
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 4

temp 25
pH 3.17
pe 12
redox pe
units mg/l
density 1
Cl 46.9
S(6) 1089.6
Al 25.6
As 5.0
Ca 201.4
Cu 35.1
Fe 170.2
K 69.2
Mg 19.8
Mn 20.6
Na 33.2
Zn 17.4
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 4

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

Elements	Molality	Moles
Al	9.504e-004	9.504e-004
As	6.685e-005	6.685e-005
Ca	5.034e-003	5.034e-003
Cl	1.325e-003	1.325e-003
Cu	5.533e-004	5.533e-004
Fe	3.053e-003	3.053e-003
K	1.773e-003	1.773e-003
Mg	8.161e-004	8.161e-004
Mn	3.756e-004	3.756e-004
Na	1.447e-003	1.447e-003
S(6)	1.136e-002	1.136e-002
Zn	2.666e-004	2.666e-004

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

```

pH = 3.170
pe = 12.000
Activity of water = 1.000
Ionic strength = 3.718e-002
Mass of water (kg) = 1.000e+000
Total alkalinity (eq/kg) = -2.718e-003
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = 3.154e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 8.05
Iterations = 8
Total H = 1.110537e+002
Total O = 5.557286e+001

```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	7.785e-004	6.761e-004	-3.109	-3.170	-0.061
OH-	1.709e-011	1.424e-011	-10.767	-10.846	-0.079
H2O	5.553e+001	9.996e-001	1.744	-0.000	0.000
Al	9.504e-004				
AlSO4+	4.577e-004	3.832e-004	-3.339	-3.417	-0.077
Al+3	3.507e-004	9.580e-005	-3.455	-4.019	-0.564
Al(SO4)2-	1.389e-004	1.163e-004	-3.857	-3.935	-0.077
AlOH+2	3.206e-006	1.587e-006	-5.494	-5.799	-0.305
Al(OH)2+	6.507e-009	5.448e-009	-8.187	-8.264	-0.077
Al2(OH)2+4	6.033e-009	4.095e-010	-8.219	-9.388	-1.168
HALO2	1.173e-011	1.173e-011	-10.931	-10.931	0.000
Al3(OH)4+5	3.369e-012	5.535e-014	-11.472	-13.257	-1.784
AlO2-	7.097e-015	5.942e-015	-14.149	-14.226	-0.077
NaAlO2	1.338e-018	1.338e-018	-17.874	-17.874	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-46.038	-49.537	-3.499

As(-3)	0.000e+000					
AsH3	0.000e+000	0.000e+000	-112.033	-112.033	0.000	
As(3)	1.610e-016					
HAsO2	8.593e-017	8.593e-017	-16.066	-16.066	0.000	
As(OH)3	7.510e-017	7.510e-017	-16.124	-16.124	0.000	
H2AsO3-	8.114e-023	6.793e-023	-22.091	-22.168	-0.077	
AsO2-	7.760e-023	6.497e-023	-22.110	-22.187	-0.077	
AsO2OH-2	2.019e-030	9.817e-031	-29.695	-30.008	-0.313	
As(5)	6.685e-005					
H2AsO4-	6.077e-005	5.088e-005	-4.216	-4.293	-0.077	
H3AsO4	6.059e-006	6.059e-006	-5.218	-5.218	0.000	
HAsO4-2	2.569e-008	1.249e-008	-7.590	-7.903	-0.313	
AsO4-3	2.411e-016	4.740e-017	-15.618	-16.324	-0.706	
Ca	5.034e-003					
Ca+2	3.882e-003	2.017e-003	-2.411	-2.695	-0.284	
CaSO4	1.152e-003	1.152e-003	-2.939	-2.939	0.000	
CaCl+	5.599e-007	4.688e-007	-6.252	-6.329	-0.077	
CaCl2	6.044e-010	6.044e-010	-9.219	-9.219	0.000	
CaOH+	5.032e-013	4.213e-013	-12.298	-12.375	-0.077	
Cl(-1)	1.325e-003					
Cl-	1.322e-003	1.096e-003	-2.879	-2.960	-0.081	
CuCl+	7.019e-007	5.877e-007	-6.154	-6.231	-0.077	
CaCl+	5.599e-007	4.688e-007	-6.252	-6.329	-0.077	
FeCl+	5.035e-007	4.215e-007	-6.298	-6.375	-0.077	
MnCl+	3.622e-007	3.033e-007	-6.441	-6.518	-0.077	
MgCl+	2.911e-007	2.438e-007	-6.536	-6.613	-0.077	
NaCl	2.275e-007	2.275e-007	-6.643	-6.643	0.000	
ZnCl+	2.134e-007	1.787e-007	-6.671	-6.748	-0.077	
HCl	1.665e-007	1.665e-007	-6.779	-6.779	0.000	
KCl	5.248e-008	5.248e-008	-7.280	-7.280	0.000	
FeCl+2	1.867e-008	9.244e-009	-7.729	-8.034	-0.305	
FeCl2+	9.799e-009	8.204e-009	-8.009	-8.086	-0.077	
CaCl2	6.044e-010	6.044e-010	-9.219	-9.219	0.000	
CuCl2	3.393e-010	3.393e-010	-9.469	-9.469	0.000	
ZnCl2	2.288e-010	2.288e-010	-9.640	-9.640	0.000	
Zn(OH)Cl	4.517e-012	4.517e-012	-11.345	-11.345	0.000	
FeCl2	2.480e-012	2.480e-012	-11.606	-11.606	0.000	
ZnCl3-	1.655e-013	1.385e-013	-12.781	-12.858	-0.077	
MnCl3-	9.510e-014	7.962e-014	-13.022	-13.099	-0.077	
CuCl2-	1.020e-014	8.543e-015	-13.991	-14.068	-0.077	
ZnCl4-2	2.368e-015	1.151e-015	-14.626	-14.939	-0.313	
CuCl3-2	1.237e-016	6.015e-017	-15.908	-16.221	-0.313	
FeCl4-2	1.771e-017	8.612e-018	-16.752	-17.065	-0.313	
FeCl4-	1.416e-017	1.185e-017	-16.849	-16.926	-0.077	
CuCl4-2	1.574e-020	7.653e-021	-19.803	-20.116	-0.313	
Cl(1)	4.682e-027					
HClO	4.682e-027	4.682e-027	-26.330	-26.330	0.000	
ClO-	2.230e-031	1.867e-031	-30.652	-30.729	-0.077	
Cl(3)	0.000e+000					
ClO2-	0.000e+000	0.000e+000	-51.315	-51.392	-0.077	
HClO2	0.000e+000	0.000e+000	-51.392	-51.392	0.000	
Cl(5)	0.000e+000					
ClO3-	0.000e+000	0.000e+000	-58.124	-58.203	-0.079	
Cl(7)	0.000e+000					
ClO4-	0.000e+000	0.000e+000	-69.237	-69.316	-0.079	
ZnClO4+	0.000e+000	0.000e+000	-71.975	-72.052	-0.077	
Cu(1)	1.385e-013					
Cu+	1.281e-013	1.073e-013	-12.892	-12.969	-0.077	
CuCl2-	1.020e-014	8.543e-015	-13.991	-14.068	-0.077	
CuCl3-2	1.237e-016	6.015e-017	-15.908	-16.221	-0.313	
Cu(2)	5.533e-004					
Cu+2	3.771e-004	1.960e-004	-3.424	-3.708	-0.284	
CuSO4	1.755e-004	1.755e-004	-3.756	-3.756	0.000	
CuCl+	7.019e-007	5.877e-007	-6.154	-6.231	-0.077	
CuOH+	1.785e-008	1.495e-008	-7.748	-7.825	-0.077	
CuCl2	3.393e-010	3.393e-010	-9.469	-9.469	0.000	
CuCl4-2	1.574e-020	7.653e-021	-19.803	-20.116	-0.313	

CuO2-2	6.844e-031	3.328e-031	-30.165	-30.478	-0.313
Fe(2)	1.343e-003				
Fe+2	1.016e-003	5.278e-004	-2.993	-3.278	-0.284
FeSO4	3.270e-004	3.270e-004	-3.486	-3.486	0.000
FeCl+	5.035e-007	4.215e-007	-6.298	-6.375	-0.077
FeOH+	2.947e-010	2.468e-010	-9.531	-9.608	-0.077
FeCl2	2.480e-012	2.480e-012	-11.606	-11.606	0.000
FeCl4-2	1.771e-017	8.612e-018	-16.752	-17.065	-0.313
Fe(OH)2	2.898e-018	2.898e-018	-17.538	-17.538	0.000
Fe(OH)3-	2.037e-025	1.706e-025	-24.691	-24.768	-0.077
Fe(OH)4-2	5.187e-037	2.522e-037	-36.285	-36.598	-0.313
Fe(3)	1.710e-003				
FeOH+2	9.759e-004	4.831e-004	-3.011	-3.316	-0.305
Fe(OH)2+	2.825e-004	2.365e-004	-3.549	-3.626	-0.077
Fe+3	1.852e-004	5.061e-005	-3.732	-4.296	-0.564
Fe2(OH)2+4	9.255e-005	6.281e-006	-4.034	-5.202	-1.168
FeSO4+	2.286e-005	1.914e-005	-4.641	-4.718	-0.077
Fe3(OH)4+5	1.889e-005	3.104e-007	-4.724	-6.508	-1.784
Fe(SO4)2-	1.510e-006	1.265e-006	-5.821	-5.898	-0.077
Fe(OH)3	1.635e-007	1.635e-007	-6.786	-6.786	0.000
FeCl+2	1.867e-008	9.244e-009	-7.729	-8.034	-0.305
FeCl2+	9.799e-009	8.204e-009	-8.009	-8.086	-0.077
Fe(OH)4-	7.254e-014	6.074e-014	-13.139	-13.217	-0.077
FeCl4-	1.416e-017	1.185e-017	-16.849	-16.926	-0.077
H(0)	7.189e-034				
H2	3.595e-034	3.627e-034	-33.444	-33.440	0.004
K	1.773e-003				
K+	1.719e-003	1.426e-003	-2.765	-2.846	-0.081
KSO4-	5.372e-005	4.497e-005	-4.270	-4.347	-0.077
KCl	5.248e-008	5.248e-008	-7.280	-7.280	0.000
KHSO4	2.683e-008	2.683e-008	-7.571	-7.571	0.000
KOH	7.308e-015	7.308e-015	-14.136	-14.136	0.000
Mg	8.161e-004				
Mg+2	5.185e-004	2.848e-004	-3.285	-3.545	-0.260
MgSO4	2.973e-004	2.973e-004	-3.527	-3.527	0.000
MgCl+	2.911e-007	2.438e-007	-6.536	-6.613	-0.077
Mg4(OH)4+4	0.000e+000	0.000e+000	-40.084	-41.252	-1.168
Mn(2)	3.756e-004				
Mn+2	2.500e-004	1.299e-004	-3.602	-3.886	-0.284
MnSO4	1.253e-004	1.253e-004	-3.902	-3.902	0.000
MnCl+	3.622e-007	3.033e-007	-6.441	-6.518	-0.077
MnOH+	5.897e-012	4.937e-012	-11.229	-11.307	-0.077
MnCl3-	9.510e-014	7.962e-014	-13.022	-13.099	-0.077
Mn2OH+3	3.232e-015	6.873e-016	-14.490	-15.163	-0.672
Mn(OH)2	1.792e-020	1.792e-020	-19.747	-19.747	0.000
Mn2(OH)3+	8.202e-023	6.867e-023	-22.086	-22.163	-0.077
Mn(OH)3-	2.968e-029	2.485e-029	-28.528	-28.605	-0.077
Mn(OH)4-2	6.398e-040	3.111e-040	-39.194	-39.507	-0.313
Mn(3)	1.630e-017				
Mn+3	1.630e-017	3.465e-018	-16.788	-17.460	-0.672
Mn(6)	0.000e+000				
MnO4-2	0.000e+000	0.000e+000	-48.661	-48.974	-0.313
Mn(7)	0.000e+000				
MnO4-	0.000e+000	0.000e+000	-46.251	-46.330	-0.079
Na	1.447e-003				
Na+	1.410e-003	1.181e-003	-2.851	-2.928	-0.077
NaSO4-	3.641e-005	3.049e-005	-4.439	-4.516	-0.077
NaCl	2.275e-007	2.275e-007	-6.643	-6.643	0.000
NaOH	2.901e-015	2.901e-015	-14.537	-14.537	0.000
NaAlO2	1.338e-018	1.338e-018	-17.874	-17.874	0.000
O(0)	9.587e-026				
O2	4.793e-026	4.837e-026	-25.319	-25.315	0.004
S(6)	1.136e-002				
SO4-2	8.038e-003	3.909e-003	-2.095	-2.408	-0.313
CaSO4	1.152e-003	1.152e-003	-2.939	-2.939	0.000
AlSO4+	4.577e-004	3.832e-004	-3.339	-3.417	-0.077
FeSO4	3.270e-004	3.270e-004	-3.486	-3.486	0.000

HSO4-	3.188e-004	2.669e-004	-3.496	-3.574	-0.077
MgSO4	2.973e-004	2.973e-004	-3.527	-3.527	0.000
CuSO4	1.755e-004	1.755e-004	-3.756	-3.756	0.000
Al(SO4)2-	1.389e-004	1.163e-004	-3.857	-3.935	-0.077
MnSO4	1.253e-004	1.253e-004	-3.902	-3.902	0.000
ZnSO4	7.968e-005	7.968e-005	-4.099	-4.099	0.000
KSO4-	5.372e-005	4.497e-005	-4.270	-4.347	-0.077
NaSO4-	3.641e-005	3.049e-005	-4.439	-4.516	-0.077
FeSO4+	2.286e-005	1.914e-005	-4.641	-4.718	-0.077
Fe(SO4)2-	1.510e-006	1.265e-006	-5.821	-5.898	-0.077
KHSO4	2.683e-008	2.683e-008	-7.571	-7.571	0.000
H2SO4	1.703e-010	1.703e-010	-9.769	-9.769	0.000
Zn	2.666e-004				
Zn+2	1.867e-004	9.702e-005	-3.729	-4.013	-0.284
ZnSO4	7.968e-005	7.968e-005	-4.099	-4.099	0.000
ZnCl+	2.134e-007	1.787e-007	-6.671	-6.748	-0.077
ZnCl2	2.288e-010	2.288e-010	-9.640	-9.640	0.000
ZnOH+	1.879e-010	1.573e-010	-9.726	-9.803	-0.077
Zn(OH)Cl	4.517e-012	4.517e-012	-11.345	-11.345	0.000
ZnCl3-	1.655e-013	1.385e-013	-12.781	-12.858	-0.077
ZnCl4-2	2.368e-015	1.151e-015	-14.626	-14.939	-0.313
Zn(OH)2	9.960e-016	9.960e-016	-15.002	-15.002	0.000
Zn(OH)3-	5.452e-024	4.565e-024	-23.263	-23.341	-0.077
Zn(OH)4-2	2.366e-033	1.151e-033	-32.626	-32.939	-0.313
ZnClO4+	0.000e+000	0.000e+000	-71.975	-72.052	-0.077

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

Phase	SI	log IAP	log KT	
Al	-125.44	24.48	149.91	Al
Al(g)	-176.14	24.48	200.62	Al
Al2(SO4)3	-34.16	-15.26	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-16.82	-15.26	1.56	Al2(SO4)3:6H2O
Alum-K	-6.71	-11.68	-4.97	KAl(SO4)2:12H2O
Alunite	-0.23	-0.70	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.75	-5.10	-4.35	CaSO4
Antarcticite	-12.71	-8.62	4.09	CaCl2:6H2O
Antlerite	-9.58	-0.85	8.73	Cu3(SO4)(OH)4
Aphthitalite	-12.39	-16.28	-3.89	NaK3(SO4)2
Arcanite	-6.26	-8.10	-1.84	K2SO4
Arsenolite	-30.83	-50.68	-19.84	As2O3
As	-49.03	-6.35	42.68	As
As2O5	-17.06	-14.93	2.14	As2O5
As4O6(cubi)	-61.53	-101.35	-39.82	As4O6
As4O6(mono)	-61.30	-101.35	-40.05	As4O6
Atacamite	-16.00	-1.73	14.26	Cu4Cl2(OH)6
Bassanite	-1.40	-5.10	-3.71	CaSO4:0.5H2O
Birnessite	-68.13	-153.67	-85.55	Mn8O14:5H2O
Bischofite	-13.86	-9.47	4.39	MgCl2:6H2O
Bixbyite	-14.94	-15.90	-0.96	Mn2O3
Bloedite	-11.74	-14.22	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-2.06	5.49	7.55	AlO2H
Brochantite	-13.64	1.78	15.42	Cu4(SO4)(OH)6
Brucite	-13.49	2.79	16.28	Mg(OH)2
Ca	-123.53	16.30	139.83	Ca
Ca(g)	-148.77	16.30	165.07	Ca
Ca2Al2O5:8H2O	-41.30	18.27	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-31.26	-4.97	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-21.80	-3.99	17.80	Ca3(AsO4)2
Ca3Al2O6	-91.12	21.92	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-104.49	35.99	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-81.70	25.56	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-78.12	25.56	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-66.01	2.32	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-32.28	14.63	46.91	CaAl2O4
CaAl2O4:10H2O	-23.37	14.63	37.99	CaAl2O4:10H2O

CaAl4O7	-42.98	25.61	68.59	CaAl4O7
Carnallite	-19.54	-15.27	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.57	-5.10	-3.54	CaSO4:0.5H2O
Chalcanthite	-3.49	-6.12	-2.63	CuSO4:5H2O
Chalcocyanite	-9.03	-6.12	2.91	CuSO4
Chloromagnesite	-31.28	-9.47	21.82	MgCl2
Cl2(g)	-27.91	-24.92	2.99	Cl2
Claudetite	-30.88	-50.68	-19.80	As2O3
Corundum	-7.31	10.98	18.29	Al2O3
Cu	-16.21	15.29	31.50	Cu
Cu(g)	-68.37	15.29	83.66	Cu
CuCl2	-13.35	-9.63	3.72	CuCl2
Cuprite	-17.69	-19.60	-1.91	Cu2O
Delafossite	1.85	-4.59	-6.44	CuFeO2
Diaspore	-1.66	5.49	7.15	AlHO2
Epsomite	-3.99	-5.95	-1.96	MgSO4:7H2O
Ettringite	-55.86	6.60	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-43.30	15.72	59.02	Fe
Fe(OH)2	-10.83	3.06	13.89	Fe(OH)2
Fe(OH)3	-0.43	5.21	5.64	Fe(OH)3
Fe2(SO4)3	-18.86	-15.82	3.05	Fe2(SO4)3
FeO	-10.46	3.06	13.52	FeO
Ferrite-Ca	-7.42	14.07	21.50	CaFe2O4
Ferrite-Cu	2.78	13.06	10.28	CuFe2O4
Ferrite-Dicalcium	-39.08	17.72	56.80	Ca2Fe2O5
Ferrite-Mg	-7.80	13.22	21.02	MgFe2O4
Ferrite-Zn	1.05	12.75	11.70	ZnFe2O4
FeSO4	-8.29	-5.69	2.61	FeSO4
Gibbsite	-2.25	5.49	7.74	Al(OH)3
Glauberite	-7.90	-13.37	-5.47	Na2Ca(SO4)2
Goethite	4.68	5.21	0.53	FeOOH
Gypsum	-0.57	-5.10	-4.53	CaSO4:2H2O
H2(g)	-30.34	-33.44	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.45	-5.89	1.56	NaCl
Hausmannite	-23.59	-13.45	10.14	Mn3O4
HCl(g)	-12.43	-6.13	6.30	HCl
Hematite	10.35	10.43	0.08	Fe2O3
Hercynite	-14.76	14.04	28.80	FeAl2O4
Hexahydrite	-4.23	-5.95	-1.73	MgSO4:6H2O
Hydrophilite	-20.36	-8.62	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	7.88	-1.53	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	3.84	-1.61	-5.45	NaFe3(SO4)2(OH)6
K	-64.32	6.65	70.98	K
K(g)	-74.93	6.65	81.58	K
K2O	-83.39	0.65	84.04	K2O
K3H(SO4)2	-12.90	-16.52	-3.62	K3H(SO4)2
Kainite	-11.45	-11.76	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-14.95	-11.68	3.27	KAl(SO4)2
Katoite	-57.03	21.91	78.94	Ca3Al2H12O12
Kieserite	-5.69	-5.95	-0.27	MgSO4:H2O
KMgCl3	-36.52	-15.27	21.25	KMgCl3
KMgCl3:2H2O	-29.23	-15.27	13.96	KMgCl3:2H2O
Lammerite	-8.58	-7.03	1.55	Cu3(AsO4)2
Lawrencite	-18.25	-9.20	9.05	FeCl2
Leonite	-9.94	-14.05	-4.11	K2Mg(SO4)2:4H2O
Lime	-28.92	3.64	32.57	CaO
Magnetite	3.07	13.49	10.42	Fe3O4
Manganite	-7.79	-7.95	-0.16	MnO(OH)
Manganosite	-15.46	2.45	17.92	MnO
Mayenite	-373.54	120.61	494.15	Ca12Al14O33
Melanterite	-3.29	-5.69	-2.40	FeSO4:7H2O
Mercallite	-6.99	-8.42	-1.44	KHSO4
Mg	-107.07	15.45	122.52	Mg
Mg(g)	-126.79	15.45	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.45	-5.25	5.20	Mg1.25SO4(OH)0.5:0.5H2O

Mg1.5SO4(OH)	-13.77	-4.56	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.20	-9.47	12.73	MgCl2:2H2O
MgCl2:4H2O	-16.77	-9.47	7.30	MgCl2:4H2O
MgCl2:H2O	-25.54	-9.47	16.07	MgCl2:H2O
MgOHCl	-19.23	-3.34	15.89	MgOHCl
MgSO4	-10.78	-5.95	4.83	MgSO4
Mirabilite	-7.11	-8.27	-1.15	Na2SO4:10H2O
Misenite	-47.57	-58.64	-11.08	K8H6(SO4)7
Mn	-67.82	15.11	82.93	Mn
Mn(OH)2(am)	-12.85	2.45	15.31	Mn(OH)2
Mn(OH)3	-14.29	-7.95	6.34	Mn(OH)3
MnCl2:2H2O	-13.80	-9.81	4.00	MnCl2:2H2O
MnCl2:4H2O	-12.56	-9.81	2.75	MnCl2:4H2O
MnCl2:H2O	-15.35	-9.81	5.54	MnCl2:H2O
MnO2(gamma)	-10.30	-26.43	-16.13	MnO2
MnSO4	-8.90	-6.29	2.61	MnSO4
Molysite	-26.65	-13.18	13.47	FeCl3
Na	-60.80	6.57	67.37	Na
Na(g)	-74.29	6.57	80.86	Na
Na2O	-66.93	0.48	67.42	Na2O
Na3H(SO4)2	-15.88	-16.77	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-15.74	-21.63	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-14.43	5.46	19.88	NaFeO2
Nantokite	-9.16	-15.93	-6.77	CuCl
O2(g)	-22.42	-25.32	-2.89	O2
Oxychloride-Mg	-26.37	-0.54	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.57	-5.95	-1.39	MgSO4:5H2O
Periclase	-18.53	2.79	21.33	MgO
Picromerite	-9.61	-14.05	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-9.95	-24.26	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-18.90	3.64	22.55	Ca(OH)2
Pyrolusite	-8.77	-26.43	-17.66	MnO2
Scacchite	-18.55	-9.81	8.74	MnCl2
Spinel	-23.83	13.78	37.61	Al2MgO4
Starkeyite	-4.95	-5.95	-1.00	MgSO4:4H2O
Sylvite	-6.63	-5.81	0.83	KCl
Syngenite	-5.60	-13.20	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-44.69	-27.55	17.14	Mg2CaCl6:12H2O
Tenorite	-5.01	2.63	7.65	CuO
Thenardite	-7.91	-8.26	-0.36	Na2SO4
Todorokite	-57.19	-103.02	-45.82	Mn7O12:3H2O
Wustite	-9.27	3.13	12.40	Fe.9470
Zincite	-8.87	2.33	11.20	ZnO
Zn	-53.80	14.98	68.79	Zn
Zn(ClO4)2:6H2O	-148.28	-142.65	5.63	Zn(ClO4)2:6H2O
Zn(g)	-70.42	14.98	85.41	Zn
Zn(OH)2(beta)	-9.61	2.33	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-9.33	2.33	11.66	Zn(OH)2
Zn(OH)2(gamma)	-9.56	2.33	11.88	Zn(OH)2
Zn2(OH)3Cl	-16.77	-1.48	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-11.68	-4.09	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-17.26	-7.95	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-29.61	-10.52	19.09	Zn3O(SO4)2
ZnCl2	-17.01	-9.93	7.08	ZnCl2
ZnSO4	-9.95	-6.42	3.53	ZnSO4
ZnSO4:6H2O	-4.72	-6.42	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-4.54	-6.42	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-5.87	-6.42	-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
Tachyhydrite	-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 4
3.000e+000 Solution 3 AS2

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

Elements	Molality	Moles
Al	2.376e-004	9.504e-004
As	1.824e-005	7.297e-005
C	1.894e-003	7.575e-003
Ca	5.727e-003	2.291e-002
Cl	1.471e-002	5.885e-002
Cu	1.383e-004	5.533e-004
Fe	7.632e-004	3.053e-003
K	1.226e-003	4.904e-003
Mg	6.273e-004	2.509e-003
Mn	9.546e-005	3.819e-004
Na	1.320e-002	5.282e-002
S	6.182e-003	2.473e-002
Zn	9.468e-005	3.787e-004

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

pH = 5.505 Charge balance
 pe = 8.036 Adjusted to redox equilibrium
 Activity of water = 0.999
 Ionic strength = 3.661e-002
 Mass of water (kg) = 4.000e+000
 Total alkalinity (eq/kg) = 9.166e-004
 Total CO2 (mol/kg) = 1.894e-003
 Temperature (deg C) = 25.000
 Electrical balance (eq) = 6.379e-003
 Percent error, $100 \cdot (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$ = 3.12
 Iterations = 12
 Total H = 4.442120e+002
 Total O = 2.222238e+002

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	3.594e-006	3.123e-006	-5.444	-5.505	-0.061
OH-	3.695e-009	3.082e-009	-8.432	-8.511	-0.079
H2O	5.553e+001	9.993e-001	1.744	-0.000	0.000
Al	2.376e-004				
Al13O4(OH)24+7	1.790e-005	5.937e-009	-4.747	-8.226	-3.479
AlOH+2	1.857e-006	9.230e-007	-5.731	-6.035	-0.304
Al+3	9.367e-007	2.575e-007	-6.028	-6.589	-0.561
Al(OH)2+	8.181e-007	6.857e-007	-6.087	-6.164	-0.077
AlSO4+	7.383e-007	6.188e-007	-6.132	-6.208	-0.077
HALO2	3.195e-007	3.195e-007	-6.496	-6.496	0.000
Al(SO4)2-	1.346e-007	1.128e-007	-6.871	-6.948	-0.077
ALO2-	4.181e-008	3.504e-008	-7.379	-7.455	-0.077
Al2(OH)2+4	2.010e-009	1.385e-010	-8.697	-9.858	-1.162
Al3(OH)4+5	1.402e-010	2.357e-012	-9.853	-11.628	-1.774
NaAlO2	7.270e-011	7.270e-011	-10.138	-10.138	0.000
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-101.900	-101.900	0.000
As(3)	3.703e-016				
HAsO2	1.976e-016	1.976e-016	-15.704	-15.704	0.000
As(OH)3	1.726e-016	1.726e-016	-15.763	-15.763	0.000
H2AsO3-	4.033e-020	3.380e-020	-19.394	-19.471	-0.077
AsO2-	3.858e-020	3.234e-020	-19.414	-19.490	-0.077
AsO2OH-2	2.165e-025	1.057e-025	-24.665	-24.976	-0.311
HAsS2	0.000e+000	0.000e+000	-171.022	-171.022	0.000
As(5)	1.824e-005				
H2AsO4-	1.671e-005	1.401e-005	-4.777	-4.854	-0.077
HAsO4-2	1.524e-006	7.444e-007	-5.817	-6.128	-0.311
H3AsO4	7.706e-009	7.706e-009	-8.113	-8.113	0.000
AsO4-3	3.079e-012	6.114e-013	-11.512	-12.214	-0.702
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-177.247	-177.247	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-135.443	-135.443	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-89.592	-89.592	0.000
C(2)	1.209e-035				
CO	1.209e-035	1.209e-035	-34.918	-34.918	0.000
C(4)	1.894e-003				
CO2	1.595e-003	1.610e-003	-2.797	-2.793	0.004
HCO3-	2.649e-004	2.220e-004	-3.577	-3.654	-0.077
FeHCO3+	1.913e-005	1.604e-005	-4.718	-4.795	-0.077
CaHCO3+	7.931e-006	6.647e-006	-5.101	-5.177	-0.077
NaHCO3	3.454e-006	3.454e-006	-5.462	-5.462	0.000
CuCO3	1.635e-006	1.635e-006	-5.787	-5.787	0.000
MgHCO3+	7.856e-007	6.584e-007	-6.105	-6.181	-0.077

ZnHCO3+	2.647e-007	2.218e-007	-6.577	-6.654	-0.077
MnHCO3+	7.611e-008	6.379e-008	-7.119	-7.195	-0.077
FeCO3+	3.117e-008	2.612e-008	-7.506	-7.583	-0.077
FeCO3	2.464e-008	2.464e-008	-7.608	-7.608	0.000
CaCO3	1.847e-008	1.847e-008	-7.734	-7.734	0.000
CO3-2	6.344e-009	3.154e-009	-8.198	-8.501	-0.304
MnCO3	4.166e-009	4.166e-009	-8.380	-8.380	0.000
ZnCO3	1.026e-009	1.026e-009	-8.989	-8.989	0.000
MgCO3	8.518e-010	8.518e-010	-9.070	-9.070	0.000
NaCO3-	1.432e-010	1.200e-010	-9.844	-9.921	-0.077
Cu(CO3)2-2	1.881e-011	9.185e-012	-10.726	-11.037	-0.311
CuCO3(OH)2-2	2.913e-015	1.423e-015	-14.536	-14.847	-0.311
Ca	5.727e-003				
Ca+2	4.844e-003	2.527e-003	-2.315	-2.597	-0.283
CaSO4	8.667e-004	8.667e-004	-3.062	-3.062	0.000
CaHCO3+	7.931e-006	6.647e-006	-5.101	-5.177	-0.077
CaCl+	7.783e-006	6.523e-006	-5.109	-5.186	-0.077
CaCl2	9.346e-008	9.346e-008	-7.029	-7.029	0.000
CaCO3	1.847e-008	1.847e-008	-7.734	-7.734	0.000
CaOH+	1.362e-010	1.142e-010	-9.866	-9.942	-0.077
Cl(-1)	1.471e-002				
Cl-	1.467e-002	1.218e-002	-1.833	-1.914	-0.081
NaCl	2.328e-005	2.328e-005	-4.633	-4.633	0.000
CaCl+	7.783e-006	6.523e-006	-5.109	-5.186	-0.077
MgCl+	2.897e-006	2.428e-006	-5.538	-5.615	-0.077
CuCl+	2.161e-006	1.811e-006	-5.665	-5.742	-0.077
FeCl+	1.457e-006	1.221e-006	-5.836	-5.913	-0.077
MnCl+	1.168e-006	9.788e-007	-5.933	-6.009	-0.077
ZnCl+	9.464e-007	7.933e-007	-6.024	-6.101	-0.077
KCl	4.086e-007	4.086e-007	-6.389	-6.389	0.000
CaCl2	9.346e-008	9.346e-008	-7.029	-7.029	0.000
CuCl2	1.162e-008	1.162e-008	-7.935	-7.935	0.000
ZnCl2	1.129e-008	1.129e-008	-7.947	-7.947	0.000
HCl	8.545e-009	8.545e-009	-8.068	-8.068	0.000
Zn(OH)Cl	4.339e-009	4.339e-009	-8.363	-8.363	0.000
CuCl2-	3.211e-009	2.691e-009	-8.493	-8.570	-0.077
CuCl3-2	4.311e-010	2.106e-010	-9.365	-9.677	-0.311
ZnCl3-	9.059e-011	7.593e-011	-10.043	-10.120	-0.077
FeCl2	7.984e-011	7.984e-011	-10.098	-10.098	0.000
MnCl3-	3.785e-011	3.173e-011	-10.422	-10.499	-0.077
FeCl2+	3.425e-011	2.871e-011	-10.465	-10.542	-0.077
ZnCl4-2	1.435e-011	7.011e-012	-10.843	-11.154	-0.311
FeCl+2	5.856e-012	2.911e-012	-11.232	-11.536	-0.304
FeCl4-2	7.009e-014	3.423e-014	-13.154	-13.466	-0.311
CuCl4-2	6.624e-017	3.235e-017	-16.179	-16.490	-0.311
FeCl4-	6.110e-018	5.121e-018	-17.214	-17.291	-0.077
Cl(1)	1.343e-031				
HClO	1.330e-031	1.330e-031	-30.876	-30.876	0.000
ClO-	1.370e-033	1.148e-033	-32.863	-32.940	-0.077
Cl(3)	0.000e+000				
ClO2-	0.000e+000	0.000e+000	-56.784	-56.860	-0.077
HClO2	0.000e+000	0.000e+000	-59.196	-59.196	0.000
Cl(5)	0.000e+000				
ClO3-	0.000e+000	0.000e+000	-66.850	-66.928	-0.079
Cl(7)	0.000e+000				
ClO4-	0.000e+000	0.000e+000	-81.220	-81.298	-0.079
ZnClO4+	0.000e+000	0.000e+000	-84.356	-84.433	-0.077
Cu(1)	3.969e-009				
CuCl2-	3.211e-009	2.691e-009	-8.493	-8.570	-0.077
CuCl3-2	4.311e-010	2.106e-010	-9.365	-9.677	-0.311
Cu+	3.266e-010	2.738e-010	-9.486	-9.563	-0.077
Cu(2)	1.383e-004				
Cu+2	1.042e-004	5.435e-005	-3.982	-4.265	-0.283
CuSO4	2.924e-005	2.924e-005	-4.534	-4.534	0.000
CuCl+	2.161e-006	1.811e-006	-5.665	-5.742	-0.077
CuCO3	1.635e-006	1.635e-006	-5.787	-5.787	0.000
CuOH+	1.070e-006	8.970e-007	-5.971	-6.047	-0.077

CuCl ₂	1.162e-008	1.162e-008	-7.935	-7.935	0.000
Cu(CO ₃) ₂₋₂	1.881e-011	9.185e-012	-10.726	-11.037	-0.311
CuCO ₃ (OH) ₂₋₂	2.913e-015	1.423e-015	-14.536	-14.847	-0.311
CuCl ₄₋₂	6.624e-017	3.235e-017	-16.179	-16.490	-0.311
CuO ₂₋₂	4.146e-022	2.025e-022	-21.382	-21.694	-0.311
Fe(2)	3.357e-004				
Fe+2	2.639e-004	1.376e-004	-3.579	-3.861	-0.283
FeSO ₄	5.123e-005	5.123e-005	-4.290	-4.290	0.000
FeHCO ₃ +	1.913e-005	1.604e-005	-4.718	-4.795	-0.077
FeCl+	1.457e-006	1.221e-006	-5.836	-5.913	-0.077
FeCO ₃	2.464e-008	2.464e-008	-7.608	-7.608	0.000
FeOH+	1.661e-008	1.393e-008	-7.780	-7.856	-0.077
FeCl ₂	7.984e-011	7.984e-011	-10.098	-10.098	0.000
FeCl ₄₋₂	7.009e-014	3.423e-014	-13.154	-13.466	-0.311
Fe(OH) ₂	3.539e-014	3.539e-014	-13.451	-13.451	0.000
Fe(OH) ₃₋	5.378e-019	4.508e-019	-18.269	-18.346	-0.077
Fe(OH) ₄₋₂	2.953e-028	1.442e-028	-27.530	-27.841	-0.311
Fe(3)	4.275e-004				
Fe(OH) ₂₊	3.745e-004	3.139e-004	-3.427	-3.503	-0.077
Fe(OH) ₃	4.697e-005	4.697e-005	-4.328	-4.328	0.000
FeOH+2	5.960e-006	2.963e-006	-5.225	-5.528	-0.304
FeCO ₃ +	3.117e-008	2.612e-008	-7.506	-7.583	-0.077
Fe+3	5.217e-009	1.434e-009	-8.283	-8.843	-0.561
Fe(OH) ₄₋	4.504e-009	3.775e-009	-8.346	-8.423	-0.077
Fe ₂ (OH) ₂₊₄	3.428e-009	2.363e-010	-8.465	-9.627	-1.162
Fe ₃ (OH) ₄₊₅	9.218e-010	1.549e-011	-9.035	-10.810	-1.774
FeSO ₄ +	3.888e-010	3.259e-010	-9.410	-9.487	-0.077
FeCl ₂ +	3.425e-011	2.871e-011	-10.465	-10.542	-0.077
Fe(SO ₄) ₂₋	1.544e-011	1.294e-011	-10.811	-10.888	-0.077
FeCl+2	5.856e-012	2.911e-012	-11.232	-11.536	-0.304
FeCl ₄₋	6.110e-018	5.121e-018	-17.214	-17.291	-0.077
H(0)	1.299e-030				
H ₂	6.496e-031	6.553e-031	-30.187	-30.184	0.004
K	1.226e-003				
K+	1.203e-003	9.988e-004	-2.920	-3.001	-0.081
KSO ₄₋	2.259e-005	1.893e-005	-4.646	-4.723	-0.077
KCl	4.086e-007	4.086e-007	-6.389	-6.389	0.000
KHSO ₄	5.217e-011	5.217e-011	-10.283	-10.283	0.000
KOH	1.108e-012	1.108e-012	-11.955	-11.955	0.000
Mg	6.273e-004				
Mg+2	4.635e-004	2.554e-004	-3.334	-3.593	-0.259
MgSO ₄	1.601e-004	1.601e-004	-3.796	-3.796	0.000
MgCl+	2.897e-006	2.428e-006	-5.538	-5.615	-0.077
MgHCO ₃ +	7.856e-007	6.584e-007	-6.105	-6.181	-0.077
MgCO ₃	8.518e-010	8.518e-010	-9.070	-9.070	0.000
Mg ₄ (OH) ₄₊₄	1.150e-031	7.922e-033	-30.939	-32.101	-1.162
Mn(2)	9.546e-005				
Mn+2	7.235e-005	3.774e-005	-4.141	-4.423	-0.283
MnSO ₄	2.187e-005	2.187e-005	-4.660	-4.660	0.000
MnCl+	1.168e-006	9.788e-007	-5.933	-6.009	-0.077
MnHCO ₃ +	7.611e-008	6.379e-008	-7.119	-7.195	-0.077
MnCO ₃	4.166e-009	4.166e-009	-8.380	-8.380	0.000
MnOH+	3.703e-010	3.103e-010	-9.431	-9.508	-0.077
MnCl ₃₋	3.785e-011	3.173e-011	-10.422	-10.499	-0.077
Mn ₂ OH+3	5.849e-014	1.255e-014	-13.233	-13.901	-0.668
Mn(OH) ₂	2.437e-016	2.437e-016	-15.613	-15.613	0.000
Mn ₂ (OH) ₃₊	7.005e-017	5.871e-017	-16.155	-16.231	-0.077
Mn(OH) ₃₋	8.727e-023	7.314e-023	-22.059	-22.136	-0.077
Mn(OH) ₄₋₂	4.057e-031	1.982e-031	-30.392	-30.703	-0.311
Mn(3)	5.099e-022				
Mn+3	5.099e-022	1.094e-022	-21.293	-21.961	-0.668
Mn(6)	0.000e+000				
MnO ₄₋₂	0.000e+000	0.000e+000	-46.372	-46.684	-0.311
Mn(7)	0.000e+000				
MnO ₄₋	0.000e+000	0.000e+000	-47.925	-48.004	-0.079
Na	1.320e-002				
Na+	1.298e-002	1.088e-002	-1.887	-1.964	-0.077

NaSO4-	2.013e-004	1.687e-004	-3.696	-3.773	-0.077
NaCl	2.328e-005	2.328e-005	-4.633	-4.633	0.000
NaHCO3	3.454e-006	3.454e-006	-5.462	-5.462	0.000
NaCO3-	1.432e-010	1.200e-010	-9.844	-9.921	-0.077
NaAlO2	7.270e-011	7.270e-011	-10.138	-10.138	0.000
NaOH	5.784e-012	5.784e-012	-11.238	-11.238	0.000
O(0)	2.935e-032				
O2	1.468e-032	1.481e-032	-31.833	-31.830	0.004
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-81.254	-81.254	0.000
HS-	0.000e+000	0.000e+000	-82.679	-82.758	-0.079
S-2	0.000e+000	0.000e+000	-89.882	-90.179	-0.296
S2-2	0.000e+000	0.000e+000	-147.862	-148.173	-0.311
HAsS2	0.000e+000	0.000e+000	-171.022	-171.022	0.000
S3-2	0.000e+000	0.000e+000	-205.898	-206.209	-0.311
S4-2	0.000e+000	0.000e+000	-264.160	-264.472	-0.311
S5-2	0.000e+000	0.000e+000	-322.640	-322.951	-0.311
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-85.772	-86.084	-0.311
HS2O3-	0.000e+000	0.000e+000	-90.498	-90.575	-0.077
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-86.630	-86.927	-0.296
S(4)	3.050e-032				
HSO3-	2.955e-032	2.477e-032	-31.529	-31.606	-0.077
SO3-2	9.359e-034	4.652e-034	-33.029	-33.332	-0.304
H2SO3	7.415e-036	7.415e-036	-35.130	-35.130	0.000
SO2	5.891e-036	5.891e-036	-35.230	-35.230	0.000
S2O6-2	0.000e+000	0.000e+000	-51.412	-51.723	-0.311
S3O6-2	0.000e+000	0.000e+000	-111.930	-112.241	-0.311
S4O6-2	0.000e+000	0.000e+000	-156.543	-156.854	-0.311
S5O6-2	0.000e+000	0.000e+000	-230.035	-230.346	-0.311
S(5)	0.000e+000				
S2O5-2	0.000e+000	0.000e+000	-67.731	-68.042	-0.311
S(6)	6.182e-003				
SO4-2	4.808e-003	2.348e-003	-2.318	-2.629	-0.311
CaSO4	8.667e-004	8.667e-004	-3.062	-3.062	0.000
NaSO4-	2.013e-004	1.687e-004	-3.696	-3.773	-0.077
MgSO4	1.601e-004	1.601e-004	-3.796	-3.796	0.000
FeSO4	5.123e-005	5.123e-005	-4.290	-4.290	0.000
CuSO4	2.924e-005	2.924e-005	-4.534	-4.534	0.000
KSO4-	2.259e-005	1.893e-005	-4.646	-4.723	-0.077
MnSO4	2.187e-005	2.187e-005	-4.660	-4.660	0.000
ZnSO4	1.913e-005	1.913e-005	-4.718	-4.718	0.000
HSO4-	8.839e-007	7.409e-007	-6.054	-6.130	-0.077
AlSO4+	7.383e-007	6.188e-007	-6.132	-6.208	-0.077
Al(SO4)2-	1.346e-007	1.128e-007	-6.871	-6.948	-0.077
FeSO4+	3.888e-010	3.259e-010	-9.410	-9.487	-0.077
KHSO4	5.217e-011	5.217e-011	-10.283	-10.283	0.000
Fe(SO4)2-	1.544e-011	1.294e-011	-10.811	-10.888	-0.077
H2SO4	2.183e-015	2.183e-015	-14.661	-14.661	0.000
S(7)	0.000e+000				
S2O8-2	0.000e+000	0.000e+000	-54.328	-54.639	-0.311
S(8)	0.000e+000				
HSO5-	0.000e+000	0.000e+000	-41.233	-41.310	-0.077
Zn	9.468e-005				
Zn+2	7.431e-005	3.876e-005	-4.129	-4.412	-0.283
ZnSO4	1.913e-005	1.913e-005	-4.718	-4.718	0.000
ZnCl+	9.464e-007	7.933e-007	-6.024	-6.101	-0.077
ZnHCO3+	2.647e-007	2.218e-007	-6.577	-6.654	-0.077
ZnOH+	1.623e-008	1.360e-008	-7.790	-7.866	-0.077
ZnCl2	1.129e-008	1.129e-008	-7.947	-7.947	0.000
Zn(OH)Cl	4.339e-009	4.339e-009	-8.363	-8.363	0.000
ZnCO3	1.026e-009	1.026e-009	-8.989	-8.989	0.000
ZnCl3-	9.059e-011	7.593e-011	-10.043	-10.120	-0.077
Zn(OH)2	1.863e-011	1.863e-011	-10.730	-10.730	0.000
ZnCl4-2	1.435e-011	7.011e-012	-10.843	-11.154	-0.311
Zn(OH)3-	2.205e-017	1.848e-017	-16.657	-16.733	-0.077

Zn(OH)4-2	2.064e-024	1.008e-024	-23.685	-23.997	-0.311
ZnClO4+	0.000e+000	0.000e+000	-84.356	-84.433	-0.077

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

Phase	SI	log IAP	log KT	
Al	-116.11	33.80	149.91	Al
Al(g)	-166.82	33.80	200.62	Al
Al2(SO4)3	-39.96	-21.07	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-22.62	-21.07	1.56	Al2(SO4)3:6H2O
Alabandite	-81.26	-81.68	-0.42	MnS
Alum-K	-9.88	-14.85	-4.97	KAl(SO4)2:12H2O
Alunite	5.47	5.00	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.88	-5.23	-4.35	CaSO4
Antarcticite	-10.52	-6.43	4.09	CaCl2:6H2O
Antlerite	-2.13	6.60	8.73	Cu3(SO4)(OH)4
Aphthitalite	-12.34	-16.22	-3.89	NaK3(SO4)2
Aragonite	-2.72	-0.75	1.97	CaCO3
Arcanite	-6.79	-8.63	-1.84	K2SO4
Arsenolite	-30.11	-49.95	-19.84	As2O3
Arsenopyrite	-130.11	-144.55	-14.45	FeAsS
Artinite	-13.95	5.68	19.63	Mg2CO3(OH)2:3H2O
As	-43.79	-1.10	42.68	As
As2O5	-22.85	-20.72	2.14	As2O5
As4O6(cubi)	-60.08	-99.90	-39.82	As4O6
As4O6(mono)	-59.85	-99.90	-40.05	As4O6
Atacamite	-2.12	12.14	14.26	Cu4Cl2(OH)6
Azurite	-7.20	1.92	9.12	Cu3(CO3)2(OH)2
Bassanite	-1.52	-5.23	-3.71	CaSO4:0.5H2O
Birnessite	-54.60	-140.15	-85.55	Mn8O14:5H2O
Bischofite	-11.82	-7.42	4.39	MgCl2:6H2O
Bixbyite	-9.93	-10.89	-0.96	Mn2O3
Bloedite	-10.30	-12.78	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	2.38	9.93	7.55	AlO2H
Bornite	-252.85	-355.39	-102.53	Cu5FeS4
Brochantite	-2.08	13.34	15.42	Cu4(SO4)(OH)6
Brucite	-8.87	7.42	16.28	Mg(OH)2
Burkeite	-24.67	-15.19	9.49	Na6CO3(SO4)2
C	-41.48	22.67	64.15	C
C(g)	-159.09	22.67	181.77	C
Ca	-115.50	24.33	139.83	Ca
Ca(g)	-140.74	24.33	165.07	Ca
Ca2Al2O5:8H2O	-22.89	36.68	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-24.30	1.99	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-13.28	4.52	17.80	Ca3(AsO4)2
Ca3Al2O6	-67.94	45.09	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-71.63	68.85	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-53.75	53.50	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-50.18	53.50	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-49.52	18.81	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-18.64	28.27	46.91	CaAl2O4
CaAl2O4:10H2O	-9.73	28.26	37.99	CaAl2O4:10H2O
CaAl4O7	-20.47	48.12	68.59	CaAl4O7
Calcite	-2.57	-0.75	1.82	CaCO3
Carnallite	-16.61	-12.34	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.69	-5.23	-3.54	CaSO4:0.5H2O
CH4(g)	-86.75	-89.59	-2.84	CH4
Chalcanthite	-4.27	-6.90	-2.63	CuSO4:5H2O
Chalcocite	-61.63	-96.38	-34.74	Cu2S
Chalcocyanite	-9.81	-6.89	2.91	CuSO4
Chalcopyrite	-130.03	-162.63	-32.60	CuFeS2
Chloromagnesite	-29.24	-7.42	21.82	MgCl2
Cl2(g)	-33.75	-30.75	2.99	Cl2
Claudetite	-30.16	-49.95	-19.80	As2O3
CO(g)	-31.92	-34.92	-3.00	CO
CO2(g)	-1.33	-9.16	-7.83	CO2

Corundum	1.56	19.85	18.29	Al ₂ O ₃
Covellite	-58.66	-81.52	-22.86	CuS
Cu	-8.84	22.66	31.50	Cu
Cu(g)	-61.00	22.66	83.66	Cu
CuCl ₂	-11.81	-8.09	3.72	CuCl ₂
Cuprite	-6.21	-8.11	-1.91	Cu ₂ O
Dawsonite	-0.03	4.31	4.34	NaAlCO ₃ (OH) ₂
Delafoosite	10.05	3.61	-6.44	CuFeO ₂
Diaspore	2.78	9.93	7.15	AlHO ₂
Dolomite	-4.96	-2.49	2.47	CaMg(CO ₃) ₂
Dolomite-dis	-6.50	-2.49	4.01	CaMg(CO ₃) ₂
Dolomite-ord	-4.95	-2.49	2.46	CaMg(CO ₃) ₂
Epsomite	-4.26	-6.22	-1.96	MgSO ₄ ·7H ₂ O
Ettringite	-33.06	29.40	62.46	Ca ₆ Al ₂ (SO ₄) ₃ (OH) ₁₂ ·26H ₂ O
Fe	-35.95	23.06	59.02	Fe
Fe(OH) ₂	-6.75	7.15	13.89	Fe(OH) ₂
Fe(OH) ₃	2.03	7.67	5.64	Fe(OH) ₃
Fe ₂ (SO ₄) ₃	-28.62	-25.57	3.05	Fe ₂ (SO ₄) ₃
FeO	-6.37	7.15	13.52	FeO
Ferrite-Ca	2.26	23.76	21.50	CaFe ₂ O ₄
Ferrite-Cu	11.81	22.09	10.28	CuFe ₂ O ₄
Ferrite-Dicalcium	-24.63	32.17	56.80	Ca ₂ Fe ₂ O ₅
Ferrite-Mg	1.74	22.76	21.02	MgFe ₂ O ₄
Ferrite-Zn	10.24	21.94	11.70	ZnFe ₂ O ₄
FeSO ₄	-9.10	-6.49	2.61	FeSO ₄
Gaylussite	-13.99	-2.82	11.16	CaNa ₂ (CO ₃) ₂ ·5H ₂ O
Gibbsite	2.19	9.93	7.74	Al(OH) ₃
Glauberite	-6.31	-11.78	-5.47	Na ₂ Ca(SO ₄) ₂
Goethite	7.14	7.67	0.53	FeOOH
Gypsum	-0.70	-5.23	-4.53	CaSO ₄ ·2H ₂ O
H ₂ (g)	-27.08	-30.18	-3.10	H ₂
H ₂ O(g)	-1.59	-0.00	1.59	H ₂ O
H ₂ S(g)	-80.27	-88.26	-7.99	H ₂ S
Halite	-5.44	-3.88	1.56	NaCl
Hausmannite	-14.45	-4.30	10.14	Mn ₃ O ₄
HCl(g)	-13.72	-7.42	6.30	HCl
Hematite	15.27	15.34	0.08	Fe ₂ O ₃
Hercynite	-1.80	27.00	28.80	FeAl ₂ O ₄
Hexahydrite	-4.50	-6.22	-1.73	MgSO ₄ ·6H ₂ O
Huntite	-16.19	-5.97	10.22	CaMg ₃ (CO ₃) ₄
Hydromagnesite	-30.29	0.45	30.74	Mg ₅ (CO ₃) ₄ (OH) ₂ ·4H ₂ O
Hydrophilite	-18.17	-6.43	11.75	CaCl ₂
Hydrozincite	-15.63	14.68	30.31	Zn ₅ (OH) ₆ (CO ₃) ₂
Ice	-0.14	-0.00	0.14	H ₂ O
Jarosite	7.65	-1.76	-9.41	KFe ₃ (SO ₄) ₂ (OH) ₆
Jarosite-Na	4.73	-0.72	-5.45	NaFe ₃ (SO ₄) ₂ (OH) ₆
K	-60.51	10.46	70.98	K
K(g)	-71.12	10.46	81.58	K
K ₂ CO ₃ ·1.5H ₂ O	-17.53	-4.15	13.38	K ₂ CO ₃ ·1.5H ₂ O
K ₂ O	-79.03	5.01	84.04	K ₂ O
K ₃ H(SO ₄) ₂	-16.14	-19.77	-3.62	K ₃ H(SO ₄) ₂
K ₈ H ₄ (CO ₃) ₆ ·3H ₂ O	-62.63	-34.92	27.71	K ₈ H ₄ (CO ₃) ₆ ·3H ₂ O
Kainite	-10.83	-11.14	-0.31	KMgClSO ₄ ·3H ₂ O
KAl(SO ₄) ₂	-18.12	-14.85	3.27	KAl(SO ₄) ₂
Kalinite	-6.94	-6.65	0.28	KHCO ₃
Katoite	-33.85	45.09	78.94	Ca ₃ Al ₂ H ₁₂ O ₁₂
Kieserite	-5.96	-6.22	-0.27	MgSO ₄ ·H ₂ O
KMgCl ₃	-33.58	-12.34	21.25	KMgCl ₃
KMgCl ₃ ·2H ₂ O	-26.30	-12.34	13.96	KMgCl ₃ ·2H ₂ O
KNaCO ₃ ·6H ₂ O	-13.37	-3.11	10.26	KNaCO ₃ ·6H ₂ O
Lammerite	-2.03	-0.48	1.55	Cu ₃ (AsO ₄) ₂
Lansfordite	-6.58	-1.74	4.84	MgCO ₃ ·5H ₂ O
Lawrencite	-16.74	-7.69	9.05	FeCl ₂
Leonite	-10.74	-14.85	-4.11	K ₂ Mg(SO ₄) ₂ ·4H ₂ O
Lime	-24.16	8.41	32.57	CaO
Magnesite	-4.01	-1.74	2.27	MgCO ₃
Magnetite	12.08	22.49	10.42	Fe ₃ O ₄

Malachite	-1.57	4.33	5.90	Cu ₂ CO ₃ (OH) ₂
Manganite	-5.28	-5.45	-0.16	MnO(OH)
Manganosite	-11.33	6.59	17.92	MnO
Mayenite	-254.22	239.93	494.15	Ca ₁₂ Al ₁₄ O ₃₃
Melanterite	-4.09	-6.49	-2.40	FeSO ₄ ·7H ₂ O
Mercallite	-9.70	-11.14	-1.44	KHSO ₄
Mg	-99.19	23.33	122.52	Mg
Mg(g)	-118.91	23.33	142.25	Mg
Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O	-9.56	-4.37	5.20	Mg _{1.25} SO ₄ (OH)0.5:0.5H ₂ O
Mg _{1.5} SO ₄ (OH)	-11.72	-2.51	9.21	Mg _{1.5} SO ₄ (OH)
MgCl ₂ :2H ₂ O	-20.15	-7.42	12.73	MgCl ₂ :2H ₂ O
MgCl ₂ :4H ₂ O	-14.72	-7.42	7.30	MgCl ₂ :4H ₂ O
MgCl ₂ :H ₂ O	-23.49	-7.42	16.07	MgCl ₂ :H ₂ O
MgOHCl	-15.89	-0.00	15.89	MgOHCl
MgSO ₄	-11.05	-6.22	4.83	MgSO ₄
Mirabilite	-5.41	-6.56	-1.15	Na ₂ SO ₄ :10H ₂ O
Misenite	-64.37	-75.44	-11.08	K ₈ H ₆ (SO ₄) ₇
Mn	-60.43	22.50	82.93	Mn
Mn(OH) ₂ (am)	-8.72	6.59	15.31	Mn(OH) ₂
Mn(OH) ₃	-11.79	-5.45	6.34	Mn(OH) ₃
MnCl ₂ :2H ₂ O	-12.25	-8.25	4.00	MnCl ₂ :2H ₂ O
MnCl ₂ :4H ₂ O	-11.00	-8.25	2.75	MnCl ₂ :4H ₂ O
MnCl ₂ :H ₂ O	-13.79	-8.25	5.54	MnCl ₂ :H ₂ O
MnO ₂ (gamma)	-9.43	-25.55	-16.13	MnO ₂
MnSO ₄	-9.66	-7.05	2.61	MnSO ₄
Molysite	-28.06	-14.59	13.47	FeCl ₃
Monohydrocalcite	-3.42	-0.75	2.68	CaCO ₃ :H ₂ O
Na	-55.87	11.50	67.37	Na
Na(g)	-69.36	11.50	80.86	Na
Na ₂ CO ₃	-13.24	-2.08	11.16	Na ₂ CO ₃
Na ₂ CO ₃ :7H ₂ O	-12.02	-2.08	9.94	Na ₂ CO ₃ :7H ₂ O
Na ₂ O	-60.33	7.08	67.42	Na ₂ O
Na ₃ H(SO ₄) ₂	-15.76	-16.65	-0.89	Na ₃ H(SO ₄) ₂
Na ₄ Ca(SO ₄) ₃ :2H ₂ O	-12.45	-18.34	-5.89	Na ₄ Ca(SO ₄) ₃ :2H ₂ O
NaFeO ₂	-8.67	11.21	19.88	NaFeO ₂
Nahcolite	-5.48	-5.62	-0.14	NaHCO ₃
Nantokite	-4.71	-11.48	-6.77	CuCl
Natron	-11.67	-2.08	9.59	Na ₂ CO ₃ :10H ₂ O
Nesquehonite	-7.03	-1.74	5.29	MgCO ₃ :3H ₂ O
O ₂ (g)	-28.94	-31.83	-2.89	O ₂
Orpiment	-235.26	-314.74	-79.49	As ₂ S ₃
Oxychloride-Mg	-18.42	7.41	25.83	Mg ₂ Cl(OH) ₃ :4H ₂ O
Pentahydrite	-4.84	-6.22	-1.39	MgSO ₄ :5H ₂ O
Periclase	-13.91	7.42	21.33	MgO
Picromerite	-10.41	-14.85	-4.44	K ₂ Mg(SO ₄) ₂ :6H ₂ O
Pirssonite	-14.14	-2.82	11.32	Na ₂ Ca(CO ₃) ₂ :2H ₂ O
Polyhalite	-10.99	-25.31	-14.31	K ₂ MgCa ₂ (SO ₄) ₄ :2H ₂ O
Portlandite	-14.13	8.41	22.55	Ca(OH) ₂
Pyrite	-126.02	-150.72	-24.70	FeS ₂
Pyrolusite	-7.89	-25.55	-17.66	MnO ₂
Pyrrhotite	-77.38	-81.11	-3.74	FeS
Realgar	-90.59	-150.87	-60.28	AsS
Rhodochrosite	-2.35	-2.57	-0.22	MnCO ₃
S	-59.07	-104.18	-45.11	S
S ₂ (g)	-132.03	-139.21	-7.19	S ₂
Scacchite	-16.99	-8.25	8.74	MnCl ₂
Siderite	-1.79	-2.01	-0.22	FeCO ₃
Smithsonite	-3.00	-2.56	0.44	ZnCO ₃
SO ₂ (g)	-35.41	-35.23	0.18	SO ₂
Sphalerite	-70.19	-81.66	-11.47	ZnS
Spinel	-10.33	27.27	37.61	Al ₂ MgO ₄
Starkeyite	-5.22	-6.22	-1.00	MgSO ₄ :4H ₂ O
Sylvite	-5.74	-4.91	0.83	KCl
Syngenite	-6.26	-13.86	-7.60	K ₂ Ca(SO ₄) ₂ :H ₂ O
Tachyhydrite	-38.42	-21.27	17.14	Mg ₂ CaCl ₆ :12H ₂ O
Tenorite	-0.90	6.75	7.65	CuO
Thenardite	-6.20	-6.56	-0.36	Na ₂ SO ₄

Thermonatrite	-13.01	-2.08	10.94	Na2CO3:H2O
Todorokite	-44.54	-90.37	-45.82	Mn7O12:3H2O
Troilite	-77.27	-81.11	-3.84	FeS
Trona-K	-21.36	-9.77	11.59	K2NaH(CO3)2:2H2O
Wurtzite	-72.50	-81.66	-9.17	ZnS
Wustite	-5.58	6.83	12.40	Fe.9470
Zincite	-4.60	6.60	11.20	ZnO
Zn	-46.27	22.51	68.79	Zn
Zn(ClO4)2:6H2O	-172.64	-167.01	5.63	Zn(ClO4)2:6H2O
Zn(g)	-62.89	22.51	85.41	Zn
Zn(OH)2(beta)	-5.33	6.60	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-5.06	6.60	11.66	Zn(OH)2
Zn(OH)2(gamma)	-5.28	6.60	11.88	Zn(OH)2
Zn2(OH)3Cl	-9.51	5.78	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-8.02	-0.44	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-10.23	-0.92	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-26.57	-7.48	19.09	Zn3O(SO4)2
ZnCl2	-15.32	-8.24	7.08	ZnCl2
ZnCO3:H2O	-2.70	-2.56	0.14	ZnCO3:H2O
ZnSO4	-10.57	-7.04	3.53	ZnSO4
ZnSO4:6H2O	-5.34	-7.04	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.17	-7.04	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.49	-7.04	-0.55	ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
