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Reading data base.  
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LLNL\_AQUEOUS\_MODEL\_PARAMETERS  
NAMED\_EXPRESSIONS  
SOLUTION\_MASTER\_SPECIES  
SOLUTION\_SPECIES  
PHASES  
EXCHANGE\_MASTER\_SPECIES  
EXCHANGE\_SPECIES  
SURFACE\_MASTER\_SPECIES  
SURFACE\_SPECIES  
RATES  
END

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Reading input data for simulation 1.  
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DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 2.18.5570\database\llnl.dat  
SOLUTION 1 Flujo 1  
temp 25  
pH 3.098  
pe 17  
redox pe  
units mg/l  
density 1  
Cl 46.4  
S(6) 830  
Al 11.6  
As 1.7  
Ca 78.4  
Cu 21.3  
Fe 133.5  
K 30.3  
Mg 8.6  
Mn 14.1  
Na 19.5  
Zn 5.2  
C(4) 0  
water 1 # kg  
SOLUTION 3 AS2  
temp 25  
units mg/l  
pe 10  
pH 6.98  
Cl 678.5  
S(6) 427.00  
Al 0.00  
As 0.1526  
Ca 238.3  
Cu 0.00  
Fe 0.00  
K 40.73  
Mg 13.69  
Mn 0.114  
Na 392.9  
Zn 2.44  
C(4) 153.72  
MIX 2  
1 1

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3      1
SELECTED_OUTPUT
file          DAM_AS2
ph            true
percent_error true
totals        Al  As  Cu  Fe  Mg  Mn  Zn
              S(6)

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Beginning of initial solution calculations.  
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Initial solution 1.      Flujo 1

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

Elements	Molality	Moles
Al	4.304e-004	4.304e-004
As	2.272e-005	2.272e-005
Ca	1.959e-003	1.959e-003
Cl	1.310e-003	1.310e-003
Cu	3.356e-004	3.356e-004
Fe	2.393e-003	2.393e-003
K	7.759e-004	7.759e-004
Mg	3.543e-004	3.543e-004
Mn	2.570e-004	2.570e-004
Na	8.492e-004	8.492e-004
S(6)	8.652e-003	8.652e-003
Zn	7.962e-005	7.962e-005

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

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pH = 3.098
pe = 17.000
Activity of water = 1.000
Ionic strength = 2.715e-002
Mass of water (kg) = 1.000e+000
Total alkalinity (eq/kg) = -3.600e-003
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000
Electrical balance (eq) = -3.759e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -13.38
Iterations = 9
Total H = 1.110544e+002
Total O = 5.556248e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	9.068e-004	7.980e-004	-3.042	-3.098	-0.056
OH-	1.417e-011	1.207e-011	-10.849	-10.918	-0.070
H2O	5.553e+001	9.997e-001	1.744	-0.000	0.000
Al	4.304e-004				
AlSO4+	2.135e-004	1.825e-004	-3.671	-3.739	-0.068
Al+3	1.537e-004	4.763e-005	-3.813	-4.322	-0.509
Al(SO4)2-	6.205e-005	5.304e-005	-4.207	-4.275	-0.068
AlOH+2	1.244e-006	6.684e-007	-5.905	-6.175	-0.270
Al(OH)2+	2.275e-009	1.944e-009	-8.643	-8.711	-0.068
Al2(OH)2+4	7.923e-010	7.265e-011	-9.101	-10.139	-1.038
HALO2	3.546e-012	3.546e-012	-11.450	-11.450	0.000
Al3(OH)4+5	1.360e-013	3.505e-015	-12.866	-14.455	-1.589
AlO2-	1.781e-015	1.522e-015	-14.749	-14.818	-0.068
NaAlO2	2.057e-019	2.057e-019	-18.687	-18.687	0.000
Al13O4(OH)24+7	0.000e+000	0.000e+000	-52.670	-55.785	-3.115

As(-3)	0.000e+000					
AsH3	0.000e+000	0.000e+000	-151.853	-151.853	0.000	
As(3)	9.018e-027					
HAsO2	4.812e-027	4.812e-027	-26.318	-26.318	0.000	
As(OH)3	4.206e-027	4.206e-027	-26.376	-26.376	0.000	
H2AsO3-	3.771e-033	3.223e-033	-32.424	-32.492	-0.068	
AsO2-	3.606e-033	3.082e-033	-32.443	-32.511	-0.068	
AsO2OH-2	0.000e+000	0.000e+000	-40.128	-40.404	-0.276	
As(5)	2.272e-005					
H2AsO4-	2.027e-005	1.733e-005	-4.693	-4.761	-0.068	
H3AsO4	2.436e-006	2.436e-006	-5.613	-5.613	0.000	
HAsO4-2	6.805e-009	3.605e-009	-8.167	-8.443	-0.276	
AsO4-3	4.856e-017	1.159e-017	-16.314	-16.936	-0.622	
Ca	1.959e-003					
Ca+2	1.500e-003	8.374e-004	-2.824	-3.077	-0.253	
CaSO4	4.580e-004	4.580e-004	-3.339	-3.339	0.000	
CaCl+	2.306e-007	1.971e-007	-6.637	-6.705	-0.068	
CaCl2	2.574e-010	2.574e-010	-9.589	-9.589	0.000	
CaOH+	1.734e-013	1.482e-013	-12.761	-12.829	-0.068	
Cl(-1)	1.310e-003					
Cl-	1.309e-003	1.110e-003	-2.883	-2.955	-0.071	
CuCl+	4.495e-007	3.842e-007	-6.347	-6.415	-0.068	
MnCl+	2.615e-007	2.235e-007	-6.583	-6.651	-0.068	
CaCl+	2.306e-007	1.971e-007	-6.637	-6.705	-0.068	
HCl	1.990e-007	1.990e-007	-6.701	-6.701	0.000	
NaCl	1.382e-007	1.382e-007	-6.859	-6.859	0.000	
MgCl+	1.323e-007	1.131e-007	-6.878	-6.946	-0.068	
ZnCl+	6.734e-008	5.756e-008	-7.172	-7.240	-0.068	
FeCl+2	3.035e-008	1.630e-008	-7.518	-7.788	-0.270	
KCl	2.383e-008	2.383e-008	-7.623	-7.623	0.000	
FeCl2+	1.715e-008	1.466e-008	-7.766	-7.834	-0.068	
CaCl2	2.574e-010	2.574e-010	-9.589	-9.589	0.000	
CuCl2	2.247e-010	2.247e-010	-9.648	-9.648	0.000	
ZnCl2	7.466e-011	7.466e-011	-10.127	-10.127	0.000	
FeCl+	8.697e-012	7.434e-012	-11.061	-11.129	-0.068	
Zn(OH)Cl	1.233e-012	1.233e-012	-11.909	-11.909	0.000	
MnCl3-	7.044e-014	6.021e-014	-13.152	-13.220	-0.068	
ZnCl3-	5.357e-014	4.579e-014	-13.271	-13.339	-0.068	
ZnCl4-2	7.275e-016	3.854e-016	-15.138	-15.414	-0.276	
FeCl2	4.430e-017	4.430e-017	-16.354	-16.354	0.000	
FeCl4-	2.542e-017	2.173e-017	-16.595	-16.663	-0.068	
CuCl2-	6.618e-020	5.657e-020	-19.179	-19.247	-0.068	
CuCl4-2	9.814e-021	5.199e-021	-20.008	-20.284	-0.276	
CuCl3-2	7.615e-022	4.034e-022	-21.118	-21.394	-0.276	
FeCl4-2	2.980e-022	1.578e-022	-21.526	-21.802	-0.276	
Cl(1)	4.019e-017					
HClO	4.019e-017	4.019e-017	-16.396	-16.396	0.000	
ClO-	1.589e-021	1.358e-021	-20.799	-20.867	-0.068	
Cl(3)	4.974e-032					
HClO2	2.497e-032	2.497e-032	-31.603	-31.603	0.000	
ClO2-	2.476e-032	2.117e-032	-31.606	-31.674	-0.068	
Cl(5)	2.757e-029					
ClO3-	2.757e-029	2.348e-029	-28.560	-28.629	-0.070	
Cl(7)	1.527e-030					
ClO4-	1.526e-030	1.300e-030	-29.816	-29.886	-0.070	
ZnClO4+	8.875e-034	7.586e-034	-33.052	-33.120	-0.068	
Cu(1)	8.770e-019					
Cu+	8.101e-019	6.924e-019	-18.091	-18.160	-0.068	
CuCl2-	6.618e-020	5.657e-020	-19.179	-19.247	-0.068	
CuCl3-2	7.615e-022	4.034e-022	-21.118	-21.394	-0.276	
Cu(2)	3.356e-004					
Cu+2	2.266e-004	1.265e-004	-3.645	-3.898	-0.253	
CuSO4	1.085e-004	1.085e-004	-3.965	-3.965	0.000	
CuCl+	4.495e-007	3.842e-007	-6.347	-6.415	-0.068	
CuOH+	9.563e-009	8.174e-009	-8.019	-8.088	-0.068	
CuCl2	2.247e-010	2.247e-010	-9.648	-9.648	0.000	
CuCl4-2	9.814e-021	5.199e-021	-20.008	-20.284	-0.276	

CuO2-2	2.089e-031	1.107e-031	-30.680	-30.956	-0.276
Fe(2)	2.193e-008				
Fe+2	1.647e-008	9.190e-009	-7.783	-8.037	-0.253
FeSO4	5.453e-009	5.453e-009	-8.263	-8.263	0.000
FeCl+	8.697e-012	7.434e-012	-11.061	-11.129	-0.068
FeOH+	4.259e-015	3.641e-015	-14.371	-14.439	-0.068
FeCl2	4.430e-017	4.430e-017	-16.354	-16.354	0.000
FeCl4-2	2.980e-022	1.578e-022	-21.526	-21.802	-0.276
Fe(OH)2	3.623e-023	3.623e-023	-22.441	-22.441	0.000
Fe(OH)3-	2.114e-030	1.807e-030	-29.675	-29.743	-0.068
Fe(OH)4-2	0.000e+000	0.000e+000	-41.369	-41.645	-0.276
Fe(3)	2.393e-003				
FeOH+2	1.327e-003	7.127e-004	-2.877	-3.147	-0.270
Fe(OH)2+	3.459e-004	2.956e-004	-3.461	-3.529	-0.068
Fe+3	2.843e-004	8.811e-005	-3.546	-4.055	-0.509
Fe2(OH)2+4	1.491e-004	1.367e-005	-3.827	-4.864	-1.038
FeSO4+	3.734e-005	3.192e-005	-4.428	-4.496	-0.068
Fe3(OH)4+5	3.276e-005	8.444e-007	-4.485	-6.073	-1.589
Fe(SO4)2-	2.364e-006	2.021e-006	-5.626	-5.695	-0.068
Fe(OH)3	1.732e-007	1.732e-007	-6.761	-6.761	0.000
FeCl+2	3.035e-008	1.630e-008	-7.518	-7.788	-0.270
FeCl2+	1.715e-008	1.466e-008	-7.766	-7.834	-0.068
Fe(OH)4-	6.378e-014	5.452e-014	-13.195	-13.263	-0.068
FeCl4-	2.542e-017	2.173e-017	-16.595	-16.663	-0.068
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-43.299	-43.296	0.003
K	7.759e-004				
K+	7.533e-004	6.391e-004	-3.123	-3.194	-0.071
KSO4-	2.260e-005	1.932e-005	-4.646	-4.714	-0.068
KCl	2.383e-008	2.383e-008	-7.623	-7.623	0.000
KHSO4	1.360e-008	1.360e-008	-7.866	-7.866	0.000
KOH	2.776e-015	2.776e-015	-14.557	-14.557	0.000
Mg	3.543e-004				
Mg+2	2.237e-004	1.305e-004	-3.650	-3.884	-0.234
MgSO4	1.305e-004	1.305e-004	-3.884	-3.884	0.000
MgCl+	1.323e-007	1.131e-007	-6.878	-6.946	-0.068
Mg4(OH)4+4	0.000e+000	0.000e+000	-41.859	-42.896	-1.038
Mn(2)	2.570e-004				
Mn+2	1.694e-004	9.453e-005	-3.771	-4.024	-0.253
MnSO4	8.733e-005	8.733e-005	-4.059	-4.059	0.000
MnCl+	2.615e-007	2.235e-007	-6.583	-6.651	-0.068
MnOH+	3.561e-012	3.044e-012	-11.448	-11.517	-0.068
MnCl3-	7.044e-014	6.021e-014	-13.152	-13.220	-0.068
Mn2OH+3	1.215e-015	3.083e-016	-14.915	-15.511	-0.596
Mn(OH)2	9.361e-021	9.361e-021	-20.029	-20.029	0.000
Mn2(OH)3+	2.588e-023	2.212e-023	-22.587	-22.655	-0.068
Mn(OH)3-	1.287e-029	1.100e-029	-28.890	-28.959	-0.068
Mn(OH)4-2	2.203e-040	1.167e-040	-39.657	-39.933	-0.276
Mn(3)	9.938e-013				
Mn+3	9.938e-013	2.521e-013	-12.003	-12.598	-0.596
Mn(6)	3.873e-030				
MnO4-2	3.873e-030	2.052e-030	-29.412	-29.688	-0.276
Mn(7)	1.061e-022				
MnO4-	1.061e-022	9.036e-023	-21.974	-22.044	-0.070
Na	8.492e-004				
Na+	8.286e-004	7.083e-004	-3.082	-3.150	-0.068
NaSO4-	2.050e-005	1.752e-005	-4.688	-4.756	-0.068
NaCl	1.382e-007	1.382e-007	-6.859	-6.859	0.000
NaOH	1.475e-015	1.475e-015	-14.831	-14.831	0.000
NaAlO2	2.057e-019	2.057e-019	-18.687	-18.687	0.000
O(0)	4.953e-006				
O2	2.476e-006	2.493e-006	-5.606	-5.603	0.003
S(6)	8.652e-003				
SO4-2	7.068e-003	3.744e-003	-2.151	-2.427	-0.276
CaSO4	4.580e-004	4.580e-004	-3.339	-3.339	0.000
HSO4-	3.531e-004	3.018e-004	-3.452	-3.520	-0.068
AlSO4+	2.135e-004	1.825e-004	-3.671	-3.739	-0.068

MgSO4	1.305e-004	1.305e-004	-3.884	-3.884	0.000
CuSO4	1.085e-004	1.085e-004	-3.965	-3.965	0.000
MnSO4	8.733e-005	8.733e-005	-4.059	-4.059	0.000
Al(SO4)2-	6.205e-005	5.304e-005	-4.207	-4.275	-0.068
FeSO4+	3.734e-005	3.192e-005	-4.428	-4.496	-0.068
ZnSO4	2.427e-005	2.427e-005	-4.615	-4.615	0.000
KSO4-	2.260e-005	1.932e-005	-4.646	-4.714	-0.068
NaSO4-	2.050e-005	1.752e-005	-4.688	-4.756	-0.068
Fe(SO4)2-	2.364e-006	2.021e-006	-5.626	-5.695	-0.068
KHSO4	1.360e-008	1.360e-008	-7.866	-7.866	0.000
FeSO4	5.453e-009	5.453e-009	-8.263	-8.263	0.000
H2SO4	2.272e-010	2.272e-010	-9.644	-9.644	0.000
Zn	7.962e-005				
Zn+2	5.528e-005	3.085e-005	-4.257	-4.511	-0.253
ZnSO4	2.427e-005	2.427e-005	-4.615	-4.615	0.000
ZnCl+	6.734e-008	5.756e-008	-7.172	-7.240	-0.068
ZnCl2	7.466e-011	7.466e-011	-10.127	-10.127	0.000
ZnOH+	4.959e-011	4.239e-011	-10.305	-10.373	-0.068
Zn(OH)Cl	1.233e-012	1.233e-012	-11.909	-11.909	0.000
ZnCl3-	5.357e-014	4.579e-014	-13.271	-13.339	-0.068
ZnCl4-2	7.275e-016	3.854e-016	-15.138	-15.414	-0.276
Zn(OH)2	2.274e-016	2.274e-016	-15.643	-15.643	0.000
Zn(OH)3-	1.033e-024	8.831e-025	-23.986	-24.054	-0.068
ZnClO4+	8.875e-034	7.586e-034	-33.052	-33.120	-0.068
Zn(OH)4-2	3.560e-034	1.886e-034	-33.448	-33.724	-0.276

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

Phase	SI	log IAP	log KT	
Al	-140.74	9.17	149.91	Al
Al(g)	-191.44	9.17	200.62	Al
Al2(SO4)3	-34.82	-15.92	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-17.48	-15.92	1.56	Al2(SO4)3:6H2O
Alum-K	-7.40	-12.37	-4.97	KAl(SO4)2:12H2O
Alunite	-1.96	-2.43	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-1.15	-5.50	-4.35	CaSO4
Antarcticite	-13.08	-8.99	4.09	CaCl2:6H2O
Antlerite	-10.46	-1.73	8.73	Cu3(SO4)(OH)4
Aphthitalite	-13.70	-17.59	-3.89	NaK3(SO4)2
Arcanite	-6.97	-8.82	-1.84	K2SO4
Arsenolite	-51.34	-71.18	-19.84	As2O3
As	-74.07	-31.39	42.68	As
As2O5	-17.85	-15.72	2.14	As2O5
As4O6(cubi)	-102.53	-142.36	-39.82	As4O6
As4O6(mono)	-102.31	-142.36	-40.05	As4O6
Atacamite	-17.18	-2.91	14.26	Cu4Cl2(OH)6
Bassanite	-1.80	-5.50	-3.71	CaSO4:0.5H2O
Birnessite	-11.25	-96.79	-85.55	Mn8O14:5H2O
Bischofite	-14.19	-9.79	4.39	MgCl2:6H2O
Bixbyite	-5.64	-6.61	-0.96	Mn2O3
Bloedite	-12.56	-15.04	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-2.58	4.97	7.55	AlO2H
Brochantite	-14.85	0.57	15.42	Cu4(SO4)(OH)6
Brucite	-13.97	2.31	16.28	Mg(OH)2
Ca	-133.91	5.92	139.83	Ca
Ca(g)	-159.15	5.92	165.07	Ca
Ca2Al2O5:8H2O	-43.39	16.18	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-32.16	-5.87	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-24.16	-6.36	17.80	Ca3(AsO4)2
Ca3Al2O6	-93.73	19.30	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-107.59	32.90	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-84.84	22.42	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-81.27	22.42	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-67.96	0.37	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-33.85	13.06	46.91	CaAl2O4
CaAl2O4:10H2O	-24.93	13.06	37.99	CaAl2O4:10H2O

CaAl4O7	-45.59	23.01	68.59	CaAl4O7
Carnallite	-20.22	-15.94	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.97	-5.50	-3.54	CaSO4:0.5H2O
Chalcanthite	-3.70	-6.33	-2.63	CuSO4:5H2O
Chalcocyanite	-9.24	-6.32	2.91	CuSO4
Chloromagnesite	-31.61	-9.79	21.82	MgCl2
Cl2(g)	-17.90	-14.91	2.99	Cl2
Claudetite	-51.38	-71.18	-19.80	As2O3
Corundum	-8.35	9.94	18.29	Al2O3
Cu	-26.40	5.10	31.50	Cu
Cu(g)	-78.56	5.10	83.66	Cu
CuCl2	-13.53	-9.81	3.72	CuCl2
Cuprite	-28.22	-30.12	-1.91	Cu2O
Delafossite	-3.39	-9.82	-6.44	CuFeO2
Diaspore	-2.17	4.97	7.15	AlHO2
Epsomite	-4.35	-6.31	-1.96	MgSO4:7H2O
Ettringite	-59.68	2.78	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-58.06	0.96	59.02	Fe
Fe(OH)2	-15.74	-1.84	13.89	Fe(OH)2
Fe(OH)3	-0.40	5.24	5.64	Fe(OH)3
Fe2(SO4)3	-18.44	-15.39	3.05	Fe2(SO4)3
FeO	-15.36	-1.84	13.52	FeO
Ferrite-Ca	-7.90	13.60	21.50	CaFe2O4
Ferrite-Cu	2.49	12.78	10.28	CuFe2O4
Ferrite-Dicalcium	-40.08	16.72	56.80	Ca2Fe2O5
Ferrite-Mg	-8.23	12.79	21.02	MgFe2O4
Ferrite-Zn	0.46	12.16	11.70	ZnFe2O4
FeSO4	-13.07	-10.46	2.61	FeSO4
Gibbsite	-2.77	4.97	7.74	Al(OH)3
Glauberite	-8.76	-14.23	-5.47	Na2Ca(SO4)2
Goethite	4.71	5.24	0.53	FeOOH
Gypsum	-0.97	-5.50	-4.53	CaSO4:2H2O
H2(g)	-40.20	-43.30	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-7.67	-6.10	1.56	NaCl
Hausmannite	-14.58	-4.44	10.14	Mn3O4
HCl(g)	-12.35	-6.05	6.30	HCl
Hematite	10.40	10.48	0.08	Fe2O3
Hercynite	-20.70	8.10	28.80	FeAl2O4
Hexahydrite	-4.59	-6.31	-1.73	MgSO4:6H2O
Hydrophilite	-20.73	-8.99	11.75	CaCl2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	7.79	-1.63	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	3.87	-1.58	-5.45	NaFe3(SO4)2(OH)6
K	-69.67	1.30	70.98	K
K(g)	-80.27	1.30	81.58	K
K2O	-84.23	-0.19	84.04	K2O
K3H(SO4)2	-13.91	-17.53	-3.62	K3H(SO4)2
Kainite	-12.15	-12.46	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-15.64	-12.37	3.27	KAl(SO4)2
Katoite	-59.64	19.30	78.94	Ca3Al2H12O12
Kieserite	-6.04	-6.31	-0.27	MgSO4:H2O
KMgCl3	-37.19	-15.94	21.25	KMgCl3
KMgCl3:2H2O	-29.90	-15.94	13.96	KMgCl3:2H2O
Lammerite	-10.38	-8.82	1.55	Cu3(AsO4)2
Lawrencite	-23.00	-13.95	9.05	FeCl2
Leonite	-11.01	-15.13	-4.11	K2Mg(SO4)2:4H2O
Lime	-29.45	3.12	32.57	CaO
Magnetite	-1.78	8.64	10.42	Fe3O4
Manganite	-3.14	-3.30	-0.16	MnO(OH)
Manganosite	-15.74	2.17	17.92	MnO
Mayenite	-387.12	107.03	494.15	Ca12Al14O33
Melanterite	-8.07	-10.46	-2.40	FeSO4:7H2O
Mercallite	-7.28	-8.72	-1.44	KHSO4
Mg	-117.41	5.11	122.52	Mg
Mg(g)	-137.13	5.11	142.25	Mg
Mg1.25SO4(OH)0.5:0.5H2O	-10.93	-5.73	5.20	Mg1.25SO4(OH)0.5:0.5H2O

Mg1.5SO4(OH)	-14.36	-5.16	9.21	Mg1.5SO4(OH)
MgCl2:2H2O	-22.53	-9.79	12.73	MgCl2:2H2O
MgCl2:4H2O	-17.10	-9.79	7.30	MgCl2:4H2O
MgCl2:H2O	-25.87	-9.79	16.07	MgCl2:H2O
MgOHCl	-19.63	-3.74	15.89	MgOHCl
MgSO4	-11.14	-6.31	4.83	MgSO4
Mirabilite	-7.57	-8.73	-1.15	Na2SO4:10H2O
Misenite	-50.05	-61.13	-11.08	K8H6(SO4)7
Mn	-77.96	4.97	82.93	Mn
Mn(OH)2(am)	-13.14	2.17	15.31	Mn(OH)2
Mn(OH)3	-9.65	-3.30	6.34	Mn(OH)3
MnCl2:2H2O	-13.93	-9.93	4.00	MnCl2:2H2O
MnCl2:4H2O	-12.69	-9.93	2.75	MnCl2:4H2O
MnCl2:H2O	-15.48	-9.93	5.54	MnCl2:H2O
MnO2(gamma)	-0.73	-16.86	-16.13	MnO2
MnSO4	-9.06	-6.45	2.61	MnSO4
Molysite	-26.39	-12.92	13.47	FeCl3
Na	-66.02	1.35	67.37	Na
Na(g)	-79.51	1.35	80.86	Na
Na2O	-67.52	-0.10	67.42	Na2O
Na3H(SO4)2	-16.51	-17.40	-0.89	Na3H(SO4)2
Na4Ca(SO4)3:2H2O	-17.06	-22.96	-5.89	Na4Ca(SO4)3:2H2O
NaFeO2	-14.70	5.19	19.88	NaFeO2
Nantokite	-14.35	-21.11	-6.77	CuCl
O2(g)	-2.71	-5.60	-2.89	O2
Oxychloride-Mg	-27.26	-1.43	25.83	Mg2Cl(OH)3:4H2O
Pentahydrate	-4.92	-6.31	-1.39	MgSO4:5H2O
Periclase	-19.01	2.31	21.33	MgO
Picromerite	-10.69	-15.13	-4.44	K2Mg(SO4)2:6H2O
Polyhalite	-11.82	-26.13	-14.31	K2MgCa2(SO4)4:2H2O
Portlandite	-19.43	3.12	22.55	Ca(OH)2
Pyrolusite	0.80	-16.86	-17.66	MnO2
Scacchite	-18.67	-9.93	8.74	MnCl2
Spinel	-25.35	12.25	37.61	Al2MgO4
Starkeyite	-5.31	-6.31	-1.00	MgSO4:4H2O
Sylvite	-6.98	-6.15	0.83	KCl
Syngenite	-6.72	-14.32	-7.60	K2Ca(SO4)2:H2O
Tachyhydrate	-45.72	-28.57	17.14	Mg2CaCl6:12H2O
Tenorite	-5.35	2.30	7.65	CuO
Thenardite	-8.37	-8.73	-0.36	Na2SO4
Todorokite	-9.89	-55.71	-45.82	Mn7O12:3H2O
Wustite	-13.40	-0.99	12.40	Fe.947O
Zincite	-9.51	1.69	11.20	ZnO
Zn	-64.30	4.49	68.79	Zn
Zn(ClO4)2:6H2O	-69.92	-64.28	5.63	Zn(ClO4)2:6H2O
Zn(g)	-80.92	4.49	85.41	Zn
Zn(OH)2(beta)	-10.25	1.69	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-9.98	1.69	11.66	Zn(OH)2
Zn(OH)2(gamma)	-10.20	1.69	11.88	Zn(OH)2
Zn2(OH)3Cl	-17.97	-2.68	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-12.83	-5.25	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-19.97	-10.66	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-31.28	-12.19	19.09	Zn3O(SO4)2
ZnCl2	-17.50	-10.42	7.08	ZnCl2
ZnSO4	-10.47	-6.94	3.53	ZnSO4
ZnSO4:6H2O	-5.24	-6.94	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.06	-6.94	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.39	-6.94	-0.55	ZnSO4:H2O

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

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

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Beginning of batch-reaction calculations.  
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Reaction step 1.

Using mix 2.

Mixture 2.

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

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

Elements	Molality	Moles
Al	2.152e-004	4.304e-004
As	1.238e-005	2.476e-005
C	1.262e-003	2.525e-003
Ca	3.958e-003	7.916e-003
Cl	1.024e-002	2.049e-002
Cu	1.678e-004	3.356e-004
Fe	1.197e-003	2.393e-003
K	9.098e-004	1.820e-003
Mg	4.593e-004	9.186e-004
Mn	1.295e-004	2.590e-004
Na	8.986e-003	1.797e-002
S	6.553e-003	1.311e-002
Zn	5.850e-005	1.170e-004

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

pH = 3.857 Charge balance  
 pe = 16.166 Adjusted to redox equilibrium  
 Activity of water = 0.999  
 Ionic strength = 3.046e-002  
 Mass of water (kg) = 2.000e+000  
 Total alkalinity (eq/kg) = -7.357e-004  
 Total CO2 (mol/kg) = 1.262e-003  
 Temperature (deg C) = 25.000  
 Electrical balance (eq) = -2.684e-003  
 Percent error,  $100 \cdot (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$  = -3.30  
 Iterations = 10  
 Total H = 2.221072e+002  
 Total O = 1.111128e+002

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	1.587e-004	1.390e-004	-3.799	-3.857	-0.058
OH-	8.196e-011	6.927e-011	-10.086	-10.159	-0.073
H2O	5.553e+001	9.994e-001	1.744	-0.000	0.000
Al	2.152e-004				
Al+3	9.704e-005	2.874e-005	-4.013	-4.541	-0.528
AlSO4+	9.392e-005	7.969e-005	-4.027	-4.099	-0.071
Al(SO4)2-	1.975e-005	1.676e-005	-4.704	-4.776	-0.071
AlOH+2	4.437e-006	2.315e-006	-5.353	-5.635	-0.282
Al(OH)2+	4.555e-008	3.865e-008	-7.342	-7.413	-0.071
Al2(OH)2+4	1.058e-008	8.715e-010	-7.976	-9.060	-1.084
HALO2	4.046e-010	4.046e-010	-9.393	-9.393	0.000
Al3(OH)4+5	3.808e-011	8.359e-013	-10.419	-12.078	-1.659
AlO2-	1.175e-012	9.971e-013	-11.930	-12.001	-0.071
NaAlO2	1.423e-015	1.423e-015	-14.847	-14.847	0.000
Al13O4(OH)24+7	7.917e-032	4.433e-035	-31.101	-34.353	-3.252
As(-3)	0.000e+000				
AsH3	0.000e+000	0.000e+000	-152.237	-152.237	0.000
As(3)	1.317e-027				
HAsO2	7.026e-028	7.026e-028	-27.153	-27.153	0.000
As(OH)3	6.140e-028	6.140e-028	-27.212	-27.212	0.000
H2AsO3-	3.183e-033	2.701e-033	-32.497	-32.568	-0.071
AsO2-	3.045e-033	2.584e-033	-32.516	-32.588	-0.071
AsO2OH-2	3.694e-040	1.898e-040	-39.433	-39.722	-0.289
HAsS2	0.000e+000	0.000e+000	-279.455	-279.455	0.000
As(5)	1.238e-005				
H2AsO4-	1.210e-005	1.027e-005	-4.917	-4.988	-0.071
H3AsO4	2.515e-007	2.515e-007	-6.600	-6.600	0.000
HAsO4-2	2.386e-008	1.226e-008	-7.622	-7.911	-0.289
AsO4-3	1.016e-015	2.263e-016	-14.993	-15.645	-0.652
C(-2)	0.000e+000				
C2H4	0.000e+000	0.000e+000	-255.230	-255.230	0.000
C(-3)	0.000e+000				
C2H6	0.000e+000	0.000e+000	-226.389	-226.389	0.000
C(-4)	0.000e+000				
CH4	0.000e+000	0.000e+000	-141.546	-141.546	0.000
C(2)	0.000e+000				
CO	0.000e+000	0.000e+000	-47.984	-47.984	0.000
C(4)	1.262e-003				
CO2	1.258e-003	1.267e-003	-2.900	-2.897	0.003
HCO3-	4.628e-006	3.927e-006	-5.335	-5.406	-0.071
CaHCO3+	9.709e-008	8.238e-008	-7.013	-7.084	-0.071
FeCO3+	4.340e-008	3.683e-008	-7.362	-7.434	-0.071
NaHCO3	4.202e-008	4.202e-008	-7.377	-7.377	0.000
MgHCO3+	9.943e-009	8.437e-009	-8.002	-8.074	-0.071
ZnHCO3+	2.879e-009	2.443e-009	-8.541	-8.612	-0.071

MnHCO3+	1.805e-009	1.532e-009	-8.743	-8.815	-0.071
CuCO3	8.066e-010	8.066e-010	-9.093	-9.093	0.000
FeHCO3+	8.797e-012	7.464e-012	-11.056	-11.127	-0.071
CaCO3	5.142e-012	5.142e-012	-11.289	-11.289	0.000
CO3-2	2.402e-012	1.253e-012	-11.619	-11.902	-0.282
MnCO3	2.248e-012	2.248e-012	-11.648	-11.648	0.000
ZnCO3	2.540e-013	2.540e-013	-12.595	-12.595	0.000
MgCO3	2.452e-013	2.452e-013	-12.610	-12.610	0.000
NaCO3-	3.866e-014	3.281e-014	-13.413	-13.484	-0.071
FeCO3	2.577e-016	2.577e-016	-15.589	-15.589	0.000
Cu(CO3)2-2	3.504e-018	1.801e-018	-17.455	-17.745	-0.289
CuCO3(OH)2-2	6.897e-022	3.545e-022	-21.161	-21.450	-0.289
Ca	3.958e-003				
Ca+2	3.253e-003	1.770e-003	-2.488	-2.752	-0.264
CaSO4	7.006e-004	7.006e-004	-3.155	-3.155	0.000
CaCl+	3.804e-006	3.228e-006	-5.420	-5.491	-0.071
CaHCO3+	9.709e-008	8.238e-008	-7.013	-7.084	-0.071
CaCl2	3.266e-008	3.266e-008	-7.486	-7.486	0.000
CaCO3	5.142e-012	5.142e-012	-11.289	-11.289	0.000
CaOH+	2.119e-012	1.798e-012	-11.674	-11.745	-0.071
Cl(-1)	1.024e-002				
Cl-	1.022e-002	8.603e-003	-1.990	-2.065	-0.075
NaCl	1.131e-005	1.131e-005	-4.946	-4.946	0.000
CaCl+	3.804e-006	3.228e-006	-5.420	-5.491	-0.071
CuCl+	1.871e-006	1.588e-006	-5.728	-5.799	-0.071
MgCl+	1.464e-006	1.242e-006	-5.834	-5.906	-0.071
MnCl+	1.106e-006	9.385e-007	-5.956	-6.028	-0.071
ZnCl+	4.110e-007	3.488e-007	-6.386	-6.457	-0.071
HCl	2.686e-007	2.686e-007	-6.571	-6.571	0.000
KCl	2.165e-007	2.165e-007	-6.665	-6.665	0.000
FeCl2+	5.987e-008	5.080e-008	-7.223	-7.294	-0.071
CaCl2	3.266e-008	3.266e-008	-7.486	-7.486	0.000
FeCl+2	1.398e-008	7.293e-009	-7.855	-8.137	-0.282
CuCl2	7.193e-009	7.193e-009	-8.143	-8.143	0.000
ZnCl2	3.505e-009	3.505e-009	-8.455	-8.455	0.000
Zn(OH)Cl	4.288e-011	4.288e-011	-10.368	-10.368	0.000
FeCl+	2.675e-011	2.270e-011	-10.573	-10.644	-0.071
ZnCl3-	1.963e-011	1.665e-011	-10.707	-10.779	-0.071
MnCl3-	1.788e-011	1.517e-011	-10.748	-10.819	-0.071
ZnCl4-2	2.113e-012	1.086e-012	-11.675	-11.964	-0.289
FeCl4-	5.327e-015	4.520e-015	-14.274	-14.345	-0.071
FeCl2	1.048e-015	1.048e-015	-14.980	-14.980	0.000
CuCl4-2	1.944e-017	9.992e-018	-16.711	-17.000	-0.289
CuCl2-	1.457e-017	1.236e-017	-16.837	-16.908	-0.071
CuCl3-2	1.329e-018	6.830e-019	-17.876	-18.166	-0.289
FeCl4-2	4.361e-019	2.241e-019	-18.360	-18.650	-0.289
Cl(1)	3.836e-017				
HClO	3.835e-017	3.835e-017	-16.416	-16.416	0.000
ClO-	8.768e-021	7.440e-021	-20.057	-20.128	-0.071
Cl(3)	1.135e-031				
ClO2-	9.666e-032	8.201e-032	-31.015	-31.086	-0.071
HClO2	1.686e-032	1.686e-032	-31.773	-31.773	0.000
Cl(5)	7.612e-029				
ClO3-	7.612e-029	6.433e-029	-28.118	-28.192	-0.073
Cl(7)	2.982e-030				
ClO4-	2.981e-030	2.519e-030	-29.526	-29.599	-0.073
ZnClO4+	1.355e-033	1.150e-033	-32.868	-32.939	-0.071
Cu(1)	1.887e-017				
CuCl2-	1.457e-017	1.236e-017	-16.837	-16.908	-0.071
Cu+	2.971e-018	2.521e-018	-17.527	-17.598	-0.071
CuCl3-2	1.329e-018	6.830e-019	-17.876	-18.166	-0.289
Cu(2)	1.678e-004				
Cu+2	1.240e-004	6.747e-005	-3.907	-4.171	-0.264
CuSO4	4.188e-005	4.188e-005	-4.378	-4.378	0.000
CuCl+	1.871e-006	1.588e-006	-5.728	-5.799	-0.071
CuOH+	2.949e-008	2.502e-008	-7.530	-7.602	-0.071
CuCl2	7.193e-009	7.193e-009	-8.143	-8.143	0.000

CuCO3	8.066e-010	8.066e-010	-9.093	-9.093	0.000
CuCl4-2	1.944e-017	9.992e-018	-16.711	-17.000	-0.289
Cu(CO3)2-2	3.504e-018	1.801e-018	-17.455	-17.745	-0.289
CuCO3(OH)2-2	6.897e-022	3.545e-022	-21.161	-21.450	-0.289
CuO2-2	1.247e-028	6.409e-029	-27.904	-28.193	-0.289
Fe(2)	8.247e-009				
Fe+2	6.656e-009	3.622e-009	-8.177	-8.441	-0.264
FeSO4	1.555e-009	1.555e-009	-8.808	-8.808	0.000
FeCl+	2.675e-011	2.270e-011	-10.573	-10.644	-0.071
FeHCO3+	8.797e-012	7.464e-012	-11.056	-11.127	-0.071
FeOH+	9.705e-015	8.235e-015	-14.013	-14.084	-0.071
FeCl2	1.048e-015	1.048e-015	-14.980	-14.980	0.000
FeCO3	2.577e-016	2.577e-016	-15.589	-15.589	0.000
FeCl4-2	4.361e-019	2.241e-019	-18.360	-18.650	-0.289
Fe(OH)2	4.703e-022	4.703e-022	-21.328	-21.328	0.000
Fe(OH)3-	1.586e-028	1.346e-028	-27.800	-27.871	-0.071
Fe(OH)4-2	1.883e-039	9.678e-040	-38.725	-39.014	-0.289
Fe(3)	1.197e-003				
Fe(OH)2+	6.627e-004	5.623e-004	-3.179	-3.250	-0.071
FeOH+2	4.526e-004	2.362e-004	-3.344	-3.627	-0.282
Fe2(OH)2+4	1.822e-005	1.501e-006	-4.739	-5.824	-1.084
Fe+3	1.718e-005	5.088e-006	-4.765	-5.293	-0.528
Fe3(OH)4+5	8.034e-006	1.764e-007	-5.095	-6.754	-1.659
Fe(OH)3	1.891e-006	1.891e-006	-5.723	-5.723	0.000
FeSO4+	1.572e-006	1.334e-006	-5.804	-5.875	-0.071
Fe(SO4)2-	7.200e-008	6.109e-008	-7.143	-7.214	-0.071
FeCl2+	5.987e-008	5.080e-008	-7.223	-7.294	-0.071
FeCO3+	4.340e-008	3.683e-008	-7.362	-7.434	-0.071
FeCl+2	1.398e-008	7.293e-009	-7.855	-8.137	-0.282
Fe(OH)4-	4.025e-012	3.415e-012	-11.395	-11.467	-0.071
FeCl4-	5.327e-015	4.520e-015	-14.274	-14.345	-0.071
H(0)	0.000e+000				
H2	0.000e+000	0.000e+000	-43.149	-43.146	0.003
K	9.098e-004				
K+	8.903e-004	7.493e-004	-3.050	-3.125	-0.075
KSO4-	1.931e-005	1.639e-005	-4.714	-4.786	-0.071
KCl	2.165e-007	2.165e-007	-6.665	-6.665	0.000
KHSO4	2.010e-009	2.010e-009	-8.697	-8.697	0.000
KOH	1.868e-014	1.868e-014	-13.729	-13.729	0.000
Mg	4.593e-004				
Mg+2	3.240e-004	1.850e-004	-3.489	-3.733	-0.243
MgSO4	1.338e-004	1.338e-004	-3.873	-3.873	0.000
MgCl+	1.464e-006	1.242e-006	-5.834	-5.906	-0.071
MgHCO3+	9.943e-009	8.437e-009	-8.002	-8.074	-0.071
MgCO3	2.452e-013	2.452e-013	-12.610	-12.610	0.000
Mg4(OH)4+4	6.752e-039	5.563e-040	-38.171	-39.255	-1.084
Mn(2)	1.295e-004				
Mn+2	9.416e-005	5.123e-005	-4.026	-4.290	-0.264
MnSO4	3.425e-005	3.425e-005	-4.465	-4.465	0.000
MnCl+	1.106e-006	9.385e-007	-5.956	-6.028	-0.071
MnHCO3+	1.805e-009	1.532e-009	-8.743	-8.815	-0.071
MnCl3-	1.788e-011	1.517e-011	-10.748	-10.819	-0.071
MnOH+	1.116e-011	9.468e-012	-10.952	-11.024	-0.071
MnCO3	2.248e-012	2.248e-012	-11.648	-11.648	0.000
Mn2OH+3	2.181e-015	5.198e-016	-14.661	-15.284	-0.623
Mn(OH)2	1.671e-019	1.671e-019	-18.777	-18.777	0.000
Mn2(OH)3+	1.447e-021	1.228e-021	-20.839	-20.911	-0.071
Mn(OH)3-	1.328e-027	1.127e-027	-26.877	-26.948	-0.071
Mn(OH)4-2	1.335e-037	6.861e-038	-36.874	-37.164	-0.289
Mn(3)	8.402e-014				
Mn+3	8.402e-014	2.002e-014	-13.076	-13.698	-0.623
Mn(6)	1.175e-027				
MnO4-2	1.175e-027	6.037e-028	-26.930	-27.219	-0.289
Mn(7)	4.608e-021				
MnO4-	4.608e-021	3.895e-021	-20.336	-20.410	-0.073
Na	8.986e-003				
Na+	8.817e-003	7.482e-003	-2.055	-2.126	-0.071

NaSO4-	1.578e-004	1.339e-004	-3.802	-3.873	-0.071
NaCl	1.131e-005	1.131e-005	-4.946	-4.946	0.000
NaHCO3	4.202e-008	4.202e-008	-7.377	-7.377	0.000
NaOH	8.941e-014	8.941e-014	-13.049	-13.049	0.000
NaCO3-	3.866e-014	3.281e-014	-13.413	-13.484	-0.071
NaAlO2	1.423e-015	1.423e-015	-14.847	-14.847	0.000
O(0)	2.475e-006				
O2	1.238e-006	1.247e-006	-5.907	-5.904	0.003
S(-2)	0.000e+000				
H2S	0.000e+000	0.000e+000	-129.746	-129.746	0.000
HS-	0.000e+000	0.000e+000	-132.825	-132.898	-0.073
S-2	0.000e+000	0.000e+000	-141.691	-141.967	-0.276
S2-2	0.000e+000	0.000e+000	-235.202	-235.491	-0.289
HAsS2	0.000e+000	0.000e+000	-279.455	-279.455	0.000
S3-2	0.000e+000	0.000e+000	-328.766	-329.055	-0.289
S4-2	0.000e+000	0.000e+000	-422.558	-422.847	-0.289
S5-2	0.000e+000	0.000e+000	-516.567	-516.856	-0.289
S(2)	0.000e+000				
S2O3-2	0.000e+000	0.000e+000	-134.224	-134.513	-0.289
HS2O3-	0.000e+000	0.000e+000	-137.285	-137.356	-0.071
S(3)	0.000e+000				
S2O4-2	0.000e+000	0.000e+000	-122.117	-122.394	-0.276
S(4)	0.000e+000				
HSO3-	0.000e+000	0.000e+000	-42.787	-42.858	-0.071
H2SO3	0.000e+000	0.000e+000	-44.734	-44.734	0.000
SO2	0.000e+000	0.000e+000	-44.834	-44.834	0.000
SO3-2	0.000e+000	0.000e+000	-45.950	-46.233	-0.282
S2O6-2	0.000e+000	0.000e+000	-60.975	-61.264	-0.289
S3O6-2	0.000e+000	0.000e+000	-157.023	-157.312	-0.289
S4O6-2	0.000e+000	0.000e+000	-237.165	-237.454	-0.289
S5O6-2	0.000e+000	0.000e+000	-346.186	-346.475	-0.289
S(5)	0.000e+000				
S2O5-2	0.000e+000	0.000e+000	-90.257	-90.546	-0.289
S(6)	6.553e-003				
SO4-2	5.272e-003	2.709e-003	-2.278	-2.567	-0.289
CaSO4	7.006e-004	7.006e-004	-3.155	-3.155	0.000
NaSO4-	1.578e-004	1.339e-004	-3.802	-3.873	-0.071
MgSO4	1.338e-004	1.338e-004	-3.873	-3.873	0.000
AlSO4+	9.392e-005	7.969e-005	-4.027	-4.099	-0.071
HSO4-	4.484e-005	3.805e-005	-4.348	-4.420	-0.071
CuSO4	4.188e-005	4.188e-005	-4.378	-4.378	0.000
MnSO4	3.425e-005	3.425e-005	-4.465	-4.465	0.000
Al(SO4)2-	1.975e-005	1.676e-005	-4.704	-4.776	-0.071
KSO4-	1.931e-005	1.639e-005	-4.714	-4.786	-0.071
ZnSO4	1.374e-005	1.374e-005	-4.862	-4.862	0.000
FeSO4+	1.572e-006	1.334e-006	-5.804	-5.875	-0.071
Fe(SO4)2-	7.200e-008	6.109e-008	-7.143	-7.214	-0.071
KHSO4	2.010e-009	2.010e-009	-8.697	-8.697	0.000
FeSO4	1.555e-009	1.555e-009	-8.808	-8.808	0.000
H2SO4	4.990e-012	4.990e-012	-11.302	-11.302	0.000
S(7)	2.163e-038				
S2O8-2	1.081e-038	5.558e-039	-37.966	-38.255	-0.289
S(8)	2.720e-027				
HSO5-	2.720e-027	2.308e-027	-26.566	-26.637	-0.071
Zn	5.850e-005				
Zn+2	4.435e-005	2.413e-005	-4.353	-4.617	-0.264
ZnSO4	1.374e-005	1.374e-005	-4.862	-4.862	0.000
ZnCl+	4.110e-007	3.488e-007	-6.386	-6.457	-0.071
ZnCl2	3.505e-009	3.505e-009	-8.455	-8.455	0.000
ZnHCO3+	2.879e-009	2.443e-009	-8.541	-8.612	-0.071
ZnOH+	2.242e-010	1.903e-010	-9.649	-9.721	-0.071
Zn(OH)Cl	4.288e-011	4.288e-011	-10.368	-10.368	0.000
ZnCl3-	1.963e-011	1.665e-011	-10.707	-10.779	-0.071
ZnCl4-2	2.113e-012	1.086e-012	-11.675	-11.964	-0.289
ZnCO3	2.540e-013	2.540e-013	-12.595	-12.595	0.000
Zn(OH)2	5.858e-015	5.858e-015	-14.232	-14.232	0.000
Zn(OH)3-	1.539e-022	1.306e-022	-21.813	-21.884	-0.071



Zn(OH)4-2	3.114e-031	1.600e-031	-30.507	-30.796	-0.289
ZnClO4+	1.355e-033	1.150e-033	-32.868	-32.939	-0.071

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

Phase	SI	log IAP	log KT	
Al	-138.46	11.46	149.91	Al
Al(g)	-189.16	11.46	200.62	Al
Al2(SO4)3	-35.68	-16.78	18.90	Al2(SO4)3
Al2(SO4)3:6H2O	-18.34	-16.79	1.56	Al2(SO4)3:6H2O
Alabandite	-132.91	-133.33	-0.42	MnS
Alum-K	-7.83	-12.80	-4.97	KAl(SO4)2:12H2O
Alunite	1.73	1.26	-0.47	KAl3(OH)6(SO4)2
Anhydrite	-0.97	-5.32	-4.35	CaSO4
Antarcticite	-10.98	-6.88	4.09	CaCl2:6H2O
Antlerite	-8.38	0.35	8.73	Cu3(SO4)(OH)4
Aphthitalite	-12.75	-16.64	-3.89	NaK3(SO4)2
Aragonite	-6.27	-4.30	1.97	CaCO3
Arcanite	-6.97	-8.82	-1.84	K2SO4
Arsenolite	-53.01	-72.85	-19.84	As2O3
Arsenopyrite	-217.37	-231.81	-14.45	FeAsS
Artinite	-20.93	-1.30	19.63	Mg2CO3(OH)2:3H2O
As	-74.68	-32.00	42.68	As
As2O5	-19.83	-17.69	2.14	As2O5
As4O6(cubi)	-105.88	-145.70	-39.82	As4O6
As4O6(mono)	-105.65	-145.70	-40.05	As4O6
Atacamite	-11.94	2.33	14.26	Cu4Cl2(OH)6
Azurite	-17.01	-7.90	9.12	Cu3(CO3)2(OH)2
Bassanite	-1.61	-5.32	-3.71	CaSO4:0.5H2O
Birnessite	-2.14	-87.68	-85.55	Mn8O14:5H2O
Bischofite	-12.26	-7.87	4.39	MgCl2:6H2O
Bixbyite	-3.29	-4.26	-0.96	Mn2O3
Bloedite	-10.64	-13.12	-2.48	Na2Mg(SO4)2:4H2O
Boehmite	-0.52	7.03	7.55	AlO2H
Bornite	-496.64	-599.17	-102.53	Cu5FeS4
Brochantite	-11.53	3.89	15.42	Cu4(SO4)(OH)6
Brucite	-12.30	3.98	16.28	Mg(OH)2
Burkeite	-28.93	-19.44	9.49	Na6CO3(SO4)2
C	-67.50	-3.36	64.15	C
C(g)	-185.12	-3.36	181.77	C
Ca	-131.92	7.91	139.83	Ca
Ca(g)	-157.16	7.91	165.07	Ca
Ca2Al2O5:8H2O	-35.59	23.98	59.57	Ca2Al2O5:8H2O
Ca2Cl2(OH)2:H2O	-28.21	-1.92	26.29	Ca2Cl2(OH)2:H2O
Ca3(AsO4)2	-20.61	-2.80	17.80	Ca3(AsO4)2
Ca3Al2O6	-84.09	28.94	113.03	Ca3Al2O6
Ca4Al2Fe2O10	-94.02	46.46	140.48	Ca4Al2Fe2O10
Ca4Al2O7:13H2O	-73.35	33.90	107.25	Ca4Al2O7:13H2O
Ca4Al2O7:19H2O	-69.78	33.90	103.68	Ca4Al2O7:19H2O
Ca4Cl2(OH)6:13H2O	-60.33	8.00	68.33	Ca4Cl2(OH)6:13H2O
CaAl2O4	-27.89	19.02	46.91	CaAl2O4
CaAl2O4:10H2O	-18.98	19.02	37.99	CaAl2O4:10H2O
CaAl4O7	-35.51	33.08	68.59	CaAl4O7
Calcite	-6.13	-4.30	1.82	CaCO3
Carnallite	-17.33	-13.06	4.27	KMgCl3:6H2O
CaSO4:0.5H2O(beta)	-1.78	-5.32	-3.54	CaSO4:0.5H2O
CH4(g)	-138.70	-141.55	-2.84	CH4
Chalcanthite	-4.11	-6.74	-2.63	CuSO4:5H2O
Chalcocite	-129.49	-164.24	-34.74	Cu2S
Chalcocyanite	-9.65	-6.74	2.91	CuSO4
Chalcopyrite	-238.09	-270.69	-32.60	CuFeS2
Chloromagnesite	-29.68	-7.86	21.82	MgCl2
Cl2(g)	-17.79	-14.80	2.99	Cl2
Claudetite	-53.05	-72.85	-19.80	As2O3
CO(g)	-44.99	-47.98	-3.00	CO
CO2(g)	-1.43	-9.26	-7.83	CO2

Corundum	-4.23	14.06	18.29	Al2O3
Covellite	-110.35	-133.21	-22.86	CuS
Cu	-25.00	6.49	31.50	Cu
Cu(g)	-77.16	6.49	83.66	Cu
CuCl2	-12.02	-8.30	3.72	CuCl2
Cuprite	-25.58	-27.48	-1.91	Cu2O
Dawsonite	-4.84	-0.50	4.34	NaAlCO3(OH)2
Delafoosite	-1.03	-7.46	-6.44	CuFeO2
Diaspore	-0.12	7.03	7.15	AlHO2
Dolomite	-12.06	-9.58	2.47	CaMg(CO3)2
Dolomite-dis	-13.59	-9.58	4.01	CaMg(CO3)2
Dolomite-ord	-12.05	-9.58	2.46	CaMg(CO3)2
Epsomite	-4.34	-6.30	-1.96	MgSO4:7H2O
Ettringite	-49.49	12.98	62.46	Ca6Al2(SO4)3(OH)12:26H2O
Fe	-56.79	2.22	59.02	Fe
Fe(OH)2	-14.62	-0.73	13.89	Fe(OH)2
Fe(OH)3	0.64	6.28	5.64	Fe(OH)3
Fe2(SO4)3	-21.34	-18.29	3.05	Fe2(SO4)3
FeO	-14.25	-0.73	13.52	FeO
Ferrite-Ca	-3.98	17.52	21.50	CaFe2O4
Ferrite-Cu	5.81	16.10	10.28	CuFe2O4
Ferrite-Dicalcium	-34.32	22.48	56.80	Ca2Fe2O5
Ferrite-Mg	-4.49	16.53	21.02	MgFe2O4
Ferrite-Zn	3.95	15.65	11.70	ZnFe2O4
FeSO4	-13.62	-11.01	2.61	FeSO4
Gaylussite	-21.27	-10.10	11.16	CaNa2(CO3)2:5H2O
Gibbsite	-0.71	7.03	7.74	Al(OH)3
Glauberite	-6.67	-12.14	-5.47	Na2Ca(SO4)2
Goethite	5.75	6.28	0.53	FeOOH
Gypsum	-0.79	-5.32	-4.53	CaSO4:2H2O
H2(g)	-40.05	-43.15	-3.10	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-128.76	-136.76	-7.99	H2S
Halite	-5.75	-4.19	1.56	NaCl
Hausmannite	-10.98	-0.83	10.14	Mn3O4
HCl(g)	-12.22	-5.92	6.30	HCl
Hematite	12.48	12.55	0.08	Fe2O3
Hercynite	-15.47	13.33	28.80	FeAl2O4
Hexahydrite	-4.57	-6.30	-1.73	MgSO4:6H2O
Huntite	-30.36	-20.15	10.22	CaMg3(CO3)4
Hydromagnesite	-47.89	-17.15	30.74	Mg5(CO3)4(OH)2:4H2O
Hydrophilite	-18.63	-6.88	11.75	CaCl2
Hydrozincite	-33.35	-3.04	30.31	Zn5(OH)6(CO3)2
Ice	-0.14	-0.00	0.14	H2O
Jarosite	8.41	-1.00	-9.41	KFe3(SO4)2(OH)6
Jarosite-Na	5.45	-0.00	-5.45	NaFe3(SO4)2(OH)6
K	-68.77	2.21	70.98	K
K(g)	-79.37	2.21	81.58	K
K2CO3:1.5H2O	-21.18	-7.80	13.38	K2CO3:1.5H2O
K2O	-82.57	1.46	84.04	K2O
K3H(SO4)2	-14.74	-18.37	-3.62	K3H(SO4)2
K8H4(CO3)6:3H2O	-77.44	-49.73	27.71	K8H4(CO3)6:3H2O
Kainite	-11.18	-11.49	-0.31	KMgClSO4:3H2O
KAl(SO4)2	-16.07	-12.80	3.27	KAl(SO4)2
Kaliginite	-8.81	-8.53	0.28	KHCO3
Katoite	-50.00	28.94	78.94	Ca3Al2H12O12
Kieserite	-6.03	-6.30	-0.27	MgSO4:H2O
KMgCl3	-34.30	-13.05	21.25	KMgCl3
KMgCl3:2H2O	-27.02	-13.05	13.96	KMgCl3:2H2O
KNaCO3:6H2O	-17.06	-6.80	10.26	KNaCO3:6H2O
Lammerite	-8.62	-7.06	1.55	Cu3(AsO4)2
Lansfordite	-10.12	-5.28	4.84	MgCO3:5H2O
Lawrencite	-21.63	-12.57	9.05	FeCl2
Leonite	-11.01	-15.12	-4.11	K2Mg(SO4)2:4H2O
Lime	-27.61	4.96	32.57	CaO
Magnesite	-7.56	-5.28	2.27	MgCO3
Magnetite	1.41	11.83	10.42	Fe3O4

Malachite	-8.08	-2.18	5.90	Cu <sub>2</sub> CO <sub>3</sub> (OH) <sub>2</sub>
Manganite	-1.96	-2.13	-0.16	MnO(OH)
Manganosite	-14.49	3.42	17.92	MnO
Mayenite	-336.20	157.95	494.15	Ca <sub>12</sub> Al <sub>14</sub> O <sub>33</sub>
Melanterite	-8.61	-11.01	-2.40	FeSO <sub>4</sub> ·7H <sub>2</sub> O
Mercallite	-8.11	-9.55	-1.44	KHSO <sub>4</sub>
Mg	-115.59	6.93	122.52	Mg
Mg(g)	-135.31	6.93	142.25	Mg
Mg <sub>1.25</sub> SO <sub>4</sub> (OH)0.5:0.5H <sub>2</sub> O	-10.50	-5.30	5.20	Mg <sub>1.25</sub> SO <sub>4</sub> (OH)0.5:0.5H <sub>2</sub> O
Mg <sub>1.5</sub> SO <sub>4</sub> (OH)	-13.52	-4.31	9.21	Mg <sub>1.5</sub> SO <sub>4</sub> (OH)
MgCl <sub>2</sub> :2H <sub>2</sub> O	-20.60	-7.86	12.73	MgCl <sub>2</sub> :2H <sub>2</sub> O
MgCl <sub>2</sub> :4H <sub>2</sub> O	-15.17	-7.86	7.30	MgCl <sub>2</sub> :4H <sub>2</sub> O
MgCl <sub>2</sub> :H <sub>2</sub> O	-23.94	-7.86	16.07	MgCl <sub>2</sub> :H <sub>2</sub> O
MgOHCl	-17.83	-1.94	15.89	MgOHCl
MgSO <sub>4</sub>	-11.13	-6.30	4.83	MgSO <sub>4</sub>
Mirabilite	-5.67	-6.82	-1.15	Na <sub>2</sub> SO <sub>4</sub> :10H <sub>2</sub> O
Misenite	-55.04	-66.11	-11.08	K <sub>8</sub> H <sub>6</sub> (SO <sub>4</sub> ) <sub>7</sub>
Mn	-76.56	6.38	82.93	Mn
Mn(OH) <sub>2</sub> (am)	-11.89	3.42	15.31	Mn(OH) <sub>2</sub>
Mn(OH) <sub>3</sub>	-8.47	-2.13	6.34	Mn(OH) <sub>3</sub>
MnCl <sub>2</sub> :2H <sub>2</sub> O	-12.42	-8.42	4.00	MnCl <sub>2</sub> :2H <sub>2</sub> O
MnCl <sub>2</sub> :4H <sub>2</sub> O	-11.17	-8.42	2.75	MnCl <sub>2</sub> :4H <sub>2</sub> O
MnCl <sub>2</sub> :H <sub>2</sub> O	-13.96	-8.42	5.54	MnCl <sub>2</sub> :H <sub>2</sub> O
MnO <sub>2</sub> (gamma)	0.37	-15.75	-16.13	MnO <sub>2</sub>
MnSO <sub>4</sub>	-9.47	-6.86	2.61	MnSO <sub>4</sub>
Molysite	-24.96	-11.49	13.47	FeCl <sub>3</sub>
Monohydrocalcite	-6.98	-4.30	2.68	CaCO <sub>3</sub> :H <sub>2</sub> O
Na	-64.16	3.21	67.37	Na
Na(g)	-77.65	3.21	80.86	Na
Na <sub>2</sub> CO <sub>3</sub>	-16.96	-5.80	11.16	Na <sub>2</sub> CO <sub>3</sub>
Na <sub>2</sub> CO <sub>3</sub> :7H <sub>2</sub> O	-15.74	-5.80	9.94	Na <sub>2</sub> CO <sub>3</sub> :7H <sub>2</sub> O
Na <sub>2</sub> O	-63.96	3.46	67.42	Na <sub>2</sub> O
Na <sub>3</sub> H(SO <sub>4</sub> ) <sub>2</sub>	-14.48	-15.37	-0.89	Na <sub>3</sub> H(SO <sub>4</sub> ) <sub>2</sub>
Na <sub>4</sub> Ca(SO <sub>4</sub> ) <sub>3</sub> :2H <sub>2</sub> O	-13.06	-18.96	-5.89	Na <sub>4</sub> Ca(SO <sub>4</sub> ) <sub>3</sub> :2H <sub>2</sub> O
NaFeO <sub>2</sub>	-11.88	8.01	19.88	NaFeO <sub>2</sub>
Nahcolite	-7.39	-7.53	-0.14	NaHCO <sub>3</sub>
Nantokite	-12.90	-19.66	-6.77	CuCl
Natron	-15.39	-5.80	9.59	Na <sub>2</sub> CO <sub>3</sub> :10H <sub>2</sub> O
Nesquehonite	-10.57	-5.28	5.29	MgCO <sub>3</sub> :3H <sub>2</sub> O
O <sub>2</sub> (g)	-3.01	-5.90	-2.89	O <sub>2</sub>
Orpiment	-403.63	-483.11	-79.49	As <sub>2</sub> S <sub>3</sub>
Oxychloride-Mg	-23.79	2.04	25.83	Mg <sub>2</sub> Cl(OH) <sub>3</sub> :4H <sub>2</sub> O
Pentahydrite	-4.91	-6.30	-1.39	MgSO <sub>4</sub> :5H <sub>2</sub> O
Periclase	-17.34	3.98	21.33	MgO
Picromerite	-10.68	-15.12	-4.44	K <sub>2</sub> Mg(SO <sub>4</sub> ) <sub>2</sub> :6H <sub>2</sub> O
Pirssonite	-21.43	-10.10	11.32	Na <sub>2</sub> Ca(CO <sub>3</sub> ) <sub>2</sub> :2H <sub>2</sub> O
Polyhalite	-11.44	-25.76	-14.31	K <sub>2</sub> MgCa <sub>2</sub> (SO <sub>4</sub> ) <sub>4</sub> :2H <sub>2</sub> O
Portlandite	-17.59	4.96	22.55	Ca(OH) <sub>2</sub>
Pyrite	-217.92	-242.62	-24.70	FeS <sub>2</sub>
Pyrolusite	1.91	-15.75	-17.66	MnO <sub>2</sub>
Pyrrhotite	-133.74	-137.48	-3.74	FeS
Realgar	-157.01	-217.29	-60.28	AsS
Rhodochrosite	-5.62	-5.84	-0.22	MnCO <sub>3</sub>
S	-94.60	-139.71	-45.11	S
S <sub>2</sub> (g)	-203.09	-210.27	-7.19	S <sub>2</sub>
Scacchite	-17.16	-8.42	8.74	MnCl <sub>2</sub>
Siderite	-9.77	-9.99	-0.22	FeCO <sub>3</sub>
Smithsonite	-6.61	-6.17	0.44	ZnCO <sub>3</sub>
SO <sub>2</sub> (g)	-45.01	-44.83	0.18	SO <sub>2</sub>
Sphalerite	-122.19	-133.66	-11.47	ZnS
Spinel	-19.57	18.04	37.61	Al <sub>2</sub> MgO <sub>4</sub>
Starkeyite	-5.30	-6.30	-1.00	MgSO <sub>4</sub> :4H <sub>2</sub> O
Sylvite	-6.02	-5.19	0.83	KCl
Syngenite	-6.54	-14.14	-7.60	K <sub>2</sub> Ca(SO <sub>4</sub> ) <sub>2</sub> :H <sub>2</sub> O
Tachyhydrite	-39.76	-22.61	17.14	Mg <sub>2</sub> CaCl <sub>6</sub> :12H <sub>2</sub> O
Tenorite	-4.10	3.54	7.65	CuO
Thenardite	-6.46	-6.82	-0.36	Na <sub>2</sub> SO <sub>4</sub>

Thermonatrite	-16.74	-5.80	10.94	Na2CO3:H2O
Todorokite	-1.88	-47.70	-45.82	Mn7O12:3H2O
Troilite	-133.64	-137.48	-3.84	FeS
Trona-K	-26.92	-15.33	11.59	K2NaH(CO3)2:2H2O
Wurtzite	-124.49	-133.66	-9.17	ZnS
Wustite	-12.35	0.05	12.40	Fe.947O
Zincite	-8.10	3.10	11.20	ZnO
Zn	-62.74	6.05	68.79	Zn
Zn(ClO4)2:6H2O	-69.45	-63.82	5.63	Zn(ClO4)2:6H2O
Zn(g)	-79.36	6.05	85.41	Zn
Zn(OH)2(beta)	-8.84	3.10	11.93	Zn(OH)2
Zn(OH)2(epsilon)	-8.56	3.10	11.66	Zn(OH)2
Zn(OH)2(gamma)	-8.79	3.10	11.88	Zn(OH)2
Zn2(OH)3Cl	-15.02	0.27	15.29	Zn2(OH)3Cl
Zn2SO4(OH)2	-11.67	-4.09	7.58	Zn2SO4(OH)2
Zn3(AsO4)2	-17.71	-8.40	9.31	Zn3(AsO4)2
Zn3O(SO4)2	-30.36	-11.27	19.09	Zn3O(SO4)2
ZnCl2	-15.83	-8.75	7.08	ZnCl2
ZnCO3:H2O	-6.31	-6.17	0.14	ZnCO3:H2O
ZnSO4	-10.72	-7.18	3.53	ZnSO4
ZnSO4:6H2O	-5.49	-7.19	-1.70	ZnSO4:6H2O
ZnSO4:7H2O	-5.31	-7.19	-1.88	ZnSO4:7H2O
ZnSO4:H2O	-6.63	-7.18	-0.55	ZnSO4:H2O

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End of simulation.  
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Reading input data for simulation 2.  
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End of run.  
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