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

```

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

```

Beginning of initial solution calculations.

Initial solution 1. Flujo 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.947O
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 4. AS3

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Beginning of batch-reaction calculations.

Reaction step 1.

Using mix 4.

Mixture 4.

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

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

Elements	Molality	Moles
Al	2.376e-004	9.504e-004
As	1.768e-005	7.072e-005
C	1.426e-003	5.703e-003
Ca	2.884e-003	1.154e-002
Cl	8.435e-004	3.374e-003
Cu	1.397e-004	5.587e-004
Fe	7.632e-004	3.053e-003
K	5.022e-004	2.009e-003
Mg	7.032e-004	2.813e-003
Mn	9.638e-005	3.855e-004
Na	1.766e-003	7.062e-003
S	4.740e-003	1.896e-002
Zn	6.888e-005	2.755e-004

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

pH	=	5.277	Charge balance
pe	=	8.455	Adjusted to redox equilibrium
Activity of water	=	1.000	
Ionic strength	=	1.682e-002	
Mass of water (kg)	=	4.000e+000	
Total alkalinity (eq/kg)	=	7.128e-004	
Total CO2 (mol/kg)	=	1.426e-003	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	3.241e-003	
Percent error, 100*(Cat- An)/(Cat+ An)	=	4.42	
Iterations	=	11	
Total H	=	4.442111e+002	
Total O	=	2.221961e+002	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	5.897e-006	5.289e-006	-5.229	-5.277	-0.047
OH-	2.077e-009	1.821e-009	-8.683	-8.740	-0.057
H2O	5.553e+001	9.998e-001	1.744	-0.000	0.000
Al	2.376e-004				
Al13O4(OH)24+7	1.737e-005	4.497e-008	-4.760	-7.347	-2.587
AlOH+2	3.880e-006	2.328e-006	-5.411	-5.633	-0.222

Al+3	2.963e-006	1.099e-006	-5.528	-5.959	-0.431
AlSO4+	2.945e-006	2.589e-006	-5.531	-5.587	-0.056
Al(OH)2+	1.162e-006	1.022e-006	-5.935	-5.991	-0.056
Al(SO4)2-	5.263e-007	4.627e-007	-6.279	-6.335	-0.056
HALO2	2.811e-007	2.811e-007	-6.551	-6.551	0.000
ALO2-	2.071e-008	1.821e-008	-7.684	-7.740	-0.056
Al2(OH)2+4	6.365e-009	8.810e-010	-8.196	-9.055	-0.859
Al3(OH)4+5	4.661e-010	2.234e-011	-9.331	-10.651	-1.320
NaAlO2	5.308e-012	5.308e-012	-11.275	-11.275	0.000
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-103.164	-103.164	0.000
As(3)	2.772e-016				
HAsO2	1.479e-016	1.479e-016	-15.830	-15.830	0.000
As(OH)3	1.293e-016	1.293e-016	-15.888	-15.888	0.000
H2AsO3-	1.700e-020	1.495e-020	-19.769	-19.825	-0.056
AsO2-	1.626e-020	1.429e-020	-19.789	-19.845	-0.056
AsO2OH-2	4.646e-026	2.761e-026	-25.333	-25.559	-0.226
HAsS2	0.000e+000	0.000e+000	-173.287	-173.287	0.000
As(5)	1.768e-005				
H2AsO4-	1.688e-005	1.484e-005	-4.773	-4.829	-0.056
HAsO4-2	7.837e-007	4.658e-007	-6.106	-6.332	-0.226
H3AsO4	1.383e-008	1.383e-008	-7.859	-7.859	0.000
AsO4-3	7.297e-013	2.259e-013	-12.137	-12.646	-0.509
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-179.711	-179.711	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-138.286	-138.286	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-91.203	-91.203	0.000
C(2)	4.065e-036				
CO	4.065e-036	4.065e-036	-35.391	-35.391	0.000
C(4)	1.426e-003				
CO2	1.292e-003	1.297e-003	-2.889	-2.887	0.002
HCO3-	1.202e-004	1.057e-004	-3.920	-3.976	-0.056
FeHCO3+	1.032e-005	9.073e-006	-4.986	-5.042	-0.056
CaHCO3+	2.095e-006	1.841e-006	-5.679	-5.735	-0.056
CuCO3	5.435e-007	5.435e-007	-6.265	-6.265	0.000
MgHCO3+	4.482e-007	3.940e-007	-6.349	-6.405	-0.056
NaHCO3	2.311e-007	2.311e-007	-6.636	-6.636	0.000
ZnHCO3+	1.011e-007	8.884e-008	-6.995	-7.051	-0.056
MnHCO3+	4.020e-008	3.534e-008	-7.396	-7.452	-0.056
FeCO3+	2.602e-008	2.287e-008	-7.585	-7.641	-0.056
FeCO3	8.233e-009	8.233e-009	-8.084	-8.084	0.000
CaCO3	3.021e-009	3.021e-009	-8.520	-8.520	0.000
CO3-2	1.478e-009	8.865e-010	-8.830	-9.052	-0.222
MnCO3	1.363e-009	1.363e-009	-8.866	-8.866	0.000
MgCO3	3.010e-010	3.010e-010	-9.521	-9.521	0.000
ZnCO3	2.428e-010	2.428e-010	-9.615	-9.615	0.000
NaCO3-	5.393e-012	4.741e-012	-11.268	-11.324	-0.056
Cu(CO3)2-2	1.444e-012	8.583e-013	-11.840	-12.066	-0.226
CuCO3(OH)2-2	2.777e-016	1.651e-016	-15.556	-15.782	-0.226
Ca	2.884e-003				
Ca+2	2.387e-003	1.470e-003	-2.622	-2.833	-0.211
CaSO4	4.944e-004	4.944e-004	-3.306	-3.306	0.000
CaHCO3+	2.095e-006	1.841e-006	-5.679	-5.735	-0.056
CaCl+	2.612e-007	2.296e-007	-6.583	-6.639	-0.056
CaCO3	3.021e-009	3.021e-009	-8.520	-8.520	0.000
CaCl2	1.991e-010	1.991e-010	-9.701	-9.701	0.000
CaOH+	4.465e-011	3.925e-011	-10.350	-10.406	-0.056
Cl(-1)	8.435e-004				
Cl-	8.425e-004	7.370e-004	-3.074	-3.133	-0.058
CaCl+	2.612e-007	2.296e-007	-6.583	-6.639	-0.056
MgCl+	2.101e-007	1.847e-007	-6.678	-6.734	-0.056
NaCl	1.980e-007	1.980e-007	-6.703	-6.703	0.000
CuCl+	1.474e-007	1.296e-007	-6.832	-6.888	-0.056
FeCl+	9.990e-008	8.782e-008	-7.000	-7.056	-0.056
MnCl+	7.839e-008	6.891e-008	-7.106	-7.162	-0.056

ZnCl+	4.593e-008	4.037e-008	-7.338	-7.394	-0.056
KCl	1.067e-008	1.067e-008	-7.972	-7.972	0.000
HCl	8.755e-010	8.755e-010	-9.058	-9.058	0.000
CaCl2	1.991e-010	1.991e-010	-9.701	-9.701	0.000
Zn(OH)Cl	1.305e-010	1.305e-010	-9.884	-9.884	0.000
CuCl2	5.028e-011	5.028e-011	-10.299	-10.299	0.000
ZnCl2	3.476e-011	3.476e-011	-10.459	-10.459	0.000
CuCl2-	5.056e-012	4.445e-012	-11.296	-11.352	-0.056
FeCl+2	9.143e-013	5.485e-013	-12.039	-12.261	-0.222
FeCl2+	3.723e-013	3.273e-013	-12.429	-12.485	-0.056
FeCl2	3.473e-013	3.473e-013	-12.459	-12.459	0.000
CuCl3-2	3.539e-014	2.104e-014	-13.451	-13.677	-0.226
ZnCl3-	1.609e-014	1.415e-014	-13.793	-13.849	-0.056
MnCl3-	9.301e-015	8.176e-015	-14.031	-14.087	-0.056
ZnCl4-2	1.329e-016	7.902e-017	-15.876	-16.102	-0.226
FeCl4-2	9.170e-019	5.451e-019	-18.038	-18.264	-0.226
CuCl4-2	8.622e-022	5.125e-022	-21.064	-21.290	-0.226
FeCl4-	2.431e-022	2.137e-022	-21.614	-21.670	-0.056
Cl(1)	3.283e-032				
HClO	3.264e-032	3.264e-032	-31.486	-31.486	0.000
ClO-	1.893e-034	1.664e-034	-33.723	-33.779	-0.056
Cl(3)	0.000e+000				
ClO2-	0.000e+000	0.000e+000	-57.264	-57.320	-0.056
HClO2	0.000e+000	0.000e+000	-59.426	-59.426	0.000
Cl(5)	0.000e+000				
ClO3-	0.000e+000	0.000e+000	-66.951	-67.008	-0.057
Cl(7)	0.000e+000				
ClO4-	0.000e+000	0.000e+000	-80.942	-80.999	-0.057
ZnClO4+	0.000e+000	0.000e+000	-84.153	-84.208	-0.056
Cu(1)	1.456e-010				
Cu+	1.405e-010	1.235e-010	-9.852	-9.908	-0.056
CuCl2-	5.056e-012	4.445e-012	-11.296	-11.352	-0.056
CuCl3-2	3.539e-014	2.104e-014	-13.451	-13.677	-0.226
Cu(2)	1.397e-004				
Cu+2	1.044e-004	6.427e-005	-3.981	-4.192	-0.211
CuSO4	3.389e-005	3.389e-005	-4.470	-4.470	0.000
CuOH+	7.128e-007	6.266e-007	-6.147	-6.203	-0.056
CuCO3	5.435e-007	5.435e-007	-6.265	-6.265	0.000
CuCl+	1.474e-007	1.296e-007	-6.832	-6.888	-0.056
CuCl2	5.028e-011	5.028e-011	-10.299	-10.299	0.000
Cu(CO3)2-2	1.444e-012	8.583e-013	-11.840	-12.066	-0.226
CuCO3(OH)2-2	2.777e-016	1.651e-016	-15.556	-15.782	-0.226
CuCl4-2	8.622e-022	5.125e-022	-21.064	-21.290	-0.226
CuO2-2	4.903e-023	2.914e-023	-22.310	-22.535	-0.226
Fe(2)	3.357e-004				
Fe+2	2.656e-004	1.636e-004	-3.576	-3.786	-0.211
FeSO4	5.968e-005	5.968e-005	-4.224	-4.224	0.000
FeHCO3+	1.032e-005	9.073e-006	-4.986	-5.042	-0.056
FeCl+	9.990e-008	8.782e-008	-7.000	-7.056	-0.056
FeOH+	1.112e-008	9.778e-009	-7.954	-8.010	-0.056
FeCO3	8.233e-009	8.233e-009	-8.084	-8.084	0.000
FeCl2	3.473e-013	3.473e-013	-12.459	-12.459	0.000
Fe(OH)2	1.468e-014	1.468e-014	-13.833	-13.833	0.000
FeCl4-2	9.170e-019	5.451e-019	-18.038	-18.264	-0.226
Fe(OH)3-	1.257e-019	1.105e-019	-18.901	-18.957	-0.056
Fe(OH)4-2	3.513e-029	2.088e-029	-28.454	-28.680	-0.226
Fe(3)	4.275e-004				
Fe(OH)2+	3.882e-004	3.412e-004	-3.411	-3.467	-0.056
Fe(OH)3	3.017e-005	3.017e-005	-4.520	-4.520	0.000
FeOH+2	9.087e-006	5.452e-006	-5.042	-5.263	-0.222
FeCO3+	2.602e-008	2.287e-008	-7.585	-7.641	-0.056
Fe+3	1.204e-008	4.467e-009	-7.919	-8.350	-0.431
Fe2(OH)2+4	5.780e-009	8.000e-010	-8.238	-9.097	-0.859
Fe(OH)4-	1.629e-009	1.432e-009	-8.788	-8.844	-0.056
Fe3(OH)4+5	1.190e-009	5.703e-011	-8.924	-10.244	-1.320
FeSO4+	1.132e-009	9.949e-010	-8.946	-9.002	-0.056
Fe(SO4)2-	4.404e-011	3.872e-011	-10.356	-10.412	-0.056

FeCl+2	9.143e-013	5.485e-013	-12.039	-12.261	-0.222
FeCl2+	3.723e-013	3.273e-013	-12.429	-12.485	-0.056
FeCl4-	2.431e-022	2.137e-022	-21.614	-21.670	-0.056
H(0)	5.451e-031				
H2	2.725e-031	2.736e-031	-30.565	-30.563	0.002
K	5.022e-004				
K+	4.930e-004	4.313e-004	-3.307	-3.365	-0.058
KSO4-	9.116e-006	8.014e-006	-5.040	-5.096	-0.056
KCl	1.067e-008	1.067e-008	-7.972	-7.972	0.000
KHSO4	3.740e-011	3.740e-011	-10.427	-10.427	0.000
KOH	2.827e-013	2.827e-013	-12.549	-12.549	0.000
Mg	7.032e-004				
Mg+2	5.053e-004	3.209e-004	-3.296	-3.494	-0.197
MgSO4	1.973e-004	1.973e-004	-3.705	-3.705	0.000
MgHCO3+	4.482e-007	3.940e-007	-6.349	-6.405	-0.056
MgCl+	2.101e-007	1.847e-007	-6.678	-6.734	-0.056
MgCO3	3.010e-010	3.010e-010	-9.521	-9.521	0.000
Mg4(OH)4+4	1.740e-032	2.409e-033	-31.759	-32.618	-0.859
Mn(2)	9.638e-005				
Mn+2	7.131e-005	4.392e-005	-4.147	-4.357	-0.211
MnSO4	2.494e-005	2.494e-005	-4.603	-4.603	0.000
MnCl+	7.839e-008	6.891e-008	-7.106	-7.162	-0.056
MnHCO3+	4.020e-008	3.534e-008	-7.396	-7.452	-0.056
MnCO3	1.363e-009	1.363e-009	-8.866	-8.866	0.000
MnOH+	2.427e-010	2.134e-010	-9.615	-9.671	-0.056
Mn2OH+3	3.112e-014	1.004e-014	-13.507	-13.998	-0.491
MnCl3-	9.301e-015	8.176e-015	-14.031	-14.087	-0.056
Mn(OH)2	9.900e-017	9.900e-017	-16.004	-16.004	0.000
Mn2(OH)3+	1.865e-017	1.640e-017	-16.729	-16.785	-0.056
Mn(OH)3-	1.997e-023	1.755e-023	-22.700	-22.756	-0.056
Mn(OH)4-2	4.727e-032	2.810e-032	-31.325	-31.551	-0.226
Mn(3)	1.034e-021				
Mn+3	1.034e-021	3.336e-022	-20.985	-21.477	-0.491
Mn(6)	0.000e+000				
MnO4-2	0.000e+000	0.000e+000	-46.548	-46.774	-0.226
Mn(7)	0.000e+000				
MnO4-	0.000e+000	0.000e+000	-47.618	-47.675	-0.057
Na	1.766e-003				
Na+	1.739e-003	1.528e-003	-2.760	-2.816	-0.056
NaSO4-	2.644e-005	2.325e-005	-4.578	-4.634	-0.056
NaHCO3	2.311e-007	2.311e-007	-6.636	-6.636	0.000
NaCl	1.980e-007	1.980e-007	-6.703	-6.703	0.000
NaCO3-	5.393e-012	4.741e-012	-11.268	-11.324	-0.056
NaAlO2	5.308e-012	5.308e-012	-11.275	-11.275	0.000
NaOH	4.802e-013	4.802e-013	-12.319	-12.319	0.000
O(0)	1.693e-031				
O2	8.466e-032	8.500e-032	-31.072	-31.071	0.002
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-82.323	-82.323	0.000
HS-	0.000e+000	0.000e+000	-83.999	-84.056	-0.057
S-2	0.000e+000	0.000e+000	-91.487	-91.705	-0.218
S2-2	0.000e+000	0.000e+000	-150.164	-150.390	-0.226
HAsS2	0.000e+000	0.000e+000	-173.287	-173.287	0.000
S3-2	0.000e+000	0.000e+000	-208.889	-209.115	-0.226
S4-2	0.000e+000	0.000e+000	-267.842	-268.068	-0.226
S5-2	0.000e+000	0.000e+000	-327.011	-327.237	-0.226
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-86.936	-87.162	-0.226
HS2O3-	0.000e+000	0.000e+000	-91.368	-91.424	-0.056
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-87.407	-87.625	-0.218
S(4)	1.985e-032				
HSO3-	1.952e-032	1.716e-032	-31.710	-31.765	-0.056
SO3-2	3.173e-034	1.903e-034	-33.499	-33.720	-0.222
H2SO3	8.700e-036	8.700e-036	-35.060	-35.060	0.000
SO2	6.908e-036	6.908e-036	-35.161	-35.161	0.000
S2O6-2	0.000e+000	0.000e+000	-51.436	-51.662	-0.226

S306-2	0.000e+000	0.000e+000	-112.645	-112.871	-0.226
S406-2	0.000e+000	0.000e+000	-157.947	-158.173	-0.226
S506-2	0.000e+000	0.000e+000	-232.129	-232.355	-0.226
S(5)	0.000e+000				
S205-2	0.000e+000	0.000e+000	-68.135	-68.361	-0.226
S(6)	4.740e-003				
SO4-2	3.873e-003	2.302e-003	-2.412	-2.638	-0.226
CaSO4	4.944e-004	4.944e-004	-3.306	-3.306	0.000
MgSO4	1.973e-004	1.973e-004	-3.705	-3.705	0.000
FeSO4	5.968e-005	5.968e-005	-4.224	-4.224	0.000
CuSO4	3.389e-005	3.389e-005	-4.470	-4.470	0.000
NaSO4-	2.644e-005	2.325e-005	-4.578	-4.634	-0.056
MnSO4	2.494e-005	2.494e-005	-4.603	-4.603	0.000
ZnSO4	1.577e-005	1.577e-005	-4.802	-4.802	0.000
KSO4-	9.116e-006	8.014e-006	-5.040	-5.096	-0.056
AlSO4+	2.945e-006	2.589e-006	-5.531	-5.587	-0.056
HSO4-	1.399e-006	1.230e-006	-5.854	-5.910	-0.056
Al(SO4)2-	5.263e-007	4.627e-007	-6.279	-6.335	-0.056
FeSO4+	1.132e-009	9.949e-010	-8.946	-9.002	-0.056
Fe(SO4)2-	4.404e-011	3.872e-011	-10.356	-10.412	-0.056
KHSO4	3.740e-011	3.740e-011	-10.427	-10.427	0.000
H2SO4	6.137e-015	6.137e-015	-14.212	-14.212	0.000
S(7)	0.000e+000				
S208-2	0.000e+000	0.000e+000	-53.593	-53.819	-0.226
S(8)	0.000e+000				
HSO5-	0.000e+000	0.000e+000	-40.654	-40.710	-0.056
Zn	6.888e-005				
Zn+2	5.295e-005	3.261e-005	-4.276	-4.487	-0.211
ZnSO4	1.577e-005	1.577e-005	-4.802	-4.802	0.000
ZnHCO3+	1.011e-007	8.884e-008	-6.995	-7.051	-0.056
ZnCl+	4.593e-008	4.037e-008	-7.338	-7.394	-0.056
ZnOH+	7.689e-009	6.759e-009	-8.114	-8.170	-0.056
ZnCO3	2.428e-010	2.428e-010	-9.615	-9.615	0.000
Zn(OH)Cl	1.305e-010	1.305e-010	-9.884	-9.884	0.000
ZnCl2	3.476e-011	3.476e-011	-10.459	-10.459	0.000
Zn(OH)2	5.472e-012	5.472e-012	-11.262	-11.262	0.000
ZnCl3-	1.609e-014	1.415e-014	-13.793	-13.849	-0.056
ZnCl4-2	1.329e-016	7.902e-017	-15.876	-16.102	-0.226
Zn(OH)3-	3.647e-018	3.206e-018	-17.438	-17.494	-0.056
Zn(OH)4-2	1.738e-025	1.033e-025	-24.760	-24.986	-0.226
ZnClO4+	0.000e+000	0.000e+000	-84.153	-84.208	-0.056

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

Phase	SI	log IAP	log KT	
Al	-116.74	33.17	149.91	Al
Al(g)	-167.44	33.17	200.62	Al
Al2(SO4)3	-38.73	-19.83	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-21.39	-19.83	1.56	Al2(SO4)3:6H2O
Alabandite	-82.72	-83.14	-0.42	MnS
Alum-K	-9.63	-14.60	-4.97	KAl(SO4)2:12H2O
Alunite	5.61	5.14	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.12	-5.47	-4.35	CaSO4
Antarcticite	-13.19	-9.10	4.09	CaCl2:6H2O
Antlerite	-2.84	5.89	8.73	Cu3(SO4)(OH)4
Aphthitalite	-14.30	-18.19	-3.89	NaK3(SO4)2
Aragonite	-3.50	-1.53	1.97	CaCO3
Arcanite	-7.52	-9.37	-1.84	K2SO4
Arsenolite	-30.36	-50.20	-19.84	As2O3
Arsenopyrite	-132.25	-146.70	-14.45	FeAsS
Artinite	-14.76	4.87	19.63	Mg2CO3(OH)2:3H2O
As	-44.48	-1.80	42.68	As
As2O5	-22.35	-20.21	2.14	As2O5
As4O6(cubi)	-60.58	-100.41	-39.82	As4O6
As4O6(mono)	-60.36	-100.41	-40.05	As4O6
Atacamite	-5.64	8.63	14.26	Cu4Cl2(OH)6

Azurite	-8.54	0.58	9.12	$\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$
Bassanite	-1.76	-5.47	-3.71	$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$
Birnessite	-55.46	-141.00	-85.55	$\text{Mn}_8\text{O}_{14} \cdot 5\text{H}_2\text{O}$
Bischofite	-14.15	-9.76	4.39	$\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$
Bixbyite	-10.33	-11.29	-0.96	Mn_2O_3
Bloedite	-11.92	-14.40	-2.48	$\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$
Boehmite	2.32	9.87	7.55	AlO_2H
Bornite	-260.20	-362.73	-102.53	Cu_5FeS_4
Brochantite	-3.17	12.25	15.42	$\text{Cu}_4(\text{SO}_4)(\text{OH})_6$
Brucite	-9.22	7.06	16.28	$\text{Mg}(\text{OH})_2$
Burkeite	-30.36	-20.87	9.49	$\text{Na}_6\text{CO}_3(\text{SO}_4)_2$
C	-42.33	21.82	64.15	C
C(g)	-159.95	21.82	181.77	C
Ca	-116.58	23.26	139.83	Ca
Ca(g)	-141.82	23.26	165.07	Ca
$\text{Ca}_2\text{Al}_2\text{O}_5 \cdot 8\text{H}_2\text{O}$	-24.39	35.18	59.57	$\text{Ca}_2\text{Al}_2\text{O}_5 \cdot 8\text{H}_2\text{O}$
$\text{Ca}_2\text{Cl}_2(\text{OH})_2 \cdot \text{H}_2\text{O}$	-27.67	-1.38	26.29	$\text{Ca}_2\text{Cl}_2(\text{OH})_2 \cdot \text{H}_2\text{O}$
$\text{Ca}_3(\text{AsO}_4)_2$	-14.85	2.95	17.80	$\text{Ca}_3(\text{AsO}_4)_2$
$\text{Ca}_3\text{Al}_2\text{O}_6$	-70.13	42.90	113.03	$\text{Ca}_3\text{Al}_2\text{O}_6$
$\text{Ca}_4\text{Al}_2\text{Fe}_2\text{O}_{10}$	-74.90	65.58	140.48	$\text{Ca}_4\text{Al}_2\text{Fe}_2\text{O}_{10}$
$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 13\text{H}_2\text{O}$	-56.63	50.62	107.25	$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 13\text{H}_2\text{O}$
$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 19\text{H}_2\text{O}$	-53.06	50.62	103.68	$\text{Ca}_4\text{Al}_2\text{O}_7 \cdot 19\text{H}_2\text{O}$
$\text{Ca}_4\text{Cl}_2(\text{OH})_6 \cdot 13\text{H}_2\text{O}$	-54.27	14.06	68.33	$\text{Ca}_4\text{Cl}_2(\text{OH})_6 \cdot 13\text{H}_2\text{O}$
CaAl_2O_4	-19.45	27.46	46.91	CaAl_2O_4
$\text{CaAl}_2\text{O}_4 \cdot 10\text{H}_2\text{O}$	-10.53	27.46	37.99	$\text{CaAl}_2\text{O}_4 \cdot 10\text{H}_2\text{O}$
CaAl_4O_7	-21.39	47.20	68.59	CaAl_4O_7
Calcite	-3.36	-1.53	1.82	CaCO_3
Carnallite	-20.53	-16.26	4.27	$\text{KMgCl}_3 \cdot 6\text{H}_2\text{O}$
$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}(\text{beta})$	-1.94	-5.47	-3.54	$\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$
$\text{CH}_4(\text{g})$	-88.36	-91.20	-2.84	CH_4
Chalcanthite	-4.20	-6.83	-2.63	$\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$
Chalcocite	-63.85	-98.60	-34.74	Cu_2S
Chalcocyanite	-9.74	-6.83	2.91	CuSO_4
Chalcopyrite	-132.93	-165.54	-32.60	CuFeS_2
Chloromagnesite	-31.57	-9.76	21.82	MgCl_2
$\text{Cl}_2(\text{g})$	-35.35	-32.35	2.99	Cl_2
Claudetite	-30.41	-50.20	-19.80	As_2O_3
$\text{CO}(\text{g})$	-32.39	-35.39	-3.00	CO
$\text{CO}_2(\text{g})$	-1.42	-9.25	-7.83	CO_2
Corundum	1.45	19.74	18.29	Al_2O_3
Covellite	-60.11	-82.97	-22.86	CuS
Cu	-9.60	21.90	31.50	Cu
$\text{Cu}(\text{g})$	-61.76	21.90	83.66	Cu
CuCl_2	-14.18	-10.46	3.72	CuCl_2
Cuprite	-7.36	-9.26	-1.91	Cu_2O
Dawsonite	-1.26	3.08	4.34	$\text{NaAlCO}_3(\text{OH})_2$
Delafossite	9.28	2.85	-6.44	CuFeO_2
Diaspore	2.72	9.87	7.15	AlHO_2
Dolomite	-6.20	-3.72	2.47	$\text{CaMg}(\text{CO}_3)_2$
Dolomite-dis	-7.74	-3.72	4.01	$\text{CaMg}(\text{CO}_3)_2$
Dolomite-ord	-6.19	-3.72	2.46	$\text{CaMg}(\text{CO}_3)_2$
Epsomite	-4.17	-6.13	-1.96	$\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$
Ettringite	-35.98	26.49	62.46	$\text{Ca}_6\text{Al}_2(\text{SO}_4)_3(\text{OH})_{12} \cdot 26\text{H}_2\text{O}$
Fe	-36.72	22.30	59.02	Fe
$\text{Fe}(\text{OH})_2$	-7.13	6.77	13.89	$\text{Fe}(\text{OH})_2$
$\text{Fe}(\text{OH})_3$	1.84	7.48	5.64	$\text{Fe}(\text{OH})_3$
$\text{Fe}_2(\text{SO}_4)_3$	-27.66	-24.61	3.05	$\text{Fe}_2(\text{SO}_4)_3$
FeO	-6.76	6.77	13.52	FeO
Ferrite-Ca	1.18	22.68	21.50	CaFe_2O_4
Ferrite-Cu	11.04	21.32	10.28	CuFe_2O_4
Ferrite-Dicalcium	-26.40	30.40	56.80	$\text{Ca}_2\text{Fe}_2\text{O}_5$
Ferrite-Mg	1.00	22.02	21.02	MgFe_2O_4
Ferrite-Zn	9.33	21.03	11.70	ZnFe_2O_4
FeSO_4	-9.03	-6.42	2.61	FeSO_4
Gaylussite	-17.03	-5.86	11.16	$\text{CaNa}_2(\text{CO}_3)_2 \cdot 5\text{H}_2\text{O}$
Gibbsite	2.13	9.87	7.74	$\text{Al}(\text{OH})_3$
Glauberite	-8.27	-13.74	-5.47	$\text{Na}_2\text{Ca}(\text{SO}_4)_2$

Goethite	6.95	7.48	0.53	FeOOH
Gypsum	-0.94	-5.47	-4.53	CaSO4:2H2O
H2(g)	-27.46	-30.56	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-81.34	-89.33	-7.99	H2S
Halite	-7.51	-5.95	1.56	NaCl
Hausmannite	-15.24	-5.10	10.14	Mn3O4
HCl(g)	-14.71	-8.41	6.30	HCl
Hematite	14.88	14.96	0.08	Fe2O3
Hercynite	-2.29	26.51	28.80	FeAl2O4
Hexahydrite	-4.41	-6.13	-1.73	MgSO4:6H2O
Huntite	-18.33	-8.11	10.22	CaMg3(CO3)4
Hydromagnesite	-32.45	-1.71	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-20.84	-9.10	11.75	CaCl2
Hydrozincite	-18.48	11.83	30.31	Zn5(OH)6(CO3)2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	7.38	-2.03	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	3.97	-1.48	-5.45	NaFe3(SO4)2(OH)6
K	-61.30	9.68	70.98	K
K(g)	-71.90	9.68	81.58	K
K2CO3:1.5H2O	-18.81	-5.43	13.38	K2CO3:1.5H2O
K2O	-80.21	3.82	84.04	K2O
K3H(SO4)2	-17.02	-20.65	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-67.93	-40.22	27.71	K8H4(CO3)6:3H2O
Kainite	-12.32	-12.63	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-17.87	-14.60	3.27	KAl(SO4)2
Kaliginite	-7.62	-7.34	0.28	KHCO3
Katoite	-36.04	42.90	78.94	Ca3Al2H12O12
Kieserite	-5.86	-6.13	-0.27	MgSO4:H2O
KMgCl3	-37.50	-16.26	21.25	KMgCl3
KMgCl3:2H2O	-30.22	-16.26	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-15.14	-4.88	10.26	KNaCO3:6H2O
Lammerite	-2.68	-1.13	1.55	Cu3(AsO4)2
Lansfordite	-7.03	-2.19	4.84	MgCO3:5H2O
Lawrencite	-19.11	-10.05	9.05	FeCl2
Leonite	-11.39	-15.50	-4.11	K2Mg(SO4)2:4H2O
Lime	-24.85	7.72	32.57	CaO
Magnesite	-4.47	-2.19	2.27	MgCO3
Magnetite	11.31	21.73	10.42	Fe3O4
Malachite	-2.43	3.47	5.90	Cu2CO3(OH)2
Manganite	-5.48	-5.65	-0.16	MnO(OH)
Manganosite	-11.72	6.20	17.92	MnO
Mayenite	-263.31	230.84	494.15	Ca12Al14O33
Melanterite	-4.03	-6.42	-2.40	FeSO4:7H2O
Mercallite	-9.84	-11.28	-1.44	KHSO4
Mg	-99.93	22.59	122.52	Mg
Mg(g)	-119.65	22.59	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-9.56	-4.37	5.20	Mg1.25SO4(OH)0.5:0.5H2O
Mg1.5SO4(OH)	-11.81	-2.60	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.49	-9.76	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.06	-9.76	7.30	MgCl2:4H2O
MgCl2:H2O	-25.83	-9.76	16.07	MgCl2:H2O
MgOHCl	-17.24	-1.35	15.89	MgOHCl
MgSO4	-10.96	-6.13	4.83	MgSO4
Mirabilite	-7.12	-8.27	-1.15	Na2SO4:10H2O
Misenite	-65.97	-77.05	-11.08	K8H6(SO4)7
Mn	-61.20	21.73	82.93	Mn
Mn(OH)2(am)	-9.11	6.20	15.31	Mn(OH)2
Mn(OH)3	-11.99	-5.65	6.34	Mn(OH)3
MnCl2:2H2O	-14.62	-10.62	4.00	MnCl2:2H2O
MnCl2:4H2O	-13.37	-10.62	2.75	MnCl2:4H2O
MnCl2:H2O	-16.16	-10.62	5.54	MnCl2:H2O
MnO2(gamma)	-9.44	-25.57	-16.13	MnO2
MnSO4	-9.60	-7.00	2.61	MnSO4
Molysite	-31.22	-17.75	13.47	FeCl3
Monohydrocalcite	-4.21	-1.53	2.68	CaCO3:H2O
Na	-57.14	10.23	67.37	Na

Na(g)	-70.63	10.23	80.86	Na
Na2CO3	-15.49	-4.33	11.16	Na2CO3
Na2CO3:7H2O	-14.27	-4.33	9.94	Na2CO3:7H2O
Na2O	-62.50	4.92	67.42	Na2O
Na3H(SO4)2	-18.11	-19.00	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-16.12	-22.01	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-9.94	9.94	19.88	NaFeO2
Nahcolite	-6.65	-6.79	-0.14	NaHCO3
Nantokite	-6.28	-13.04	-6.77	CuCl
Natron	-13.92	-4.33	9.59	Na2CO3:10H2O
Nesquehonite	-7.48	-2.19	5.29	MgCO3:3H2O
O2(g)	-28.18	-31.07	-2.89	O2
Orpiment	-238.72	-318.20	-79.49	As2S3
Oxychloride-Mg	-20.12	5.71	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.74	-6.13	-1.39	MgSO4:5H2O
Periclase	-14.27	7.06	21.33	MgO
Picromerite	-11.06	-15.50	-4.44	K2Mg(SO4)2:6H2O
Pirssonite	-17.19	-5.86	11.32	Na2Ca(CO3)2:2H2O
Polyhalite	-12.13	-26.44	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-14.83	7.72	22.55	Ca(OH)2
Pyrite	-128.16	-152.86	-24.70	FeS2
Pyrolusite	-7.90	-25.57	-17.66	MnO2
Pyrrhotite	-78.83	-82.57	-3.74	FeS
Realgar	-91.98	-152.25	-60.28	AsS
Rhodochrosite	-2.84	-3.06	-0.22	MnCO3
S	-59.76	-104.87	-45.11	S
S2(g)	-133.41	-140.59	-7.19	S2
Scacchite	-19.36	-10.62	8.74	MnCl2
Siderite	-2.27	-2.49	-0.22	FeCO3
Smithsonite	-3.63	-3.19	0.44	ZnCO3
SO2(g)	-35.34	-35.16	0.18	SO2
Sphalerite	-71.80	-83.27	-11.47	ZnS
Spinel	-10.80	26.80	37.61	Al2MgO4
Starkeyite	-5.13	-6.13	-1.00	MgSO4:4H2O
Sylvite	-7.32	-6.50	0.83	KCl
Syngenite	-7.24	-14.84	-7.60	K2Ca(SO4)2:H2O
Tachyhydrite	-45.76	-28.62	17.14	Mg2CaCl6:12H2O
Tenorite	-1.29	6.36	7.65	CuO
Thenardite	-7.91	-8.27	-0.36	Na2SO4
Thermonatrite	-15.27	-4.33	10.94	Na2CO3:H2O
Todorokite	-45.39	-91.21	-45.82	Mn7O12:3H2O
Troilite	-78.72	-82.57	-3.84	FeS
Trona-K	-23.81	-12.22	11.59	K2NaH(CO3)2:2H2O
Wurtzite	-74.10	-83.27	-9.17	ZnS
Wustite	-5.92	6.48	12.40	Fe.947O
Zincite	-5.13	6.07	11.20	ZnO
Zn	-47.19	21.60	68.79	Zn
Zn(ClO4)2:6H2O	-172.12	-166.48	5.63	Zn(ClO4)2:6H2O
Zn(g)	-63.81	21.60	85.41	Zn
Zn(OH)2(beta)	-5.87	6.07	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-5.59	6.07	11.66	Zn(OH)2
Zn(OH)2(gamma)	-5.82	6.07	11.88	Zn(OH)2
Zn2(OH)3Cl	-11.57	3.72	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-8.64	-1.06	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-11.32	-2.01	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-27.27	-8.18	19.09	Zn3O(SO4)2
ZnCl2	-17.83	-10.75	7.08	ZnCl2
ZnCO3:H2O	-3.33	-3.19	0.14	ZnCO3:H2O
ZnSO4	-10.66	-7.12	3.53	ZnSO4
ZnSO4:6H2O	-5.43	-7.13	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.25	-7.13	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.57	-7.12	-0.55	ZnSO4:H2O

End of simulation.

Reading input data for simulation 2.

End of run.
