Leonite	-12.09	-16.20	-4.11	K2Mg(SO4)2:4H2O
Lime	-24.58	7.99	32.57	CaO
Magnesite	-4.16	-1.89	2.27	MgCO3
Magnetite	6.08	16.49	10.42	Fe3O4
Malachite	-2.08	3.82	5.90	Cu2CO3(OH)2
Manganite	0.97	0.81	-0.16	MnO(OH)
Manganosite	-11.48	6.44	17.92	MnO
Mayenite	-258.82	235.33	494.15	Ca12Al14O33
Melanterite	-10.32	-12.72	-2.40	FeSO4:7H2O
Mercallite	-10.35	-11.79	-1.44	KHSO4
Mg	-112.03	10.49	122.52	Mg
Mg(g)	-131.76	10.49	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-9.57	-4.37	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-11.74	-2.53	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.54	-9.81	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.11	-9.81	7.30	MgCl2:4H2O
MgCl2:H2O	-25.88	-9.81	16.07	MgCl2:H2O
MgOHCl	-17.11	-1.21	15.89	MgOHCl
MgSO4	-11.05	-6.22	4.83	MgSO4
Mirabilite	-7.21	-8.36	-1.15	Na2SO4:10H2O
Misenite	-69.64	-80.72	-11.08	K8H6(SO4)7
Mn	-73.39	9.54	82.93	Mn
Mn(OH)2(am)	-8.87	6.44	15.31	Mn(OH)2
Mn(OH)3	-5.53	0.81	6.34	Mn(OH)3
MnCl2:2H2O	-14.75	-10.76	4.00	MnCl2:2H2O
MnCl2:4H2O	-13.51	-10.76	2.75	MnCl2:4H2O
MnCl2:H2O	-16.30	-10.76	5.54	MnCl2:H2O
MnO2(gamma)	3.23	-12.89	-16.13	MnO2
MnSO4	-9.77	-7.16	2.61	MnSO4
Molysite	-31.45	-17.98	13.47	FeCl3
Monohydrocalcite	-3.96	-1.28	2.68	CaCO3:H2O
Na	-63.20	4.17	67.37	Na

Na(g)	-76.69	4.17	80.86	Na
Na2CO3	-15.19	-4.03	11.16	Na2CO3
Na2CO3:7H2O	-13.97	-4.03	9.94	Na2CO3:7H2O
Na2O	-62.18	5.24	67.42	Na2O
Na3H(SO4)2	-18.45	-19.34	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.44	-22.34	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-9.46	10.43	19.88	NaFeO2
Nahcolite	-6.51	-6.65	-0.14	NaHCO3
Nantokite	-12.49	-19.26	-6.77	CuCl
Natron	-13.62	-4.03	9.59	Na2CO3:10H2O
Nesquehonite	-7.18	-1.89	5.29	MgCO3:3H2O
O2(g)	-3.32	-6.21	-2.89	O2
Orpiment	-415.22	-494.71	-79.49	As2S3
Oxychloride-Mg	-19.67	6.17	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.83	-6.22	-1.39	MgSO4:5H2O
Periclase	-13.94	7.38	21.33	MgO
Picromerite	-11.76	-16.20	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-16.64	-5.32	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-13.11	-27.42	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-14.56	7.99	22.55	Ca(OH)2
Pyrite	-221.89	-246.59	-24.70	FeS2
Pyrolusite	4.77	-12.89	-17.66	MnO2
Pyrrhotite	-134.85	-138.59	-3.74	FeS
Realgar	-161.38	-221.65	-60.28	AsS
Rhodochrosite	-2.61	-2.83	-0.22	MnCO3
S	-97.46	-142.57	-45.11	S
S2(g)	-208.81	-216.00	-7.19	S2
Scacchite	-19.50	-10.76	8.74	MnCl2
Siderite	-8.17	-8.39	-0.22	FeCO3
Smithsonite	-3.74	-3.29	0.44	ZnCO3
SO2(g)	-48.18	-48.00	0.18	SO2
Sphalerite	-122.02	-133.49	-11.47	ZnS
Spinel	-10.30	27.31	37.61	Al2MgO4
Starkeyite	-5.22	-6.22	-1.00	MgSO4:4H2O
Sylvite	-7.61	-6.79	0.83	KCl
Syngenite	-7.99	-15.59	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-45.97	-28.83	17.14	Mg2CaCl6:12H2O
Tenorite	-1.10	6.54	7.65	CuO
Thenardite	-8.00	-8.36	-0.36	Na2SO4
Thermonatrite	-14.97	-4.03	10.94	Na2CO3:H2O
Todorokite	18.46	-27.36	-45.82	Mn7O12:3H2O
Troilite	-134.74	-138.59	-3.84	FeS
Trona-K	-23.89	-12.30	11.59	K2NaH(CO3)2:2H2O
Wurtzite	-124.32	-133.49	-9.17	ZnS
Wustite	-10.84	1.57	12.40	Fe.947O
Zincite	-5.22	5.97	11.20	ZnO
Zn	-59.71	9.08	68.79	Zn
Zn(ClO4)2:6H2O	-73.13	-67.50	5.63	Zn(ClO4)2:6H2O
Zn(g)	-76.33	9.08	85.41	Zn
Zn(OH)2(beta)	-5.96	5.97	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-5.69	5.97	11.66	Zn(OH)2
Zn(OH)2(gamma)	-5.91	5.97	11.88	Zn(OH)2
Zn2(OH)3Cl	-11.94	3.35	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-9.23	-1.65	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-12.84	-3.53	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-28.37	-9.28	19.09	Zn3O(SO4)2
ZnCl2	-18.30	-11.22	7.08	ZnCl2
ZnCO3:H2O	-3.43	-3.29	0.14	ZnCO3:H2O
ZnSO4	-11.16	-7.63	3.53	ZnSO4
ZnSO4:6H2O	-5.93	-7.63	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.75	-7.63	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-7.07	-7.63	-0.55	ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
