

Input file: C:\phreeqc\exmpls\Medard.pqi
Output file: C:\phreeqc\exmpls\Medard.pgo
Database file: c:\phreeqc\database\wateq4f.dat

Reading data base.

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:\phreeqc\database\wateq4f.dat
SOLUTION_MASTER_SPECIES
N(-3) NH4+ 0.0 N
SOLUTION_SPECIES
NH4+ = NH3 + H+
log_k -9.252
delta_h 12.48 kcal
analytical_expression 0.6322 -0.001225 -2835.76
NO3- + 10 H+ + 8 e- = NH4+ + 3 H2O
log_k 119.077
delta_h -187.055 kcal
gamma 2.5000 0.0000
SOLUTION 1 LAKE MEDARD MONIMOLIMNION'S WATER (quite imbalanced)
units ppm # unless otherwise stated
pH 7.6
density 1.002
temp 8.0
pe -3
Ca 6.09
Mg 15.01
Na 163591 ppb
K 8004 ppb
Al 0.0027
Mn 1.78 pe
Si 5274 ppb
Cl 192073 ppb
S(6) 1575.4
S(-2) 4.263 ppb # L.Q. AVS
N(5) 1.116 ppm as NO3
N(-3) 2.345 ppm as NH4
Fe 1.83 pe
C(4) 397
END

Beginning of initial solution calculations.

Initial solution 1. LAKE MEDARD MONIMOLIMNION'S WATER (quite imbalanced)

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

Elements	Molality	Moles
Al	1.003e-07	1.003e-07
C(4)	6.522e-03	6.522e-03
Ca	1.523e-04	1.523e-04
Cl	5.431e-03	5.431e-03

Fe	3.285e-05	3.285e-05
K	2.052e-04	2.052e-04
Mg	6.189e-04	6.189e-04
Mn	3.248e-05	3.248e-05
N(-3)	1.303e-04	1.303e-04
N(5)	1.804e-05	1.804e-05
Na	7.133e-03	7.133e-03
S(-2)	1.333e-07	1.333e-07
S(6)	1.644e-02	1.644e-02
Si	8.799e-05	8.799e-05

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

pH	=	7.600
pe	=	-3.000
Activity of water	=	0.999
Ionic strength (mol/kgw)	=	4.230e-02
Mass of water (kg)	=	1.000e+00
Total alkalinity (eq/kg)	=	6.155e-03
Total CO2 (mol/kg)	=	6.522e-03
Temperature (°C)	=	8.00
Electrical balance (eq)	=	-3.534e-02
Percent error, 100*(Cat- An)/(Cat+ An)	=	-68.23
Iterations	=	8
Total H	=	1.110194e+02
Total O	=	5.559156e+01

-----Redox couples-----

Redox couple	pe	Eh (volts)
N(-3)/N(5)	6.3193	0.3525
S(-2)/S(6)	-3.3819	-0.1887

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm ³ /mol
OH-	1.176e-07	9.724e-08	-6.929	-7.012	-0.083	(0)
H+	2.909e-08	2.512e-08	-7.536	-7.600	-0.064	0.00
H2O	5.551e+01	9.994e-01	1.744	-0.000	0.000	18.02
Al	1.003e-07					
Al(OH)4-	9.799e-08	8.180e-08	-7.009	-7.087	-0.078	(0)
Al(OH)3	1.246e-09	1.258e-09	-8.905	-8.900	0.004	(0)
Al(OH)2+	1.041e-09	8.762e-10	-8.982	-9.057	-0.075	(0)
AlOH+2	2.906e-11	1.457e-11	-10.537	-10.837	-0.300	(0)
AlSO4+	2.725e-12	2.274e-12	-11.565	-11.643	-0.078	(0)
Al(SO4)2-	6.198e-13	5.174e-13	-12.208	-12.286	-0.078	(0)
Al+3	4.347e-13	1.162e-13	-12.362	-12.935	-0.573	(0)
AlHSO4+2	9.346e-21	4.541e-21	-20.029	-20.343	-0.313	(0)
C(4)	6.522e-03					
HCO3-	6.073e-03	5.110e-03	-2.217	-2.292	-0.075	(0)
CO2	3.872e-04	3.910e-04	-3.412	-3.408	0.004	(0)
NaHCO3	1.638e-05	1.654e-05	-4.786	-4.781	0.004	(0)
MgHCO3+	1.348e-05	1.120e-05	-4.870	-4.951	-0.081	(0)
CO3-2	1.244e-05	6.235e-06	-4.905	-5.205	-0.300	(0)
FeHCO3+	5.408e-06	4.515e-06	-5.267	-5.345	-0.078	(0)
MnHCO3+	4.423e-06	3.709e-06	-5.354	-5.431	-0.076	(0)
MnCO3	3.994e-06	4.033e-06	-5.399	-5.394	0.004	(0)
CaHCO3+	2.402e-06	2.031e-06	-5.619	-5.692	-0.073	(0)
FeCO3	1.309e-06	1.321e-06	-5.883	-5.879	0.004	(0)
MgCO3	8.875e-07	8.962e-07	-6.052	-6.048	0.004	(0)
CaCO3	3.778e-07	3.815e-07	-6.423	-6.418	0.004	(0)
NaCO3-	3.199e-07	2.692e-07	-6.495	-6.570	-0.075	(0)
Ca	1.523e-04					
Ca+2	9.028e-05	4.536e-05	-4.044	-4.343	-0.299	(0)
CaSO4	5.925e-05	5.983e-05	-4.227	-4.223	0.004	(0)

	CaHCO3+	2.402e-06	2.031e-06	-5.619	-5.692	-0.073	(0)
	CaCO3	3.778e-07	3.815e-07	-6.423	-6.418	0.004	(0)
	CaOH+	3.542e-10	2.995e-10	-9.451	-9.524	-0.073	(0)
	CaHSO4+	8.854e-12	7.392e-12	-11.053	-11.131	-0.078	(0)
Cl	5.431e-03						
	Cl-	5.430e-03	4.495e-03	-2.265	-2.347	-0.082	(0)
	MnCl+	1.779e-07	1.491e-07	-6.750	-6.826	-0.076	(0)
	FeCl+	6.538e-08	5.482e-08	-7.185	-7.261	-0.076	(0)
	MnCl2	2.898e-10	2.927e-10	-9.538	-9.534	0.004	(0)
	MnCl3-	4.321e-13	3.624e-13	-12.364	-12.441	-0.076	(0)
	FeCl+2	4.871e-23	2.409e-23	-22.312	-22.618	-0.306	(0)
	FeCl2+	1.026e-24	8.565e-25	-23.989	-24.067	-0.078	(0)
	FeCl3	3.813e-28	3.850e-28	-27.419	-27.415	0.004	(0)
Fe (2)	3.285e-05						
	Fe+2	1.728e-05	8.835e-06	-4.763	-5.054	-0.291	(0)
	FeSO4	8.753e-06	8.838e-06	-5.058	-5.054	0.004	(0)
	FeHCO3+	5.408e-06	4.515e-06	-5.267	-5.345	-0.078	(0)
	FeCO3	1.309e-06	1.321e-06	-5.883	-5.879	0.004	(0)
	FeCl+	6.538e-08	5.482e-08	-7.185	-7.261	-0.076	(0)
	FeOH+	3.446e-08	2.890e-08	-7.463	-7.539	-0.076	(0)
	Fe (HS) 2	4.761e-11	4.808e-11	-10.322	-10.318	0.004	(0)
	Fe (OH) 2	2.020e-12	2.040e-12	-11.695	-11.690	0.004	(0)
	FeHSO4+	1.725e-12	1.440e-12	-11.763	-11.842	-0.078	(0)
	Fe (OH) 3-	3.013e-15	2.526e-15	-14.521	-14.598	-0.076	(0)
	Fe (HS) 3-	4.900e-16	4.091e-16	-15.310	-15.388	-0.078	(0)
Fe (3)	6.593e-13						
	Fe (OH) 3	4.295e-13	4.337e-13	-12.367	-12.363	0.004	(0)
	Fe (OH) 2+	2.207e-13	1.857e-13	-12.656	-12.731	-0.075	(0)
	Fe (OH) 4-	9.063e-15	7.626e-15	-14.043	-14.118	-0.075	(0)
	FeOH+2	5.647e-17	2.792e-17	-16.248	-16.554	-0.306	(0)
	FeSO4+	2.156e-20	1.808e-20	-19.666	-19.743	-0.076	(0)
	Fe (SO4) 2-	3.454e-21	2.884e-21	-20.462	-20.540	-0.078	(0)
	Fe+3	1.176e-21	3.142e-22	-20.930	-21.503	-0.573	(0)
	FeCl+2	4.871e-23	2.409e-23	-22.312	-22.618	-0.306	(0)
	FeCl2+	1.026e-24	8.565e-25	-23.989	-24.067	-0.078	(0)
	FeHSO4+2	2.647e-27	1.286e-27	-26.577	-26.891	-0.313	(0)
	FeCl3	3.813e-28	3.850e-28	-27.419	-27.415	0.004	(0)
	Fe2 (OH) 2+4	7.934e-31	4.421e-32	-30.100	-31.354	-1.254	(0)
	Fe3 (OH) 4+5	8.243e-40	0.000e+00	-39.084	-41.043	-1.959	(0)
H (0)	1.059e-12						
	H2	5.293e-13	5.345e-13	-12.276	-12.272	0.004	(0)
K	2.052e-04						
	K+	1.974e-04	1.634e-04	-3.705	-3.787	-0.082	(0)
	KSO4-	7.792e-06	6.557e-06	-5.108	-5.183	-0.075	(0)
Mg	6.189e-04						
	Mg+2	3.813e-04	1.956e-04	-3.419	-3.709	-0.290	(0)
	MgSO4	2.232e-04	2.254e-04	-3.651	-3.647	0.004	(0)
	MgHCO3+	1.348e-05	1.120e-05	-4.870	-4.951	-0.081	(0)
	MgCO3	8.875e-07	8.962e-07	-6.052	-6.048	0.004	(0)
	MgOH+	6.534e-09	5.547e-09	-8.185	-8.256	-0.071	(0)
Mn (2)	3.248e-05						
	Mn+2	1.593e-05	8.144e-06	-4.798	-5.089	-0.291	(0)
	MnSO4	7.954e-06	8.032e-06	-5.099	-5.095	0.004	(0)
	MnHCO3+	4.423e-06	3.709e-06	-5.354	-5.431	-0.076	(0)
	MnCO3	3.994e-06	4.033e-06	-5.399	-5.394	0.004	(0)
	MnCl+	1.779e-07	1.491e-07	-6.750	-6.826	-0.076	(0)
	MnOH+	2.285e-09	1.916e-09	-8.641	-8.718	-0.076	(0)
	MnCl2	2.898e-10	2.927e-10	-9.538	-9.534	0.004	(0)
	MnCl3-	4.321e-13	3.624e-13	-12.364	-12.441	-0.076	(0)
	Mn (NO3) 2	7.357e-15	7.429e-15	-14.133	-14.129	0.004	(0)
	Mn (OH) 3-	9.694e-18	8.129e-18	-17.013	-17.090	-0.076	(0)
Mn (3)	6.769e-35						
	Mn+3	6.769e-35	1.809e-35	-34.170	-34.743	-0.573	(0)
Mn (6)	0.000e+00						
	MnO4-2	0.000e+00	0.000e+00	-81.073	-81.379	-0.306	(0)
Mn (7)	0.000e+00						
	MnO4-	0.000e+00	0.000e+00	-94.857	-94.942	-0.085	(0)
N (-3)	1.303e-04						

NH4+	1.181e-04	9.656e-05	-3.928	-4.015	-0.087	(0)
NH4SO4-	1.160e-05	9.730e-06	-4.935	-5.012	-0.076	(0)
NH3	6.054e-07	6.114e-07	-6.218	-6.214	0.004	(0)
N (5)	1.804e-05					
NO3-	1.804e-05	1.483e-05	-4.744	-4.829	-0.085	(0)
Mn (NO3) 2	7.357e-15	7.429e-15	-14.133	-14.129	0.004	(0)
Na	7.133e-03					
Na+	6.877e-03	5.755e-03	-2.163	-2.240	-0.077	(0)
NaSO4-	2.392e-04	2.013e-04	-3.621	-3.696	-0.075	(0)
NaHCO3	1.638e-05	1.654e-05	-4.786	-4.781	0.004	(0)
NaCO3-	3.199e-07	2.692e-07	-6.495	-6.570	-0.075	(0)
O (0)	0.000e+00					
O2	0.000e+00	0.000e+00	-73.659	-73.655	0.004	(0)
S (-2)	1.333e-07					
HS-	9.453e-08	7.814e-08	-7.024	-7.107	-0.083	(0)
H2S	3.088e-08	3.118e-08	-7.510	-7.506	0.004	(0)
S6-2	6.646e-10	4.091e-10	-9.177	-9.388	-0.211	(0)
S5-2	5.152e-10	3.060e-10	-9.288	-9.514	-0.226	(0)
S4-2	3.009e-10	1.714e-10	-9.522	-9.766	-0.245	(0)
Fe (HS) 2	4.761e-11	4.808e-11	-10.322	-10.318	0.004	(0)
S-2	2.210e-13	1.093e-13	-12.656	-12.961	-0.306	(0)
S3-2	1.037e-13	5.622e-14	-12.984	-13.250	-0.266	(0)
S2-2	5.547e-15	2.881e-15	-14.256	-14.540	-0.284	(0)
Fe (HS) 3-	4.900e-16	4.091e-16	-15.310	-15.388	-0.078	(0)
S (6)	1.644e-02					
SO4-2	1.588e-02	7.822e-03	-1.799	-2.107	-0.308	(0)
NaSO4-	2.392e-04	2.013e-04	-3.621	-3.696	-0.075	(0)
MgSO4	2.232e-04	2.254e-04	-3.651	-3.647	0.004	(0)
CaSO4	5.925e-05	5.983e-05	-4.227	-4.223	0.004	(0)
NH4SO4-	1.160e-05	9.730e-06	-4.935	-5.012	-0.076	(0)
FeSO4	8.753e-06	8.838e-06	-5.058	-5.054	0.004	(0)
MnSO4	7.954e-06	8.032e-06	-5.099	-5.095	0.004	(0)
KSO4-	7.792e-06	6.557e-06	-5.108	-5.183	-0.075	(0)
HSO4-	1.624e-08	1.355e-08	-7.789	-7.868	-0.078	(0)
CaHSO4+	8.854e-12	7.392e-12	-11.053	-11.131	-0.078	(0)
AlSO4+	2.725e-12	2.274e-12	-11.565	-11.643	-0.078	(0)
FeHSO4+	1.725e-12	1.440e-12	-11.763	-11.842	-0.078	(0)
Al (SO4) 2-	6.198e-13	5.174e-13	-12.208	-12.286	-0.078	(0)
FeSO4+	2.156e-20	1.808e-20	-19.666	-19.743	-0.076	(0)
AlHSO4+2	9.346e-21	4.541e-21	-20.029	-20.343	-0.313	(0)
Fe (SO4) 2-	3.454e-21	2.884e-21	-20.462	-20.540	-0.078	(0)
FeHSO4+2	2.647e-27	1.286e-27	-26.577	-26.891	-0.313	(0)
Si	8.799e-05					
H4SiO4	8.766e-05	8.852e-05	-4.057	-4.053	0.004	(0)
H3SiO4-	3.223e-07	2.678e-07	-6.492	-6.572	-0.081	(0)
H2SiO4-2	4.246e-13	2.129e-13	-12.372	-12.672	-0.300	(0)

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

Phase	SI**	log IAP	log K(281 K,	1 atm)
Adularia	-1.09	-23.03	-21.94	KAlSi3O8
Al (OH) 3(a)	-2.11	9.86	11.97	Al (OH) 3
Albite	-2.33	-21.48	-19.15	NaAlSi3O8
AlumK	-15.45	-20.94	-5.49	KAl (SO4) 2:12H2O
Alunite	-2.03	-1.21	0.83	KAl3 (SO4) 2 (OH) 6
Analcime	-3.92	-17.43	-13.51	NaAlSi2O6:H2O
Anhydrite	-2.11	-6.45	-4.34	CaSO4
Annite	8.15	-80.26	-88.41	KFe3AlSi3O10 (OH) 2
Anorthite	-6.39	-26.62	-20.23	CaAl2Si2O8
Aragonite	-1.30	-9.55	-8.25	CaCO3
Artinite	-8.30	2.58	10.87	MgCO3:Mg (OH) 2:3H2O
Basaluminite	-0.55	22.15	22.70	Al4 (OH) 10SO4
Beidellite	0.50	-47.45	-47.95	(NaKMg0.5) 0.11Al2.33Si3.67O10 (OH) 2
Birnessite	-24.29	19.31	43.60	MnO2
Bixbyite	-23.95	-23.89	0.06	Mn2O3
Boehmite	0.03	9.86	9.83	AlOOH
Brucite	-6.55	11.49	18.04	Mg (OH) 2

Calcite	-1.14	-9.55	-8.40	CaCO3
Chalcedony	-0.29	-4.05	-3.76	SiO2
Chloritel4A	-10.07	65.03	75.09	Mg5Al2Si3O10(OH)8
Chlorite7A	-13.61	65.03	78.63	Mg5Al2Si3O10(OH)8
Chrysotile	-8.06	26.37	34.43	Mg3Si2O5(OH)4
Clinoenstatite	-4.79	7.44	12.23	MgSiO3
CO2(g)	-2.17	-3.41	-1.24	CO2
Cristobalite	-0.22	-4.05	-3.83	SiO2
Diaspore	1.89	9.86	7.97	AlOOH
Diopside	-7.09	14.24	21.33	CaMgSi2O6
Dolomite	-1.79	-18.46	-16.67	CaMg(CO3)2
Dolomite(d)	-2.41	-18.46	-16.05	CaMg(CO3)2
Epsomite	-3.55	-5.82	-2.26	MgSO4·7H2O
Fe(OH)2.7Cl.3	1.35	-1.69	-3.04	Fe(OH)2.7Cl0.3
Fe(OH)3(a)	-3.59	1.30	4.89	Fe(OH)3
Fe3(OH)8	-7.48	12.74	20.22	Fe3(OH)8
FeS(ppt)	-0.65	-4.56	-3.92	FeS
Forsterite	-11.53	18.93	30.46	Mg2SiO4
Gibbsite	0.74	9.86	9.12	Al(OH)3
Goethite	1.65	1.30	-0.36	FeOOH
Greenalite	1.52	22.33	20.81	Fe3Si2O5(OH)4
Greigite	-1.05	-46.09	-45.03	Fe3S4
Gypsum	-1.86	-6.45	-4.60	CaSO4·2H2O
H2(g)	-9.20	-12.27	-3.07	H2
H2O(g)	-1.98	-0.00	1.98	H2O
H2S(g)	-6.71	-7.51	-0.79	H2S
Halite	-6.13	-4.59	1.54	NaCl
Halloysite	-2.64	11.62	14.27	Al2Si2O5(OH)4
Hausmannite	-25.96	39.53	65.49	Mn3O4
Hematite	5.23	2.59	-2.64	Fe2O3
Huntite	-7.46	-36.29	-28.83	CaMg3(CO3)4
Hydromagnesite	-17.72	-24.17	-6.45	Mg5(CO3)4(OH)2·4H2O
Illite	-0.11	-42.80	-42.69	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite(ss)	-17.80	-27.63	-9.83	(K0.77Na0.03H0.2)Fe3(SO4)2(OH)6
Jarosite-K	-19.09	-26.91	-7.82	KFe3(SO4)2(OH)6
Jarosite-Na	-21.69	-25.36	-3.68	NaFe3(SO4)2(OH)6
JarositeH	-27.78	-30.72	-2.95	(H3O)Fe3(SO4)2(OH)6
Jurbanite	-4.21	-7.44	-3.23	AlOHSO4
Kaolinite	2.62	11.62	9.00	Al2Si2O5(OH)4
Kmica	5.91	21.25	15.33	KAl3Si3O10(OH)2
Laumontite	-2.01	-34.73	-32.72	CaAl2Si4O12·4H2O
Leonhardite	4.29	-69.45	-73.75	Ca2Al4Si8O24·7H2O
Mackinawite	0.09	-4.56	-4.65	FeS
Magadiite	-8.71	-23.01	-14.30	NaSi7O13(OH)3·3H2O
Maghemite	-3.79	2.59	6.39	Fe2O3
Magnesite	-1.16	-8.91	-7.76	MgCO3
Magnetite	6.77	12.74	5.97	Fe3O4
Manganite	-10.63	14.71	25.34	MnOOH
Melanterite	-4.72	-7.16	-2.44	FeSO4·7H2O
Mirabilite	-4.63	-6.59	-1.96	Na2SO4·10H2O
Mn2(SO4)3	-71.83	-75.81	-3.98	Mn2(SO4)3
MnCl2·4H2O	-11.72	-9.78	1.94	MnCl2·4H2O
MnS(Green)	-8.65	-4.60	4.06	MnS
MnSO4	-10.55	-7.20	3.36	MnSO4
Montmorillonite-Aberdeen	-0.50	-30.19	-29.69	(HNaK)0.14Mg0.45Fe0.33Al1.47Si3.82O10(OH)2
Montmorillonite-BelleFourche	0.40	-34.52	-34.91	(HNaK)0.09Mg0.29Fe0.24Al1.57Si3.93O10(OH)2
Montmorillonite-Ca	0.31	-47.30	-47.61	Ca0.165Al2.33Si3.67O10(OH)2
Nahcolite	-3.82	-4.53	-0.71	NaHCO3
Natron	-7.68	-9.69	-2.01	Na2CO3·10H2O
Nesquehonite	-3.55	-8.91	-5.36	MgCO3·3H2O
NH3(g)	-8.35	-6.21	2.13	NH3
Nsutite	-23.25	19.31	42.56	MnO2
O2(g)	-70.91	-73.65	-2.75	O2
Phillipsite	-2.38	-22.26	-19.87	Na0.5K0.5AlSi3O8·H2O
Phlogopite	-9.18	35.99	45.17	KMg3AlSi3O10(OH)2
Portlandite	-13.32	10.86	24.17	Ca(OH)2

Prehnite	-7.66	-19.82	-12.16	Ca ₂ Al ₂ Si ₃ O ₁₀ (OH) ₂
Pyrite	8.91	-10.07	-18.98	FeS ₂
Pyrochroite	-5.09	10.11	15.20	Mn(OH) ₂
Pyrolusite	-24.96	19.31	44.27	MnO ₂
Pyrophyllite	2.73	-45.58	-48.31	Al ₂ Si ₄ O ₁₀ (OH) ₂
Quartz	0.19	-4.05	-4.25	SiO ₂
Rhodochrosite	0.77	-10.29	-11.07	MnCO ₃
Rhodochrosite(d)	0.10	-10.29	-10.39	MnCO ₃
Sepiolite	-5.41	10.82	16.23	Mg ₂ Si ₃ O ₇ .5OH:3H ₂ O
Sepiolite(d)	-7.84	10.82	18.66	Mg ₂ Si ₃ O ₇ .5OH:3H ₂ O
Siderite	0.52	-10.26	-10.78	FeCO ₃
Siderite(d) (3)	0.19	-10.26	-10.45	FeCO ₃
Silicagel	-0.84	-4.05	-3.21	SiO ₂
SiO ₂ (a)	-1.19	-4.05	-2.86	SiO ₂
Sulfur	-3.59	-18.96	-15.38	S
Talc	-5.19	18.26	23.45	Mg ₃ Si ₄ O ₁₀ (OH) ₂
Thenardite	-6.43	-6.59	-0.15	Na ₂ SO ₄
Thermonatrite	-9.93	-9.69	0.25	Na ₂ CO ₃ :H ₂ O
Tremolite	-14.12	46.75	60.87	Ca ₂ Mg ₅ Si ₈ O ₂₂ (OH) ₂
Trona	-14.22	-14.22	0.00	NaHCO ₃ :Na ₂ CO ₃ :2H ₂ O
Wairakite	-6.86	-34.73	-27.87	CaAl ₂ Si ₄ O ₁₂ :2H ₂ O

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

```

EQUILIBRIUM PHASES 1
Calcite 0.0 CO2(g) 1      # Add CO2(g) until calcite saturation
    FIX_H+ -7.6 NaOH 10   # Add NaOH to pH 7.6
Halite -3.7 10           # Optimze conduct. to environmentally relevant
values.
Dolomite -1.87 0
PHASES
FIX_H+
    H+ = H+
        logK 0
END

```

End of simulation.

Reading input data for simulation 3.

```

TITLE pH is adjusted to measured monimolimic values
    conductance and pe OK, envirooneemntally relevant [C(4)] levels obtained by
iteration of dolomite SI: error significantly optimized
USE solution 1
USE equilibrium_phases 1
END

```

TITLE

```

pH is adjusted to measured monimolimic values
    conductance and pe OK, envirooneemntally relevant [C(4)] levels obtained by iteration of
dolomite SI: error significantly optimized

```

Beginning of batch-reaction calculations.

Reaction step 1.

WARNING: Calcite, Pure phase with add formula has not converged.
SI may be a local minimum. Residual: 2.729569e+00

Using solution 1. LAKE MEDARD MONIMOLIMNION'S WATER (quite imbalanced)
Using pure phase assemblage 1.

-----Phase assemblage-----

Phase	SI	log IAP	log K(T, P)	Moles in assemblage		
				Initial	Final	Delta
Calcite	-1.19	-9.59	-8.40			
CO2		is reactant		1.000e+00	9.994e-01	-6.017e-04
Dolomite	-1.87	-18.54	-16.67	0.000e+00	0	0.000e+00
FIX_H+	-7.60	-7.60	0.00			
NaOH		is reactant		1.000e+01	9.999e+00	-6.708e-04
Halite	-3.70	-2.16	1.54	1.000e+01	9.895e+00	-1.051e-01

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

Elements	Molality	Moles
Al	1.003e-07	1.003e-07
C	7.123e-03	7.124e-03
Ca	1.523e-04	1.523e-04
Cl	1.105e-01	1.105e-01
Fe	3.285e-05	3.285e-05
K	2.052e-04	2.052e-04
Mg	6.189e-04	6.189e-04
Mn	3.248e-05	3.248e-05
N	1.483e-04	1.483e-04
Na	1.129e-01	1.129e-01
S	1.644e-02	1.644e-02
Si	8.798e-05	8.799e-05

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

pH	=	7.600	Charge balance
pe	=	-3.680	Adjusted to redox equilibrium
Activity of water	=	0.996	
Ionic strength (mol/kgw)	=	1.441e-01	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	6.799e-03	
Total CO2 (mol/kg)	=	7.123e-03	
Temperature (°C)	=	8.00	
Electrical balance (eq)	=	-3.534e-02	
Percent error, 100*(Cat- An)/(Cat+ An)	=	-13.64	
Iterations	=	52	
Total H	=	1.110201e+02	
Total O	=	5.559343e+01	

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

Species	Molality	Activity	Log	Log	Log	mole V cm ³ /mol
			Molality	Activity	Gamma	
OH-	1.312e-07	9.690e-08	-6.882	-7.014	-0.132	(0)
H+	3.084e-08	2.512e-08	-7.511	-7.600	-0.089	0.00
H2O	5.551e+01	9.958e-01	1.744	-0.002	0.000	18.02
Al	1.003e-07					
Al(OH)4-	9.812e-08	7.425e-08	-7.008	-7.129	-0.121	(0)
Al(OH)3	1.108e-09	1.146e-09	-8.955	-8.941	0.014	(0)
Al(OH)2+	1.039e-09	8.011e-10	-8.983	-9.096	-0.113	(0)
AlOH+2	3.784e-11	1.337e-11	-10.422	-10.874	-0.452	(0)

AlSO4+	1.665e-12	1.260e-12	-11.779	-11.900	-0.121	(0)
Al+3	6.788e-13	1.070e-13	-12.168	-12.971	-0.803	(0)
Al (SO4) 2-	2.279e-13	1.725e-13	-12.642	-12.763	-0.121	(0)
AlHSO4+2	7.263e-21	2.515e-21	-20.139	-20.599	-0.461	(0)
C (-4)	9.803e-09					
CH4	9.803e-09	1.013e-08	-8.009	-7.994	0.014	(0)
C (4)	7.123e-03					
HCO3-	6.471e-03	4.989e-03	-2.189	-2.302	-0.113	(0)
CO2	3.706e-04	3.831e-04	-3.431	-3.417	0.014	(0)
NaHCO3	2.296e-04	2.373e-04	-3.639	-3.625	0.014	(0)
CO3-2	1.723e-05	6.086e-06	-4.764	-5.216	-0.452	(0)
MgHCO3+	1.368e-05	1.024e-05	-4.864	-4.990	-0.126	(0)
NaCO3-	5.010e-06	3.862e-06	-5.300	-5.413	-0.113	(0)
FeHCO3+	4.911e-06	3.767e-06	-5.309	-5.424	-0.115	(0)
MnHCO3+	3.950e-06	3.021e-06	-5.403	-5.520	-0.116	(0)
MnCO3	3.178e-06	3.285e-06	-5.498	-5.483	0.014	(0)
CaHCO3+	2.373e-06	1.850e-06	-5.625	-5.733	-0.108	(0)
FeCO3	1.067e-06	1.103e-06	-5.972	-5.958	0.014	(0)
MgCO3	7.926e-07	8.194e-07	-6.101	-6.087	0.014	(0)
CaCO3	3.362e-07	3.475e-07	-6.473	-6.459	0.014	(0)
Ca	1.523e-04					
Ca+2	1.171e-04	4.233e-05	-3.931	-4.373	-0.442	(0)
CaSO4	3.249e-05	3.359e-05	-4.488	-4.474	0.014	(0)
CaHCO3+	2.373e-06	1.850e-06	-5.625	-5.733	-0.108	(0)
CaCO3	3.362e-07	3.475e-07	-6.473	-6.459	0.014	(0)
CaOH+	3.573e-10	2.785e-10	-9.447	-9.555	-0.108	(0)
CaHSO4+	5.410e-12	4.150e-12	-11.267	-11.382	-0.115	(0)
Cl	1.105e-01					
Cl-	1.105e-01	8.202e-02	-0.957	-1.086	-0.129	(0)
MnCl+	2.968e-06	2.270e-06	-5.527	-5.644	-0.116	(0)
FeCl+	1.118e-06	8.550e-07	-5.952	-6.068	-0.116	(0)
MnCl2	7.863e-08	8.129e-08	-7.104	-7.090	0.014	(0)
MnCl3-	2.401e-09	1.836e-09	-8.620	-8.736	-0.116	(0)
FeCl+2	2.294e-22	7.849e-23	-21.639	-22.105	-0.466	(0)
FeCl2+	6.638e-23	5.093e-23	-22.178	-22.293	-0.115	(0)
FeCl3	4.041e-25	4.177e-25	-24.394	-24.379	0.014	(0)
Fe (2)	3.285e-05					
Fe+2	2.045e-05	7.552e-06	-4.689	-5.122	-0.433	(0)
FeHCO3+	4.911e-06	3.767e-06	-5.309	-5.424	-0.115	(0)
FeSO4	4.397e-06	4.545e-06	-5.357	-5.342	0.014	(0)
FeCl+	1.118e-06	8.550e-07	-5.952	-6.068	-0.116	(0)
FeCO3	1.067e-06	1.103e-06	-5.972	-5.958	0.014	(0)
Fe (HS) 2	8.698e-07	8.991e-07	-6.061	-6.046	0.014	(0)
FeOH+	3.218e-08	2.461e-08	-7.492	-7.609	-0.116	(0)
Fe (HS) 3-	1.475e-09	1.132e-09	-8.831	-8.946	-0.115	(0)
Fe (OH) 2	1.675e-12	1.731e-12	-11.776	-11.762	0.014	(0)
FeHSO4+	9.652e-13	7.404e-13	-12.015	-12.131	-0.115	(0)
Fe (OH) 3-	2.793e-15	2.136e-15	-14.554	-14.670	-0.116	(0)
Fe (3)	1.186e-13					
Fe (OH) 3	7.414e-14	7.664e-14	-13.130	-13.116	0.014	(0)
Fe (OH) 2+	4.271e-14	3.293e-14	-13.369	-13.482	-0.113	(0)
Fe (OH) 4-	1.742e-15	1.343e-15	-14.759	-14.872	-0.113	(0)
FeOH+2	1.452e-17	4.969e-18	-16.838	-17.304	-0.466	(0)
FeSO4+	2.540e-21	1.943e-21	-20.595	-20.712	-0.116	(0)
Fe+3	3.561e-22	5.611e-23	-21.448	-22.251	-0.803	(0)
Fe (SO4) 2-	2.430e-22	1.864e-22	-21.614	-21.729	-0.115	(0)
FeCl+2	2.294e-22	7.849e-23	-21.639	-22.105	-0.466	(0)
FeCl2+	6.638e-23	5.093e-23	-22.178	-22.293	-0.115	(0)
FeCl3	4.041e-25	4.177e-25	-24.394	-24.379	0.014	(0)
FeHSO4+2	3.990e-28	1.382e-28	-27.399	-27.860	-0.461	(0)
Fe2 (OH) 2+4	9.732e-32	1.400e-33	-31.012	-32.854	-1.842	(0)
Fe3 (OH) 4+5	0.000e+00	0.000e+00	-40.416	-43.294	-2.878	(0)
H (0)	2.369e-11					
H2	1.184e-11	1.224e-11	-10.927	-10.912	0.014	(0)
K	2.052e-04					
K+	2.005e-04	1.489e-04	-3.698	-3.827	-0.129	(0)
KSO4-	4.662e-06	3.594e-06	-5.331	-5.444	-0.113	(0)
Mg	6.189e-04					

Mg+2	4.815e-04	1.832e-04	-3.317	-3.737	-0.420	(0)
MgSO4	1.229e-04	1.270e-04	-3.911	-3.896	0.014	(0)
MgHCO3+	1.368e-05	1.024e-05	-4.864	-4.990	-0.126	(0)
MgCO3	7.926e-07	8.194e-07	-6.101	-6.087	0.014	(0)
MgOH+	6.584e-09	5.176e-09	-8.182	-8.286	-0.104	(0)
Mn (2)	3.248e-05					
Mn+2	1.840e-05	6.794e-06	-4.735	-5.168	-0.433	(0)
MnHCO3+	3.950e-06	3.021e-06	-5.403	-5.520	-0.116	(0)
MnSO4	3.900e-06	4.031e-06	-5.409	-5.395	0.014	(0)
MnCO3	3.178e-06	3.285e-06	-5.498	-5.483	0.014	(0)
MnCl+	2.968e-06	2.270e-06	-5.527	-5.644	-0.116	(0)
MnCl2	7.863e-08	8.129e-08	-7.104	-7.090	0.014	(0)
MnCl3-	2.401e-09	1.836e-09	-8.620	-8.736	-0.116	(0)
MnOH+	2.082e-09	1.593e-09	-8.681	-8.798	-0.116	(0)
Mn (OH) 3-	8.772e-18	6.709e-18	-17.057	-17.173	-0.116	(0)
Mn (NO3) 2	0.000e+00	0.000e+00	-175.338	-175.324	0.014	(0)
Mn (3)	2.001e-35					
Mn+3	2.001e-35	3.153e-36	-34.699	-35.501	-0.803	(0)
Mn (6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-83.718	-84.184	-0.466	(0)
Mn (7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-98.289	-98.427	-0.137	(0)
N (-3)	3.940e-05					
NH4+	3.712e-05	2.665e-05	-4.430	-4.574	-0.144	(0)
NH4SO4-	2.112e-06	1.616e-06	-5.675	-5.792	-0.116	(0)
NH3	1.632e-07	1.687e-07	-6.787	-6.773	0.014	(0)
N (0)	1.090e-04					
N2	5.448e-05	5.631e-05	-4.264	-4.249	0.014	(0)
N (3)	0.000e+00					
NO2-	0.000e+00	0.000e+00	-62.600	-62.716	-0.115	(0)
N (5)	0.000e+00					
NO3-	0.000e+00	0.000e+00	-85.249	-85.387	-0.137	(0)
Mn (NO3) 2	0.000e+00	0.000e+00	-175.338	-175.324	0.014	(0)
Na	1.129e-01					
Na+	1.103e-01	8.460e-02	-0.957	-1.073	-0.115	(0)
NaSO4-	2.309e-03	1.780e-03	-2.637	-2.750	-0.113	(0)
NaHCO3	2.296e-04	2.373e-04	-3.639	-3.625	0.014	(0)
NaCO3-	5.010e-06	3.862e-06	-5.300	-5.413	-0.113	(0)
O (0)	0.000e+00					
O2	0.000e+00	0.000e+00	-76.392	-76.377	0.014	(0)
S (-2)	2.321e-05					
HS-	1.565e-05	1.156e-05	-4.806	-4.937	-0.132	(0)
H2S	4.462e-06	4.613e-06	-5.350	-5.336	0.014	(0)
Fe (HS) 2	8.698e-07	8.991e-07	-6.061	-6.046	0.014	(0)
S6-2	1.142e-07	6.052e-08	-6.942	-7.218	-0.276	(0)
S5-2	9.102e-08	4.526e-08	-7.041	-7.344	-0.303	(0)
S4-2	5.507e-08	2.535e-08	-7.259	-7.596	-0.337	(0)
Fe (HS) 3-	1.475e-09	1.132e-09	-8.831	-8.946	-0.115	(0)
S-2	4.724e-11	1.617e-11	-10.326	-10.791	-0.466	(0)
S3-2	1.990e-11	8.317e-12	-10.701	-11.080	-0.379	(0)
S2-2	1.115e-12	4.262e-13	-11.953	-12.370	-0.418	(0)
S (6)	1.642e-02					
SO4-2	1.394e-02	4.706e-03	-1.856	-2.327	-0.471	(0)
NaSO4-	2.309e-03	1.780e-03	-2.637	-2.750	-0.113	(0)
MgSO4	1.229e-04	1.270e-04	-3.911	-3.896	0.014	(0)
CaSO4	3.249e-05	3.359e-05	-4.488	-4.474	0.014	(0)
KSO4-	4.662e-06	3.594e-06	-5.331	-5.444	-0.113	(0)
FeSO4	4.397e-06	4.545e-06	-5.357	-5.342	0.014	(0)
MnSO4	3.900e-06	4.031e-06	-5.409	-5.395	0.014	(0)
NH4SO4-	2.112e-06	1.616e-06	-5.675	-5.792	-0.116	(0)
HSO4-	1.078e-08	8.155e-09	-7.968	-8.089	-0.121	(0)
CaHSO4+	5.410e-12	4.150e-12	-11.267	-11.382	-0.115	(0)
AlSO4+	1.665e-12	1.260e-12	-11.779	-11.900	-0.121	(0)
FeHSO4+	9.652e-13	7.404e-13	-12.015	-12.131	-0.115	(0)
Al (SO4) 2-	2.279e-13	1.725e-13	-12.642	-12.763	-0.121	(0)
AlHSO4+2	7.263e-21	2.515e-21	-20.139	-20.599	-0.461	(0)
FeSO4+	2.540e-21	1.943e-21	-20.595	-20.712	-0.116	(0)
Fe (SO4) 2-	2.430e-22	1.864e-22	-21.614	-21.729	-0.115	(0)

FeHSO4+2	3.990e-28	1.382e-28	-27.399	-27.860	-0.461	(0)
Si	8.798e-05					
H4SiO4	8.762e-05	9.057e-05	-4.057	-4.043	0.014	(0)
H3SiO4-	3.663e-07	2.740e-07	-6.436	-6.562	-0.126	(0)
H2SiO4-2	6.165e-13	2.178e-13	-12.210	-12.662	-0.452	(0)

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

Phase	SI**	log IAP	log K(281 K, 1 atm)	
Adularia	-1.13	-23.07	-21.94	KAlSi3O8
Al (OH) 3 (a)	-2.15	9.82	11.97	Al (OH) 3
Albite	-1.17	-20.32	-19.15	NaAlSi3O8
AlumK	-15.98	-21.47	-5.49	KAl (SO4) 2:12H2O
Alunite	-2.63	-1.81	0.83	KAl3 (SO4) 2 (OH) 6
Analcime	-2.77	-16.28	-13.51	NaAlSi2O6:H2O
Anhydrite	-2.36	-6.70	-4.34	CaSO4
Annite	7.90	-80.52	-88.41	KFe3AlSi3O10 (OH) 2
Anorthite	-6.48	-26.70	-20.23	CaAl2Si2O8
Aragonite	-1.34	-9.59	-8.25	CaCO3
Artinite	-8.37	2.50	10.87	MgCO3:Mg (OH) 2:3H2O
Basaluminite	-0.93	21.77	22.70	Al4 (OH) 10SO4
Beidellite	0.58	-47.37	-47.95	(NaKMg0.5) 0.11Al2.33Si3.67O10 (OH) 2
Birnessite	-25.73	17.87	43.60	MnO2
Bixbyite	-25.47	-25.41	0.06	Mn2O3
Boehmite	-0.01	9.83	9.83	AlOOH
Brucite	-6.58	11.46	18.04	Mg (OH) 2
Calcite	-1.19	-9.59	-8.40	CaCO3
CH4 (g)	-5.28	-7.99	-2.71	CH4
Chalcedony	-0.28	-4.04	-3.76	SiO2
Chloritel4A	-10.26	64.83	75.09	Mg5Al2Si3O10 (OH) 8
Chlorite7A	-13.80	64.83	78.63	Mg5Al2Si3O10 (OH) 8
Chrysotile	-8.13	26.30	34.43	Mg3Si2O5 (OH) 4
Clinoenstatite	-4.81	7.42	12.23	MgSiO3
CO2 (g)	-2.18	-3.42	-1.24	CO2
Cristobalite	-0.21	-4.04	-3.83	SiO2
Diaspore	1.85	9.83	7.97	AlOOH
Diopside	-7.12	14.21	21.33	CaMgSi2O6
Dolomite	-1.87	-18.54	-16.67	CaMg (CO3) 2
Dolomite (d)	-2.49	-18.54	-16.05	CaMg (CO3) 2
Epsomite	-3.81	-6.08	-2.26	MgSO4:7H2O
Fe (OH) 2.7Cl1.3	0.98	-2.06	-3.04	Fe (OH) 2.7Cl10.3
Fe (OH) 3 (a)	-4.35	0.54	4.89	Fe (OH) 3
Fe3 (OH) 8	-9.06	11.16	20.22	Fe3 (OH) 8
FeS (ppt)	1.46	-2.46	-3.92	FeS
FIX_H+	-7.60	-7.60	0.00	H+
Forsterite	-11.58	18.88	30.46	Mg2SiO4
Gibbsite	0.70	9.82	9.12	Al (OH) 3
Goethite	0.90	0.55	-0.36	FeOOH
Greenalite	1.34	22.15	20.81	Fe3Si2O5 (OH) 4
Greigite	6.06	-38.97	-45.03	Fe3S4
Gypsum	-2.11	-6.70	-4.60	CaSO4:2H2O
H2 (g)	-7.84	-10.91	-3.07	H2
H2O (g)	-1.98	-0.00	1.98	H2O
H2S (g)	-4.54	-5.34	-0.79	H2S
Halite	-3.70	-2.16	1.54	NaCl
Halloysite	-2.70	11.57	14.27	Al2Si2O5 (OH) 4
Hausmannite	-27.56	37.93	65.49	Mn3O4
Hematite	3.73	1.09	-2.64	Fe2O3
Huntite	-7.62	-36.45	-28.83	CaMg3 (CO3) 4
Hydromagnesite	-17.91	-24.36	-6.45	Mg5 (CO3) 4 (OH) 2:4H2O
Illite	-0.19	-42.88	-42.69	K0.6Mg0.25Al2.3Si3.5O10 (OH) 2
Jarosite (ss)	-20.49	-30.32	-9.83	(K0.77Na0.03H0.2) Fe3 (SO4) 2 (OH) 6
Jarosite-K	-21.82	-29.65	-7.82	KFe3 (SO4) 2 (OH) 6
Jarosite-Na	-23.21	-26.89	-3.68	NaFe3 (SO4) 2 (OH) 6
JarositeH	-30.47	-33.42	-2.95	(H3O) Fe3 (SO4) 2 (OH) 6
Jurbanite	-4.47	-7.70	-3.23	AlOHSO4
Kaolinite	2.57	11.57	9.00	Al2Si2O5 (OH) 4

Kmica	5.80	21.13	15.33	KAl3Si3O10(OH)2
Laumontite	-2.07	-34.79	-32.72	CaAl2Si4O12:4H2O
Leonhardite	4.17	-69.58	-73.75	Ca2Al4Si8O24:7H2O
Mackinawite	2.19	-2.46	-4.65	FeS
Magadiite	-7.46	-21.76	-14.30	NaSi7O13(OH)3:3H2O
Maghemite	-5.29	1.09	6.39	Fe2O3
Magnesite	-1.20	-8.95	-7.76	MgCO3
Magnetite	5.20	11.17	5.97	Fe3O4
Manganite	-11.39	13.95	25.34	MnOOH
Melanterite	-5.02	-7.46	-2.44	FeSO4:7H2O
Mirabilite	-2.54	-4.49	-1.96	Na2SO4:10H2O
Mn2(SO4)3	-74.00	-77.98	-3.98	Mn2(SO4)3
MnCl2:4H2O	-9.29	-7.35	1.94	MnCl2:4H2O
MnS(Green)	-6.56	-2.50	4.06	MnS
MnSO4	-10.85	-7.50	3.36	MnSO4
Montmorillonite-Aberdeen	-0.61	-30.30	-29.69	(HNaK)0.14Mg0.45Fe0.33Al1.47Si3.82O10(OH)2
Montmorillonite-BelleFourche	0.30	-34.61	-34.91	(HNaK)0.09Mg0.29Fe0.24Al1.57Si3.93O10(OH)2
Montmorillonite-Ca	0.27	-47.35	-47.61	Ca0.165Al2.33Si3.67O10(OH)2
N2(g)	-1.05	-4.25	-3.20	N2
Nahcolite	-2.66	-3.37	-0.71	NaHCO3
Natron	-5.37	-7.38	-2.01	Na2CO3:10H2O
Nesquehonite	-3.59	-8.96	-5.36	MgCO3:3H2O
NH3(g)	-8.90	-6.77	2.13	NH3
Nsutite	-24.70	17.87	42.56	MnO2
O2(g)	-73.63	-76.38	-2.75	O2
Phillipsite	-1.82	-21.70	-19.87	Na0.5K0.5AlSi3O8:H2O
Phlogopite	-9.31	35.86	45.17	KMg3AlSi3O10(OH)2
Portlandite	-13.35	10.82	24.17	Ca(OH)2
Prehnite	-7.76	-19.92	-12.16	Ca2Al2Si3O10(OH)2
Pyrite	11.82	-7.16	-18.98	FeS2
Pyrochroite	-5.17	10.03	15.20	Mn(OH)2
Pyrolusite	-26.40	17.87	44.27	MnO2
Pyrophyllite	2.71	-45.61	-48.31	Al2Si4O10(OH)2
Quartz	0.21	-4.04	-4.25	SiO2
Rhodochrosite	0.68	-10.38	-11.07	MnCO3
Rhodochrosite(d)	0.01	-10.38	-10.39	MnCO3
Sepiolite	-5.44	10.80	16.23	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-7.86	10.80	18.66	Mg2Si3O7.5OH:3H2O
Siderite	0.44	-10.34	-10.78	FeCO3
Siderite(d)(3)	0.11	-10.34	-10.45	FeCO3
Silicagel	-0.82	-4.04	-3.21	SiO2
SiO2(a)	-1.18	-4.04	-2.86	SiO2
Sulfur	-2.78	-18.15	-15.38	S
Talc	-5.23	18.22	23.45	Mg3Si4O10(OH)2
Thenardite	-4.32	-4.47	-0.15	Na2SO4
Thermonatrite	-7.61	-7.36	0.25	Na2CO3:H2O
Tremolite	-14.23	46.64	60.87	Ca2Mg5Si8O22(OH)2
Trona	-10.74	-10.74	0.00	NaHCO3:Na2CO3:2H2O
Wairakite	-6.92	-34.79	-27.87	CaAl2Si4O12:2H2O

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 4.

End of Run after 0.104 Seconds.
