
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 3 AS2
temp 25
units mg/l
pe 10
pH 6.98
Cl 678.5
S(6) 427.00
Al 0.00
As 0.1526
Ca 238.3
Cu 0.00
Fe 0.00
K 40.73
Mg 13.69
Mn 0.114
Na 392.9
Zn 2.44
C(4) 153.72
MIX 2
1 1

```

3      3
SELECTED_OUTPUT
file          DAM_AS2
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.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 3. AS2

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

Elements	Molality	Moles
As	2.041e-006	2.041e-006
C(4)	2.525e-003	2.525e-003

Ca	5.958e-003	5.958e-003
Cl	1.918e-002	1.918e-002
K	1.044e-003	1.044e-003
Mg	5.644e-004	5.644e-004
Mn	2.079e-006	2.079e-006
Na	1.712e-002	1.712e-002
S(6)	4.455e-003	4.455e-003
Zn	3.739e-005	3.739e-005

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

pH	=	6.980
pe	=	10.000
Activity of water	=	0.999
Ionic strength	=	3.800e-002
Mass of water (kg)	=	1.000e+000
Total alkalinity (eq/kg)	=	2.128e-003
Total CO2 (mol/kg)	=	2.525e-003
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	1.075e-003
Percent error, 100*(Cat- An)/(Cat+ An)	=	1.86
Iterations	=	4
Total H	=	1.110528e+002
Total O	=	5.555032e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	1.207e-007	1.047e-007	-6.918	-6.980	-0.062
OH-	1.105e-007	9.193e-008	-6.957	-7.037	-0.080
H2O	5.553e+001	9.992e-001	1.744	-0.000	0.000
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-132.370	-132.370	0.000
As(3)	5.398e-026				
HAsO2	2.863e-026	2.863e-026	-25.543	-25.543	0.000
As(OH)3	2.501e-026	2.501e-026	-25.602	-25.602	0.000
H2AsO3-	1.747e-028	1.461e-028	-27.758	-27.835	-0.078
AsO2-	1.672e-028	1.398e-028	-27.777	-27.855	-0.078
AsO2OH-2	2.820e-032	1.363e-032	-31.550	-31.866	-0.316
As(5)	2.041e-006				
HAsO4-2	1.495e-006	7.226e-007	-5.825	-6.141	-0.316
H2AsO4-	5.453e-007	4.559e-007	-6.263	-6.341	-0.078
AsO4-3	9.134e-011	1.770e-011	-10.039	-10.752	-0.713
H3AsO4	8.408e-012	8.408e-012	-11.075	-11.075	0.000
C(4)	2.525e-003				
HCO3-	2.009e-003	1.680e-003	-2.697	-2.775	-0.078
CO2	4.046e-004	4.084e-004	-3.393	-3.389	0.004
CaHCO3+	6.422e-005	5.369e-005	-4.192	-4.270	-0.078
NaHCO3	3.387e-005	3.387e-005	-4.470	-4.470	0.000
MgHCO3+	5.687e-006	4.755e-006	-5.245	-5.323	-0.078
CaCO3	4.449e-006	4.449e-006	-5.352	-5.352	0.000
CO3-2	1.446e-006	7.117e-007	-5.840	-6.148	-0.308
ZnHCO3+	8.088e-007	6.762e-007	-6.092	-6.170	-0.078
MgCO3	1.835e-007	1.835e-007	-6.736	-6.736	0.000
ZnCO3	9.333e-008	9.333e-008	-7.030	-7.030	0.000
NaCO3-	4.199e-008	3.511e-008	-7.377	-7.455	-0.078
MnCO3	2.132e-008	2.132e-008	-7.671	-7.671	0.000
MnHCO3+	1.309e-008	1.095e-008	-7.883	-7.961	-0.078
Ca	5.958e-003				
Ca+2	5.216e-003	2.697e-003	-2.283	-2.569	-0.286
CaSO4	6.619e-004	6.619e-004	-3.179	-3.179	0.000
CaHCO3+	6.422e-005	5.369e-005	-4.192	-4.270	-0.078
CaCl+	1.082e-005	9.048e-006	-4.966	-5.043	-0.078
CaCO3	4.449e-006	4.449e-006	-5.352	-5.352	0.000
CaCl2	1.685e-007	1.685e-007	-6.774	-6.774	0.000

CaOH+	4.348e-009	3.635e-009	-8.362	-8.439	-0.078
Cl(-1)	1.918e-002				
Cl-	1.912e-002	1.583e-002	-1.719	-1.801	-0.082
NaCl	3.922e-005	3.922e-005	-4.407	-4.407	0.000
CaCl+	1.082e-005	9.048e-006	-4.966	-5.043	-0.078
MgCl+	3.602e-006	3.011e-006	-5.443	-5.521	-0.078
ZnCl+	4.967e-007	4.153e-007	-6.304	-6.382	-0.078
KCl	4.530e-007	4.530e-007	-6.344	-6.344	0.000
CaCl2	1.685e-007	1.685e-007	-6.774	-6.774	0.000
Zn(OH)Cl	6.775e-008	6.775e-008	-7.169	-7.169	0.000
MnCl+	3.450e-008	2.885e-008	-7.462	-7.540	-0.078
ZnCl2	7.678e-009	7.678e-009	-8.115	-8.115	0.000
HCl	3.723e-010	3.723e-010	-9.429	-9.429	0.000
ZnCl3-	8.028e-011	6.712e-011	-10.095	-10.173	-0.078
ZnCl4-2	1.666e-011	8.053e-012	-10.778	-11.094	-0.316
MnCl3-	1.888e-012	1.579e-012	-11.724	-11.802	-0.078
Cl(1)	5.707e-026				
HClO	4.363e-026	4.363e-026	-25.360	-25.360	0.000
ClO-	1.344e-026	1.124e-026	-25.872	-25.949	-0.078
Cl(3)	0.000e+000				
ClO2-	0.000e+000	0.000e+000	-42.915	-42.993	-0.078
HClO2	0.000e+000	0.000e+000	-46.803	-46.803	0.000
Cl(5)	0.000e+000				
ClO3-	0.000e+000	0.000e+000	-46.104	-46.184	-0.080
Cl(7)	0.000e+000				
ClO4-	0.000e+000	0.000e+000	-53.597	-53.677	-0.080
ZnClO4+	0.000e+000	0.000e+000	-57.129	-57.207	-0.078
H(0)	1.724e-037				
H2	8.621e-038	8.701e-038	-37.064	-37.060	0.004
K	1.044e-003				
K+	1.029e-003	8.522e-004	-2.987	-3.069	-0.082
KSO4-	1.382e-005	1.156e-005	-4.859	-4.937	-0.078
KCl	4.530e-007	4.530e-007	-6.344	-6.344	0.000
KOH	2.820e-011	2.820e-011	-10.550	-10.550	0.000
KHSO4	1.068e-012	1.068e-012	-11.972	-11.972	0.000
Mg	5.644e-004				
Mg+2	4.456e-004	2.437e-004	-3.351	-3.613	-0.262
MgSO4	1.093e-004	1.093e-004	-3.961	-3.961	0.000
MgHCO3+	5.687e-006	4.755e-006	-5.245	-5.323	-0.078
MgCl+	3.602e-006	3.011e-006	-5.443	-5.521	-0.078
MgCO3	1.835e-007	1.835e-007	-6.736	-6.736	0.000
Mg4(OH)4+4	7.829e-026	5.199e-027	-25.106	-26.284	-1.178
Mn(2)	2.079e-006				
Mn+2	1.655e-006	8.558e-007	-5.781	-6.068	-0.286
MnSO4	3.548e-007	3.548e-007	-6.450	-6.450	0.000
MnCl+	3.450e-008	2.885e-008	-7.462	-7.540	-0.078
MnCO3	2.132e-008	2.132e-008	-7.671	-7.671	0.000
MnHCO3+	1.309e-008	1.095e-008	-7.883	-7.961	-0.078
MnOH+	2.511e-010	2.099e-010	-9.600	-9.678	-0.078
MnCl3-	1.888e-012	1.579e-012	-11.724	-11.802	-0.078
Mn(OH)2	4.917e-015	4.917e-015	-14.308	-14.308	0.000
Mn2(OH)3+	9.583e-016	8.011e-016	-15.019	-15.096	-0.078
Mn2OH+3	9.169e-016	1.925e-016	-15.038	-15.716	-0.678
Mn(OH)3-	5.264e-020	4.400e-020	-19.279	-19.357	-0.078
Mn(OH)4-2	7.358e-027	3.556e-027	-26.133	-26.449	-0.316
Mn(3)	1.087e-021				
Mn+3	1.087e-021	2.283e-022	-20.964	-21.642	-0.678
Mn(6)	4.364e-029				
MnO4-2	4.364e-029	2.109e-029	-28.360	-28.676	-0.316
Mn(7)	1.116e-028				
MnO4-	1.116e-028	9.286e-029	-27.952	-28.032	-0.080
Na	1.712e-002				
Na+	1.686e-002	1.410e-002	-1.773	-1.851	-0.078
NaSO4-	1.872e-004	1.565e-004	-3.728	-3.806	-0.078
NaCl	3.922e-005	3.922e-005	-4.407	-4.407	0.000
NaHCO3	3.387e-005	3.387e-005	-4.470	-4.470	0.000
NaCO3-	4.199e-008	3.511e-008	-7.377	-7.455	-0.078

NaOH	2.236e-010	2.236e-010	-9.651	-9.651	0.000
O(0)	1.664e-018				
O2	8.321e-019	8.398e-019	-18.080	-18.076	0.004
S(6)	4.455e-003				
SO4-2	3.477e-003	1.680e-003	-2.459	-2.775	-0.316
CaSO4	6.619e-004	6.619e-004	-3.179	-3.179	0.000
NaSO4-	1.872e-004	1.565e-004	-3.728	-3.806	-0.078
MgSO4	1.093e-004	1.093e-004	-3.961	-3.961	0.000
KSO4-	1.382e-005	1.156e-005	-4.859	-4.937	-0.078
ZnSO4	5.512e-006	5.512e-006	-5.259	-5.259	0.000
MnSO4	3.548e-007	3.548e-007	-6.450	-6.450	0.000
HSO4-	2.126e-008	1.777e-008	-7.673	-7.750	-0.078
KHSO4	1.068e-012	1.068e-012	-11.972	-11.972	0.000
H2SO4	1.756e-018	1.756e-018	-17.756	-17.756	0.000
Zn	3.739e-005				
Zn+2	3.020e-005	1.561e-005	-4.520	-4.806	-0.286
ZnSO4	5.512e-006	5.512e-006	-5.259	-5.259	0.000
ZnHCO3+	8.088e-007	6.762e-007	-6.092	-6.170	-0.078
ZnCl+	4.967e-007	4.153e-007	-6.304	-6.382	-0.078
ZnOH+	1.955e-007	1.634e-007	-6.709	-6.787	-0.078
ZnCO3	9.333e-008	9.333e-008	-7.030	-7.030	0.000
Zn(OH)Cl	6.775e-008	6.775e-008	-7.169	-7.169	0.000
ZnCl2	7.678e-009	7.678e-009	-8.115	-8.115	0.000
Zn(OH)2	6.677e-009	6.677e-009	-8.175	-8.175	0.000
ZnCl3-	8.028e-011	6.712e-011	-10.095	-10.173	-0.078
ZnCl4-2	1.666e-011	8.053e-012	-10.778	-11.094	-0.316
Zn(OH)3-	2.362e-013	1.975e-013	-12.627	-12.704	-0.078
Zn(OH)4-2	6.648e-019	3.213e-019	-18.177	-18.493	-0.316
ZnClO4+	0.000e+000	0.000e+000	-57.129	-57.207	-0.078

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

Phase	SI	log IAP	log KT	
Anhydrite	-0.99	-5.34	-4.35	CaSO4
Antarcticite	-10.27	-6.17	4.09	CaCl2:6H2O
Aphthitalite	-12.72	-16.61	-3.89	NaK3(SO4)2
Aragonite	-0.33	1.64	1.97	CaCO3
Arcanite	-7.07	-8.91	-1.84	K2SO4
Arsenolite	-49.79	-69.63	-19.84	As2O3
Artinite	-8.69	10.94	19.63	Mg2CO3(OH)2:3H2O
As	-63.94	-21.26	42.68	As
As2O5	-28.78	-26.64	2.14	As2O5
As4O6(cubi)	-99.44	-139.26	-39.82	As4O6
As4O6(mono)	-99.21	-139.26	-40.05	As4O6
Bassanite	-1.64	-5.34	-3.71	CaSO4:0.5H2O
Birnessite	-2.90	-88.45	-85.55	Mn8O14:5H2O
Bischofite	-11.61	-7.22	4.39	MgCl2:6H2O
Bixbyite	-0.44	-1.40	-0.96	Mn2O3
Bloedite	-10.39	-12.87	-2.48	Na2Mg(SO4)2:4H2O
Brucite	-5.94	10.35	16.28	Mg(OH)2
Burkeite	-21.94	-12.45	9.49	Na6CO3(SO4)2
C	-55.82	8.32	64.15	C
C(g)	-173.44	8.32	181.77	C
Ca	-119.40	20.43	139.83	Ca
Ca(g)	-144.64	20.43	165.07	Ca
Ca2Cl2(OH)2:H2O	-21.07	5.22	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-10.27	7.53	17.80	Ca3(AsO4)2
Ca4Cl2(OH)6:13H2O	-40.33	28.00	68.33	Ca4Cl2(OH)6:13H2O
Calcite	-0.19	1.64	1.82	CaCO3
Carnallite	-16.36	-12.09	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.81	-5.34	-3.54	CaSO4:0.5H2O
Chloromagnesite	-29.03	-7.21	21.82	MgCl2
Cl2(g)	-29.59	-26.60	2.99	Cl2
Claudetite	-49.83	-69.63	-19.80	As2O3
CO2(g)	-1.93	-9.75	-7.83	CO2
Dolomite	-0.25	2.23	2.47	CaMg(CO3)2

Dolomite-dis	-1.78	2.23	4.01	CaMg(CO ₃) ₂
Dolomite-ord	-0.24	2.23	2.46	CaMg(CO ₃) ₂
Epsomite	-4.43	-6.39	-1.96	MgSO ₄ :7H ₂ O
Gaylussite	-9.03	2.14	11.16	CaNa ₂ (CO ₃) ₂ :5H ₂ O
Glauberite	-6.35	-11.82	-5.47	Na ₂ Ca(SO ₄) ₂
Gypsum	-0.81	-5.34	-4.53	CaSO ₄ :2H ₂ O
H ₂ (g)	-33.96	-37.06	-3.10	H ₂
H ₂ O(g)	-1.59	-0.00	1.59	H ₂ O
Halite	-5.21	-3.65	1.56	NaCl
Hausmannite	-3.66	6.49	10.14	Mn ₃ O ₄
HCl(g)	-15.08	-8.78	6.30	HCl
Hexahydrate	-4.66	-6.39	-1.73	MgSO ₄ :6H ₂ O
Huntite	-6.81	3.41	10.22	CaMg ₃ (CO ₃) ₄
Hydromagnesite	-18.03	12.71	30.74	Mg ₅ (CO ₃) ₄ (OH) ₂ :4H ₂ O
Hydrophilite	-17.92	-6.17	11.75	CaCl ₂
Hydrozincite	-4.05	26.26	30.31	Zn ₅ (OH) ₆ (CO ₃) ₂
Ice	-0.14	-0.00	0.14	H ₂ O
K	-62.55	8.43	70.98	K
K(g)	-73.15	8.43	81.58	K
K ₂ CO ₃ :1.5H ₂ O	-15.31	-1.93	13.38	K ₂ CO ₃ :1.5H ₂ O
K ₂ O	-76.21	7.82	84.04	K ₂ O
K ₃ H(SO ₄) ₂	-18.11	-21.74	-3.62	K ₃ H(SO ₄) ₂
K ₈ H ₄ (CO ₃) ₆ :3H ₂ O	-54.95	-27.24	27.71	K ₈ H ₄ (CO ₃) ₆ :3H ₂ O
Kainite	-10.95	-11.26	-0.31	KMgClSO ₄ :3H ₂ O
Kaliginite	-6.13	-5.84	0.28	KHCO ₃
Kieserite	-6.12	-6.39	-0.27	MgSO ₄ :H ₂ O
KMgCl ₃	-33.33	-12.08	21.25	KMgCl ₃
KMgCl ₃ :2H ₂ O	-26.05	-12.08	13.96	KMgCl ₃ :2H ₂ O
KNaCO ₃ :6H ₂ O	-10.98	-0.72	10.26	KNaCO ₃ :6H ₂ O
Lansfordite	-4.25	0.59	4.84	MgCO ₃ :5H ₂ O
Leonite	-11.19	-15.30	-4.11	K ₂ Mg(SO ₄) ₂ :4H ₂ O
Lime	-21.18	11.39	32.57	CaO
Magnesite	-1.68	0.59	2.27	MgCO ₃
Manganite	-0.54	-0.70	-0.16	MnO(OH)
Manganosite	-10.02	7.89	17.92	MnO
Mercallite	-11.39	-12.82	-1.44	KHSO ₄
Mg	-103.14	19.38	122.52	Mg
Mg(g)	-122.86	19.38	142.25	Mg
Mg _{1.25} SO ₄ (OH) _{0.5} :0.5H ₂ O	-9.00	-3.80	5.20	Mg _{1.25} SO ₄ (OH) _{0.5} :0.5H ₂ O
Mg _{1.5} SO ₄ (OH)	-10.42	-1.21	9.21	Mg _{1.5} SO ₄ (OH)
MgCl ₂ :2H ₂ O	-19.95	-7.21	12.73	MgCl ₂ :2H ₂ O
MgCl ₂ :4H ₂ O	-14.52	-7.22	7.30	MgCl ₂ :4H ₂ O
MgCl ₂ :H ₂ O	-23.29	-7.21	16.07	MgCl ₂ :H ₂ O
MgOHCl	-14.33	1.57	15.89	MgOHCl
MgSO ₄	-11.22	-6.39	4.83	MgSO ₄
Mirabilite	-5.33	-6.48	-1.15	Na ₂ SO ₄ :10H ₂ O
Misenite	-74.78	-85.86	-11.08	K ₈ H ₆ (SO ₄) ₇
Mn	-66.00	16.93	82.93	Mn
Mn(OH) ₂ (am)	-7.42	7.89	15.31	Mn(OH) ₂
Mn(OH) ₃	-7.04	-0.70	6.34	Mn(OH) ₃
MnCl ₂ :2H ₂ O	-13.67	-9.67	4.00	MnCl ₂ :2H ₂ O
MnCl ₂ :4H ₂ O	-12.42	-9.67	2.75	MnCl ₂ :4H ₂ O
MnCl ₂ :H ₂ O	-15.21	-9.67	5.54	MnCl ₂ :H ₂ O
MnO ₂ (gamma)	-1.25	-17.37	-16.13	MnO ₂
MnSO ₄	-11.45	-8.84	2.61	MnSO ₄
Monohydrocalcite	-1.04	1.64	2.68	CaCO ₃ :H ₂ O
Na	-57.72	9.65	67.37	Na
Na(g)	-71.21	9.65	80.86	Na
Na ₂ CO ₃	-10.66	0.50	11.16	Na ₂ CO ₃
Na ₂ CO ₃ :7H ₂ O	-9.44	0.50	9.94	Na ₂ CO ₃ :7H ₂ O
Na ₂ O	-57.16	10.26	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-17.19	-18.08	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-12.40	-18.30	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
Nahcolite	-4.48	-4.63	-0.14	NaHCO ₃
Natron	-9.09	0.50	9.59	Na ₂ CO ₃ :10H ₂ O
Nesquehonite	-4.70	0.59	5.29	MgCO ₃ :3H ₂ O
O ₂ (g)	-15.18	-18.08	-2.89	O ₂

Oxychloride-Mg	-13.92	11.91	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-5.00	-6.39	-1.39	MgSO4:5H2O
Periclase	-10.98	10.35	21.33	MgO
Picromerite	-10.86	-15.30	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-9.18	2.14	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-11.68	-25.99	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-11.16	11.39	22.55	Ca(OH)2
Pyrolusite	0.29	-17.37	-17.66	MnO2
Rhodochrosite	-1.64	-1.86	-0.22	MnCO3
Scacchite	-18.41	-9.67	8.74	MnCl2
Smithsonite	-1.05	-0.60	0.44	ZnCO3
Starkeyite	-5.39	-6.39	-1.00	MgSO4:4H2O
Sylvite	-5.70	-4.87	0.83	KCl
Syngenite	-6.66	-14.26	-7.60	K2Ca(SO4)2:H2O
Tachyhydrate	-37.75	-20.60	17.14	Mg2CaCl6:12H2O
Thenardite	-6.12	-6.48	-0.36	Na2SO4
Thermonatrite	-10.43	0.50	10.94	Na2CO3:H2O
Todorokite	-1.03	-46.85	-45.82	Mn7O12:3H2O
Trona-K	-18.15	-6.56	11.59	K2NaH(CO3)2:2H2O
Zincite	-2.05	9.15	11.20	ZnO
Zn	-50.60	18.19	68.79	Zn
Zn(ClO4)2:6H2O	-117.80	-112.16	5.63	Zn(ClO4)2:6H2O
Zn(g)	-67.22	18.19	85.41	Zn
Zn(OH)2(beta)	-2.78	9.15	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-2.51	9.15	11.66	Zn(OH)2
Zn(OH)2(gamma)	-2.73	9.15	11.88	Zn(OH)2
Zn2(OH)3Cl	-5.77	9.53	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-6.01	1.57	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-8.49	0.82	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-25.10	-6.01	19.09	Zn3O(SO4)2
ZnCl2	-15.49	-8.41	7.08	ZnCl2
ZnCO3:H2O	-0.74	-0.60	0.14	ZnCO3:H2O
ZnSO4	-11.11	-7.58	3.53	ZnSO4
ZnSO4:6H2O	-5.88	-7.58	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.71	-7.58	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-7.03	-7.58	-0.55	ZnSO4:H2O

Beginning of batch-reaction calculations.

Reaction step 1.

Using mix 2.

Mixture 2.

1.000e+000 Solution 1 Flujo 1
3.000e+000 Solution 3 AS2

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

Elements	Molality	Moles
Al	1.076e-004	4.304e-004
As	7.210e-006	2.884e-005
C	1.894e-003	7.575e-003
Ca	4.958e-003	1.983e-002
Cl	1.471e-002	5.884e-002
Cu	8.390e-005	3.356e-004
Fe	5.983e-004	2.393e-003
K	9.768e-004	3.907e-003
Mg	5.118e-004	2.047e-003
Mn	6.580e-005	2.632e-004
Na	1.305e-002	5.222e-002
S	5.504e-003	2.202e-002
Zn	4.794e-005	1.918e-004

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

pH	=	5.631	Charge balance
pe	=	14.316	Adjusted to redox equilibrium
Activity of water	=	0.999	
Ionic strength	=	3.330e-002	
Mass of water (kg)	=	4.000e+000	
Total alkalinity (eq/kg)	=	6.962e-004	
Total CO2 (mol/kg)	=	1.894e-003	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	-5.339e-004	
Percent error, 100*(Cat- An)/(Cat+ An)	=	-0.28	
Iterations	=	11	
Total H	=	4.442127e+002	
Total O	=	2.222134e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	2.678e-006	2.337e-006	-5.572	-5.631	-0.059
OH-	4.906e-009	4.120e-009	-8.309	-8.385	-0.076
H2O	5.553e+001	9.993e-001	1.744	-0.000	0.000
Al	1.076e-004				
Al13O4(OH)24+7	8.043e-006	3.503e-009	-5.095	-8.456	-3.361
AlOH+2	1.137e-006	5.799e-007	-5.944	-6.237	-0.293
Al(OH)2+	6.827e-007	5.759e-007	-6.166	-6.240	-0.074
Al+3	4.236e-007	1.210e-007	-6.373	-6.917	-0.544
HA1O2	3.587e-007	3.587e-007	-6.445	-6.445	0.000
AlSO4+	3.245e-007	2.737e-007	-6.489	-6.563	-0.074
AlO2-	6.233e-008	5.258e-008	-7.205	-7.279	-0.074
Al(SO4)2-	5.565e-008	4.694e-008	-7.255	-7.328	-0.074
Al2(OH)2+4	7.231e-010	5.469e-011	-9.141	-10.262	-1.121
NaAlO2	1.086e-010	1.086e-010	-9.964	-9.964	0.000
Al3(OH)4+5	4.046e-011	7.814e-013	-10.393	-12.107	-1.714
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-153.685	-153.685	0.000
As(3)	1.656e-029				
HAsO2	8.838e-030	8.838e-030	-29.054	-29.054	0.000
As(OH)3	7.722e-030	7.722e-030	-29.112	-29.112	0.000
H2AsO3-	2.396e-033	2.021e-033	-32.621	-32.694	-0.074
AsO2-	2.292e-033	1.933e-033	-32.640	-32.714	-0.074
AsO2OH-2	1.685e-038	8.450e-039	-37.773	-38.073	-0.300
HAsS2	0.000e+000	0.000e+000	-287.424	-287.424	0.000
As(5)	7.210e-006				
H2AsO4-	6.438e-006	5.431e-006	-5.191	-5.265	-0.074
HAsO4-2	7.692e-007	3.858e-007	-6.114	-6.414	-0.300
H3AsO4	2.235e-009	2.235e-009	-8.651	-8.651	0.000
AsO4-3	2.009e-012	4.236e-013	-11.697	-12.373	-0.676
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-254.151	-254.151	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-225.158	-225.158	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-140.856	-140.856	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-47.746	-47.746	0.000
C(4)	1.894e-003				
CO2	1.538e-003	1.551e-003	-2.813	-2.809	0.004
HCO3-	3.390e-004	2.859e-004	-3.470	-3.544	-0.074
CaHCO3+	9.029e-006	7.617e-006	-5.044	-5.118	-0.074
NaHCO3	4.429e-006	4.429e-006	-5.354	-5.354	0.000
CuCO3	1.738e-006	1.738e-006	-5.760	-5.760	0.000
MgHCO3+	8.441e-007	7.120e-007	-6.074	-6.148	-0.074
ZnHCO3+	1.765e-007	1.488e-007	-6.753	-6.827	-0.074

MnHCO3+	6.918e-008	5.836e-008	-7.160	-7.234	-0.074
FeCO3+	4.064e-008	3.428e-008	-7.391	-7.465	-0.074
CaCO3	2.828e-008	2.828e-008	-7.548	-7.548	0.000
CO3-2	1.065e-008	5.428e-009	-7.973	-8.265	-0.293
MnCO3	5.095e-009	5.095e-009	-8.293	-8.293	0.000
MgCO3	1.231e-009	1.231e-009	-8.910	-8.910	0.000
ZnCO3	9.207e-010	9.207e-010	-9.036	-9.036	0.000
NaCO3-	2.439e-010	2.057e-010	-9.613	-9.687	-0.074
Cu(CO3)2-2	3.351e-011	1.681e-011	-10.475	-10.775	-0.300
FeHCO3+	9.797e-012	8.264e-012	-11.009	-11.083	-0.074
FeCO3	1.697e-014	1.697e-014	-13.770	-13.770	0.000
CuCO3(OH)2-2	5.387e-015	2.702e-015	-14.269	-14.568	-0.300
Ca	4.958e-003				
Ca+2	4.216e-003	2.248e-003	-2.375	-2.648	-0.273
CaSO4	7.256e-004	7.256e-004	-3.139	-3.139	0.000
CaHCO3+	9.029e-006	7.617e-006	-5.044	-5.118	-0.074
CaCl+	6.930e-006	5.846e-006	-5.159	-5.233	-0.074
CaCl2	8.436e-008	8.436e-008	-7.074	-7.074	0.000
CaCO3	2.828e-008	2.828e-008	-7.548	-7.548	0.000
CaOH+	1.610e-010	1.358e-010	-9.793	-9.867	-0.074
Cl(-1)	1.471e-002				
Cl-	1.467e-002	1.227e-002	-1.833	-1.911	-0.078
NaCl	2.335e-005	2.335e-005	-4.632	-4.632	0.000
CaCl+	6.930e-006	5.846e-006	-5.159	-5.233	-0.074
MgCl+	2.435e-006	2.054e-006	-5.614	-5.687	-0.074
CuCl+	1.335e-006	1.126e-006	-5.874	-5.948	-0.074
MnCl+	8.302e-007	7.003e-007	-6.081	-6.155	-0.074
ZnCl+	4.935e-007	4.163e-007	-6.307	-6.381	-0.074
KCl	3.305e-007	3.305e-007	-6.481	-6.481	0.000
CaCl2	8.436e-008	8.436e-008	-7.074	-7.074	0.000
CuCl2	7.277e-009	7.277e-009	-8.138	-8.138	0.000
HCl	6.439e-009	6.439e-009	-8.191	-8.191	0.000
ZnCl2	5.966e-009	5.966e-009	-8.224	-8.224	0.000
Zn(OH)Cl	3.044e-009	3.044e-009	-8.517	-8.517	0.000
ZnCl3-	4.792e-011	4.042e-011	-10.319	-10.393	-0.074
MnCl3-	2.730e-011	2.303e-011	-10.564	-10.638	-0.074
FeCl2+	2.632e-011	2.220e-011	-10.580	-10.654	-0.074
ZnCl4-2	7.495e-012	3.759e-012	-11.125	-11.425	-0.300
FeCl+2	4.384e-012	2.235e-012	-11.358	-11.651	-0.293
FeCl+	5.836e-013	4.923e-013	-12.234	-12.308	-0.074
CuCl2-	1.049e-015	8.849e-016	-14.979	-15.053	-0.074
CuCl3-2	1.390e-016	6.973e-017	-15.857	-16.157	-0.300
CuCl4-2	4.099e-017	2.056e-017	-16.387	-16.687	-0.300
FeCl2	3.241e-017	3.241e-017	-16.489	-16.489	0.000
FeCl4-	4.763e-018	4.018e-018	-17.322	-17.396	-0.074
FeCl4-2	2.811e-020	1.410e-020	-19.551	-19.851	-0.300
Cl(1)	6.587e-019				
HClO	6.499e-019	6.499e-019	-18.187	-18.187	0.000
ClO-	8.890e-021	7.499e-021	-20.051	-20.125	-0.074
Cl(3)	6.947e-032				
ClO2-	6.926e-032	5.843e-032	-31.159	-31.233	-0.074
HClO2	2.018e-034	2.018e-034	-33.695	-33.695	0.000
Cl(5)	3.857e-029				
ClO3-	3.857e-029	3.239e-029	-28.414	-28.490	-0.076
Cl(7)	1.068e-030				
ClO4-	1.067e-030	8.964e-031	-29.972	-30.047	-0.076
ZnClO4+	4.059e-034	3.424e-034	-33.392	-33.465	-0.074
Cu(1)	1.293e-015				
CuCl2-	1.049e-015	8.849e-016	-14.979	-15.053	-0.074
CuCl3-2	1.390e-016	6.973e-017	-15.857	-16.157	-0.300
Cu+	1.052e-016	8.873e-017	-15.978	-16.052	-0.074
Cu(2)	8.390e-005				
Cu+2	6.295e-005	3.356e-005	-4.201	-4.474	-0.273
CuSO4	1.699e-005	1.699e-005	-4.770	-4.770	0.000
CuCO3	1.738e-006	1.738e-006	-5.760	-5.760	0.000
CuCl+	1.335e-006	1.126e-006	-5.874	-5.948	-0.074
CuOH+	8.777e-007	7.404e-007	-6.057	-6.131	-0.074

CuCl ₂	7.277e-009	7.277e-009	-8.138	-8.138	0.000
Cu(CO ₃) ₂₋₂	3.351e-011	1.681e-011	-10.475	-10.775	-0.300
CuCO ₃ (OH) ₂₋₂	5.387e-015	2.702e-015	-14.269	-14.568	-0.300
CuCl ₄₋₂	4.099e-017	2.056e-017	-16.387	-16.687	-0.300
CuO ₂₋₂	7.958e-022	3.992e-022	-21.099	-21.399	-0.300
Fe(2)	1.330e-010				
Fe+2	1.033e-010	5.507e-011	-9.986	-10.259	-0.273
FeSO ₄	1.929e-011	1.929e-011	-10.715	-10.715	0.000
FeHCO ₃ +	9.797e-012	8.264e-012	-11.009	-11.083	-0.074
FeCl+	5.836e-013	4.923e-013	-12.234	-12.308	-0.074
FeCO ₃	1.697e-014	1.697e-014	-13.770	-13.770	0.000
FeOH+	8.830e-015	7.448e-015	-14.054	-14.128	-0.074
FeCl ₂	3.241e-017	3.241e-017	-16.489	-16.489	0.000
FeCl ₄₋₂	2.811e-020	1.410e-020	-19.551	-19.851	-0.300
Fe(OH) ₂	2.530e-020	2.530e-020	-19.597	-19.597	0.000
Fe(OH) ₃₋	5.106e-025	4.307e-025	-24.292	-24.366	-0.074
Fe(OH) ₄₋₂	3.673e-034	1.842e-034	-33.435	-33.735	-0.300
Fe(3)	5.983e-004				
Fe(OH) ₂₊	5.068e-004	4.275e-004	-3.295	-3.369	-0.074
Fe(OH) ₃	8.552e-005	8.552e-005	-4.068	-4.068	0.000
FeOH+2	5.922e-006	3.019e-006	-5.228	-5.520	-0.293
FeCO ₃ +	4.064e-008	3.428e-008	-7.391	-7.465	-0.074
Fe(OH) ₄₋	1.089e-008	9.186e-009	-7.963	-8.037	-0.074
Fe+3	3.827e-009	1.093e-009	-8.417	-8.961	-0.544
Fe ₂ (OH) ₂₊₄	3.244e-009	2.453e-010	-8.489	-9.610	-1.121
Fe ₃ (OH) ₄₊₅	1.135e-009	2.191e-011	-8.945	-10.659	-1.714
FeSO ₄ +	2.771e-010	2.338e-010	-9.557	-9.631	-0.074
FeCl ₂ +	2.632e-011	2.220e-011	-10.580	-10.654	-0.074
Fe(SO ₄) ₂₋	1.035e-011	8.732e-012	-10.985	-11.059	-0.074
FeCl+2	4.384e-012	2.235e-012	-11.358	-11.651	-0.293
FeCl ₄₋	4.763e-018	4.018e-018	-17.322	-17.396	-0.074
H(0)	0.000e+000				
H ₂	0.000e+000	0.000e+000	-42.999	-42.995	0.004
K	9.768e-004				
K+	9.595e-004	8.023e-004	-3.018	-3.096	-0.078
KSO ₄₋	1.696e-005	1.431e-005	-4.771	-4.844	-0.074
KCl	3.305e-007	3.305e-007	-6.481	-6.481	0.000
KHSO ₄	2.950e-011	2.950e-011	-10.530	-10.530	0.000
KOH	1.190e-012	1.190e-012	-11.925	-11.925	0.000
Mg	5.118e-004				
Mg+2	3.820e-004	2.144e-004	-3.418	-3.669	-0.251
MgSO ₄	1.265e-004	1.265e-004	-3.898	-3.898	0.000
MgCl+	2.435e-006	2.054e-006	-5.614	-5.687	-0.074
MgHCO ₃ +	8.441e-007	7.120e-007	-6.074	-6.148	-0.074
MgCO ₃	1.231e-009	1.231e-009	-8.910	-8.910	0.000
Mg ₄ (OH) ₄₊₄	1.662e-031	1.257e-032	-30.779	-31.901	-1.121
Mn(2)	6.580e-005				
Mn+2	5.028e-005	2.681e-005	-4.299	-4.572	-0.273
MnSO ₄	1.462e-005	1.462e-005	-4.835	-4.835	0.000
MnCl+	8.302e-007	7.003e-007	-6.081	-6.155	-0.074
MnHCO ₃ +	6.918e-008	5.836e-008	-7.160	-7.234	-0.074
MnCO ₃	5.095e-009	5.095e-009	-8.293	-8.293	0.000
MnOH+	3.493e-010	2.947e-010	-9.457	-9.531	-0.074
MnCl ₃₋	2.730e-011	2.303e-011	-10.564	-10.638	-0.074
Mn ₂ OH+3	3.736e-014	8.465e-015	-13.428	-14.072	-0.645
Mn(OH) ₂	3.093e-016	3.093e-016	-15.510	-15.510	0.000
Mn ₂ (OH) ₃₊	8.389e-017	7.076e-017	-16.076	-16.150	-0.074
Mn(OH) ₃₋	1.471e-022	1.241e-022	-21.832	-21.906	-0.074
Mn(OH) ₄₋₂	8.960e-031	4.494e-031	-30.048	-30.347	-0.300
Mn(3)	6.534e-016				
Mn+3	6.534e-016	1.481e-016	-15.185	-15.830	-0.645
Mn(6)	3.939e-021				
MnO ₄₋₂	3.939e-021	1.976e-021	-20.405	-20.704	-0.300
Mn(7)	2.145e-016				
MnO ₄₋	2.145e-016	1.801e-016	-15.669	-15.744	-0.076
Na	1.305e-002				
Na+	1.284e-002	1.083e-002	-1.891	-1.965	-0.074

NaSO4-	1.874e-004	1.581e-004	-3.727	-3.801	-0.074
NaCl	2.335e-005	2.335e-005	-4.632	-4.632	0.000
NaHCO3	4.429e-006	4.429e-006	-5.354	-5.354	0.000
NaCO3-	2.439e-010	2.057e-010	-9.613	-9.687	-0.074
NaAlO2	1.086e-010	1.086e-010	-9.964	-9.964	0.000
NaOH	7.699e-012	7.699e-012	-11.114	-11.114	0.000
O(0)	1.236e-006				
O2	6.178e-007	6.228e-007	-6.209	-6.206	0.004
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-132.780	-132.780	0.000
HS-	0.000e+000	0.000e+000	-134.083	-134.158	-0.076
S-2	0.000e+000	0.000e+000	-141.167	-141.453	-0.286
S2-2	0.000e+000	0.000e+000	-237.862	-238.162	-0.300
HAsS2	0.000e+000	0.000e+000	-287.424	-287.424	0.000
S3-2	0.000e+000	0.000e+000	-334.612	-334.912	-0.300
S4-2	0.000e+000	0.000e+000	-431.589	-431.889	-0.300
S5-2	0.000e+000	0.000e+000	-528.783	-529.082	-0.300
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-137.337	-137.636	-0.300
HS2O3-	0.000e+000	0.000e+000	-142.180	-142.254	-0.074
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-125.382	-125.667	-0.286
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-44.497	-44.570	-0.074
SO3-2	0.000e+000	0.000e+000	-45.878	-46.171	-0.293
H2SO3	0.000e+000	0.000e+000	-48.220	-48.220	0.000
SO2	0.000e+000	0.000e+000	-48.320	-48.320	0.000
S2O6-2	0.000e+000	0.000e+000	-64.540	-64.840	-0.300
S3O6-2	0.000e+000	0.000e+000	-163.773	-164.072	-0.300
S4O6-2	0.000e+000	0.000e+000	-247.100	-247.400	-0.300
S5O6-2	0.000e+000	0.000e+000	-359.306	-359.606	-0.300
S(5)	0.000e+000				
S2O5-2	0.000e+000	0.000e+000	-93.671	-93.971	-0.300
S(6)	5.504e-003				
SO4-2	4.406e-003	2.210e-003	-2.356	-2.656	-0.300
CaSO4	7.256e-004	7.256e-004	-3.139	-3.139	0.000
NaSO4-	1.874e-004	1.581e-004	-3.727	-3.801	-0.074
MgSO4	1.265e-004	1.265e-004	-3.898	-3.898	0.000
CuSO4	1.699e-005	1.699e-005	-4.770	-4.770	0.000
KSO4-	1.696e-005	1.431e-005	-4.771	-4.844	-0.074
MnSO4	1.462e-005	1.462e-005	-4.835	-4.835	0.000
ZnSO4	9.377e-006	9.377e-006	-5.028	-5.028	0.000
HSO4-	6.183e-007	5.216e-007	-6.209	-6.283	-0.074
AlSO4+	3.245e-007	2.737e-007	-6.489	-6.563	-0.074
Al(SO4)2-	5.565e-008	4.694e-008	-7.255	-7.328	-0.074
FeSO4+	2.771e-010	2.338e-010	-9.557	-9.631	-0.074
KHSO4	2.950e-011	2.950e-011	-10.530	-10.530	0.000
FeSO4	1.929e-011	1.929e-011	-10.715	-10.715	0.000
Fe(SO4)2-	1.035e-011	8.732e-012	-10.985	-11.059	-0.074
H2SO4	1.150e-015	1.150e-015	-14.939	-14.939	0.000
S(7)	0.000e+000				
S2O8-2	0.000e+000	0.000e+000	-41.832	-42.132	-0.300
S(8)	2.651e-029				
HSO5-	2.651e-029	2.236e-029	-28.577	-28.651	-0.074
Zn	4.794e-005				
Zn+2	3.788e-005	2.020e-005	-4.422	-4.695	-0.273
ZnSO4	9.377e-006	9.377e-006	-5.028	-5.028	0.000
ZnCl+	4.935e-007	4.163e-007	-6.307	-6.381	-0.074
ZnHCO3+	1.765e-007	1.488e-007	-6.753	-6.827	-0.074
ZnOH+	1.123e-008	9.472e-009	-7.950	-8.024	-0.074
ZnCl2	5.966e-009	5.966e-009	-8.224	-8.224	0.000
Zn(OH)Cl	3.044e-009	3.044e-009	-8.517	-8.517	0.000
ZnCO3	9.207e-010	9.207e-010	-9.036	-9.036	0.000
ZnCl3-	4.792e-011	4.042e-011	-10.319	-10.393	-0.074
Zn(OH)2	1.735e-011	1.735e-011	-10.761	-10.761	0.000
ZnCl4-2	7.495e-012	3.759e-012	-11.125	-11.425	-0.300
Zn(OH)3-	2.726e-017	2.299e-017	-16.564	-16.638	-0.074

Zn(OH)4-2	3.343e-024	1.677e-024	-23.476	-23.776	-0.300
ZnClO4+	4.059e-034	3.424e-034	-33.392	-33.465	-0.074

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

Phase	SI	log IAP	log KT	
Al	-135.28	14.63	149.91	Al
Al(g)	-185.99	14.63	200.62	Al
Al2(SO4)3	-40.70	-21.80	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-23.36	-21.80	1.56	Al2(SO4)3:6H2O
Alabandite	-132.68	-133.10	-0.42	MnS
Alum-K	-10.36	-15.33	-4.97	KAl(SO4)2:12H2O
Alunite	5.10	4.63	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.95	-5.30	-4.35	CaSO4
Antarcticite	-10.57	-6.47	4.09	CaCl2:6H2O
Antlerite	-2.28	6.45	8.73	Cu3(SO4)(OH)4
Aphthitalite	-12.68	-16.56	-3.89	NaK3(SO4)2
Aragonite	-2.53	-0.56	1.97	CaCO3
Arcanite	-7.00	-8.85	-1.84	K2SO4
Arsenolite	-56.81	-76.65	-19.84	As2O3
Arsenopyrite	-220.35	-234.79	-14.45	FeAsS
Artinite	-13.62	6.01	19.63	Mg2CO3(OH)2:3H2O
As	-76.35	-33.67	42.68	As
As2O5	-23.93	-21.79	2.14	As2O5
As4O6(cubi)	-113.48	-153.30	-39.82	As4O6
As4O6(mono)	-113.25	-153.30	-40.05	As4O6
Atacamite	-2.20	12.07	14.26	Cu4Cl2(OH)6
Azurite	-7.10	2.02	9.12	Cu3(CO3)2(OH)2
Bassanite	-1.60	-5.30	-3.71	CaSO4:0.5H2O
Birnessite	23.10	-62.45	-85.55	Mn8O14:5H2O
Bischofite	-11.89	-7.49	4.39	MgCl2:6H2O
Bixbyite	3.09	2.13	-0.96	Mn2O3
Bloedite	-10.43	-12.91	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	2.43	9.98	7.55	AlO2H
Bornite	-490.52	-593.05	-102.53	Cu5FeS4
Brochantite	-2.19	13.23	15.42	Cu4(SO4)(OH)6
Brucite	-8.69	7.59	16.28	Mg(OH)2
Burkeite	-24.50	-15.02	9.49	Na6CO3(SO4)2
C	-67.12	-2.97	64.15	C
C(g)	-184.73	-2.97	181.77	C
Ca	-128.11	11.72	139.83	Ca
Ca(g)	-153.35	11.72	165.07	Ca
Ca2Al2O5:8H2O	-22.39	37.18	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-24.15	2.14	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-13.75	4.05	17.80	Ca3(AsO4)2
Ca3Al2O6	-67.24	45.80	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-70.21	70.28	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-52.85	54.41	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-49.28	54.40	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-48.96	19.37	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-18.34	28.57	46.91	CaAl2O4
CaAl2O4:10H2O	-9.43	28.56	37.99	CaAl2O4:10H2O
CaAl4O7	-20.07	48.52	68.59	CaAl4O7
Calcite	-2.39	-0.56	1.82	CaCO3
Carnallite	-16.77	-12.50	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.77	-5.30	-3.54	CaSO4:0.5H2O
CH4(g)	-138.01	-140.86	-2.84	CH4
Chalcanthite	-4.50	-7.13	-2.63	CuSO4:5H2O
Chalcocite	-125.89	-160.63	-34.74	Cu2S
Chalcocyanite	-10.04	-7.13	2.91	CuSO4
Chalcopyrite	-239.18	-271.79	-32.60	CuFeS2
Chloromagnesite	-29.31	-7.49	21.82	MgCl2
Cl2(g)	-21.18	-18.19	2.99	Cl2
Claudetite	-56.86	-76.65	-19.80	As2O3
CO(g)	-44.75	-47.75	-3.00	CO
CO2(g)	-1.35	-9.17	-7.83	CO2

Corundum	1.66	19.95	18.29	Al ₂ O ₃
Covellite	-110.14	-133.00	-22.86	CuS
Cu	-21.61	9.89	31.50	Cu
Cu(g)	-73.76	9.89	83.66	Cu
CuCl ₂	-12.02	-8.30	3.72	CuCl ₂
Cuprite	-18.93	-20.84	-1.91	Cu ₂ O
Dawsonite	0.13	4.47	4.34	NaAlCO ₃ (OH) ₂
Delafoosite	3.95	-2.49	-6.44	CuFeO ₂
Diaspore	2.83	9.98	7.15	AlHO ₂
Dolomite	-4.62	-2.14	2.47	CaMg(CO ₃) ₂
Dolomite-dis	-6.15	-2.14	4.01	CaMg(CO ₃) ₂
Dolomite-ord	-4.61	-2.14	2.46	CaMg(CO ₃) ₂
Epsomite	-4.36	-6.33	-1.96	MgSO ₄ ·7H ₂ O
Ettringite	-32.59	29.87	62.46	Ca ₆ Al ₂ (SO ₄) ₃ (OH) ₁₂ ·26H ₂ O
Fe	-54.91	4.11	59.02	Fe
Fe(OH) ₂	-12.89	1.00	13.89	Fe(OH) ₂
Fe(OH) ₃	2.29	7.93	5.64	Fe(OH) ₃
Fe ₂ (SO ₄) ₃	-28.94	-25.89	3.05	Fe ₂ (SO ₄) ₃
FeO	-12.52	1.00	13.52	FeO
Ferrite-Ca	2.98	24.48	21.50	CaFe ₂ O ₄
Ferrite-Cu	12.37	22.65	10.28	CuFe ₂ O ₄
Ferrite-Dicalcium	-23.71	33.09	56.80	Ca ₂ Fe ₂ O ₅
Ferrite-Mg	2.44	23.46	21.02	MgFe ₂ O ₄
Ferrite-Zn	10.73	22.43	11.70	ZnFe ₂ O ₄
FeSO ₄	-15.52	-12.91	2.61	FeSO ₄
Gaylussite	-13.57	-2.41	11.16	CaNa ₂ (CO ₃) ₂ ·5H ₂ O
Gibbsite	2.24	9.98	7.74	Al(OH) ₃
Glauberite	-6.42	-11.89	-5.47	Na ₂ Ca(SO ₄) ₂
Goethite	7.40	7.93	0.53	FeOOH
Gypsum	-0.77	-5.30	-4.53	CaSO ₄ ·2H ₂ O
H ₂ (g)	-39.89	-43.00	-3.10	H ₂
H ₂ O(g)	-1.59	-0.00	1.59	H ₂ O
H ₂ S(g)	-131.80	-139.79	-7.99	H ₂ S
Halite	-5.44	-3.88	1.56	NaCl
Hausmannite	-1.33	8.82	10.14	Mn ₃ O ₄
HCl(g)	-13.84	-7.54	6.30	HCl
Hematite	15.79	15.87	0.08	Fe ₂ O ₃
Hercynite	-7.85	20.96	28.80	FeAl ₂ O ₄
Hexahydrite	-4.60	-6.33	-1.73	MgSO ₄ ·6H ₂ O
Huntite	-15.52	-5.30	10.22	CaMg ₃ (CO ₃) ₄
Hydromagnesite	-29.47	1.27	30.74	Mg ₅ (CO ₃) ₄ (OH) ₂ ·4H ₂ O
Hydrophilite	-18.22	-6.47	11.75	CaCl ₂
Hydrozincite	-15.82	14.49	30.31	Zn ₅ (OH) ₆ (CO ₃) ₂
Ice	-0.14	-0.00	0.14	H ₂ O
Jarosite	7.91	-1.50	-9.41	KFe ₃ (SO ₄) ₂ (OH) ₆
Jarosite-Na	5.07	-0.37	-5.45	NaFe ₃ (SO ₄) ₂ (OH) ₆
K	-66.89	4.09	70.98	K
K(g)	-77.49	4.09	81.58	K
K ₂ CO ₃ ·1.5H ₂ O	-17.48	-4.10	13.38	K ₂ CO ₃ ·1.5H ₂ O
K ₂ O	-78.96	5.07	84.04	K ₂ O
K ₃ H(SO ₄) ₂	-16.61	-20.23	-3.62	K ₃ H(SO ₄) ₂
K ₈ H ₄ (CO ₃) ₆ ·3H ₂ O	-62.48	-34.77	27.71	K ₈ H ₄ (CO ₃) ₆ ·3H ₂ O
Kainite	-11.02	-11.33	-0.31	KMgClSO ₄ ·3H ₂ O
KAl(SO ₄) ₂	-18.60	-15.32	3.27	KAl(SO ₄) ₂
Kalichinite	-6.92	-6.64	0.28	KHCO ₃
Katoite	-33.15	45.79	78.94	Ca ₃ Al ₂ H ₁₂ O ₁₂
Kieserite	-6.06	-6.32	-0.27	MgSO ₄ ·H ₂ O
KMgCl ₃	-33.74	-12.50	21.25	KMgCl ₃
KMgCl ₃ ·2H ₂ O	-26.46	-12.50	13.96	KMgCl ₃ ·2H ₂ O
KNaCO ₃ ·6H ₂ O	-13.23	-2.98	10.26	KNaCO ₃ ·6H ₂ O
Lammerite	-2.98	-1.43	1.55	Cu ₃ (AsO ₄) ₂
Lansfordite	-6.42	-1.58	4.84	MgCO ₃ ·5H ₂ O
Lawrencite	-23.14	-14.08	9.05	FeCl ₂
Leonite	-11.06	-15.17	-4.11	K ₂ Mg(SO ₄) ₂ ·4H ₂ O
Lime	-23.95	8.61	32.57	CaO
Magnesite	-3.85	-1.58	2.27	MgCO ₃
Magnetite	6.45	16.87	10.42	Fe ₃ O ₄

Malachite	-1.50	4.40	5.90	Cu ₂ CO ₃ (OH) ₂
Manganite	1.23	1.06	-0.16	MnO(OH)
Manganosite	-11.23	6.69	17.92	MnO
Mayenite	-251.11	243.04	494.15	Ca ₁₂ Al ₁₄ O ₃₃
Melanterite	-10.52	-12.92	-2.40	FeSO ₄ ·7H ₂ O
Mercallite	-9.94	-11.38	-1.44	KHSO ₄
Mg	-111.82	10.70	122.52	Mg
Mg(g)	-131.55	10.70	142.25	Mg
Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O	-9.62	-4.43	5.20	Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O
Mg _{1.5} SO ₄ (OH)	-11.74	-2.53	9.21	Mg _{1.5} SO ₄ (OH)
MgCl ₂ :2H ₂ O	-20.22	-7.49	12.73	MgCl ₂ :2H ₂ O
MgCl ₂ :4H ₂ O	-14.79	-7.49	7.30	MgCl ₂ :4H ₂ O
MgCl ₂ :H ₂ O	-23.56	-7.49	16.07	MgCl ₂ :H ₂ O
MgOHCl	-15.84	0.05	15.89	MgOHCl
MgSO ₄	-11.15	-6.32	4.83	MgSO ₄
Mirabilite	-5.44	-6.59	-1.15	Na ₂ SO ₄ :10H ₂ O
Misenite	-66.07	-77.14	-11.08	K ₈ H ₆ (SO ₄) ₇
Mn	-73.14	9.79	82.93	Mn
Mn(OH) ₂ (am)	-8.62	6.69	15.31	Mn(OH) ₂
Mn(OH) ₃	-5.28	1.06	6.34	Mn(OH) ₃
MnCl ₂ :2H ₂ O	-12.39	-8.39	4.00	MnCl ₂ :2H ₂ O
MnCl ₂ :4H ₂ O	-11.15	-8.40	2.75	MnCl ₂ :4H ₂ O
MnCl ₂ :H ₂ O	-13.94	-8.39	5.54	MnCl ₂ :H ₂ O
MnO ₂ (gamma)	3.49	-12.64	-16.13	MnO ₂
MnSO ₄	-9.84	-7.23	2.61	MnSO ₄
Molysite	-28.17	-14.69	13.47	FeCl ₃
Monohydrocalcite	-3.24	-0.56	2.68	CaCO ₃ :H ₂ O
Na	-62.15	5.22	67.37	Na
Na(g)	-75.64	5.22	80.86	Na
Na ₂ CO ₃	-13.01	-1.84	11.16	Na ₂ CO ₃
Na ₂ CO ₃ :7H ₂ O	-11.78	-1.85	9.94	Na ₂ CO ₃ :7H ₂ O
Na ₂ O	-60.09	7.33	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-15.95	-16.84	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-12.58	-18.48	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
NaFeO ₂	-8.29	11.60	19.88	NaFeO ₂
Nahcolite	-5.37	-5.51	-0.14	NaHCO ₃
Nantokite	-11.20	-17.96	-6.77	CuCl
Natron	-11.43	-1.85	9.59	Na ₂ CO ₃ :10H ₂ O
Nesquehonite	-6.87	-1.58	5.29	MgCO ₃ :3H ₂ O
O ₂ (g)	-3.31	-6.21	-2.89	O ₂
Orpiment	-416.53	-496.02	-79.49	As ₂ S ₃
Oxychloride-Mg	-18.19	7.64	25.83	Mg ₂ Cl(OH) ₃ :4H ₂ O
Pentahydrate	-4.94	-6.33	-1.39	MgSO ₄ :5H ₂ O
Periclase	-13.73	7.59	21.33	MgO
Picromerite	-10.73	-15.17	-4.44	K ₂ Mg(SO ₄) ₂ :6H ₂ O
Pirssonite	-13.73	-2.40	11.32	Na ₂ Ca(CO ₃) ₂ :2H ₂ O
Polyhalite	-11.47	-25.78	-14.31	K ₂ MgCa ₂ (SO ₄) ₄ :2H ₂ O
Portlandite	-13.93	8.61	22.55	Ca(OH) ₂
Pyrite	-222.41	-247.11	-24.70	FeS ₂
Pyrolusite	5.02	-12.64	-17.66	MnO ₂
Pyrrhotite	-135.05	-138.79	-3.74	FeS
Realgar	-161.87	-222.15	-60.28	AsS
Rhodochrosite	-2.27	-2.48	-0.22	MnCO ₃
S	-97.78	-142.89	-45.11	S
S ₂ (g)	-209.46	-216.64	-7.19	S ₂
Scacchite	-17.14	-8.39	8.74	MnCl ₂
Siderite	-7.95	-8.17	-0.22	FeCO ₃
Smithsonite	-3.05	-2.61	0.44	ZnCO ₃
SO ₂ (g)	-48.50	-48.32	0.18	SO ₂
Sphalerite	-121.75	-133.22	-11.47	ZnS
Spinel	-10.06	27.55	37.61	Al ₂ MgO ₄
Starkeyite	-5.33	-6.33	-1.00	MgSO ₄ :4H ₂ O
Sylvite	-5.83	-5.01	0.83	KCl
Syngenite	-6.55	-14.15	-7.60	K ₂ Ca(SO ₄) ₂ :H ₂ O
Tachyhydrite	-38.60	-21.46	17.14	Mg ₂ CaCl ₆ :12H ₂ O
Tenorite	-0.86	6.79	7.65	CuO
Thenardite	-6.23	-6.59	-0.36	Na ₂ SO ₄

Thermonatrite	-12.78	-1.84	10.94	Na2CO3:H2O
Todorokite	20.24	-25.58	-45.82	Mn7O12:3H2O
Troilite	-134.94	-138.79	-3.84	FeS
Trona-K	-21.20	-9.61	11.59	K2NaH(CO3)2:2H2O
Wurtzite	-124.05	-133.22	-9.17	ZnS
Wustite	-10.72	1.68	12.40	Fe.947O
Zincite	-4.63	6.57	11.20	ZnO
Zn	-59.12	9.67	68.79	Zn
Zn(ClO4)2:6H2O	-70.42	-64.79	5.63	Zn(ClO4)2:6H2O
Zn(g)	-75.74	9.67	85.41	Zn
Zn(OH)2(beta)	-5.36	6.57	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-5.09	6.57	11.66	Zn(OH)2
Zn(OH)2(gamma)	-5.32	6.57	11.88	Zn(OH)2
Zn2(OH)3Cl	-9.70	5.59	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-8.36	-0.78	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-11.40	-2.09	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-27.22	-8.13	19.09	Zn3O(SO4)2
ZnCl2	-15.60	-8.52	7.08	ZnCl2
ZnCO3:H2O	-2.75	-2.61	0.14	ZnCO3:H2O
ZnSO4	-10.88	-7.35	3.53	ZnSO4
ZnSO4:6H2O	-5.65	-7.35	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.48	-7.35	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.80	-7.35	-0.55	ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
