```
   Input file: H:\dos\Conferences&Publications\Paper for Building and environment\C32_@_
1C.pqi
  Output file: H:\dos\Conferences&Publications\Paper for Building and environment\C32_@_
1C.pqo
Database file: C:\Program Files\USGS\Phreeqc Interactive 3.1.7-9213\database\llnl.dat

------------------
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\USGS\Phreeqc Interactive 3.1.7-9213\database\llnl.dat
      SOLUTION 1
          temp      25
          pH        7 charge
          pe        4
          redox     pe
          units     mol/kgw
          density   1
          Alkalinity 0
          water    1 # kg
      EQUILIBRIUM_PHASES 1
          Calcite 0 1000
          CO2(g)    -3.408822658 100
          SO2(g)    -5.149185349 100
      END
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

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

      Elements           Molality       Moles

      Pure water

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

                                       pH  =   7.008      Charge balance
                                       pe  =   4.000
                          Activity of water  =   1.000
                             Ionic strength  =   9.819e-08
                            Mass of water (kg)  =   1.000e+00
                  Total alkalinity (eq/kg)  =   1.060e-17
                     Total carbon (mol/kg)  =   0.000e+00
                        Total CO2 (mol/kg)  =   0.000e+00
                          Temperature (°C)  =  25.00
                   Electrical balance (eq)  =  -1.060e-17
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                                Iterations  =   2
```

```
                                  Total H  = 1.110507e+02
                                  Total O  = 5.552533e+01

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

                                                 Log       Log       Log    mole V
   Species          Molality    Activity  Molality  Activity     Gamma   cm³/mol

   OH-             9.819e-08   9.816e-08    -7.008    -7.008    -0.000     (0)
   H+              9.819e-08   9.816e-08    -7.008    -7.008    -0.000      0.00
   H2O             5.553e+01   1.000e+00     1.744    -0.000     0.000     18.07
H(0)          1.529e-25
   H2              7.645e-26   7.645e-26   -25.117   -25.117     0.000     (0)
O(0)          0.000e+00
   O2              0.000e+00   0.000e+00   -41.963   -41.963     0.000     (0)

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

  Phase               SI** log IAP   log K(298 K,   1 atm)

  H2(g)           -22.02    -25.12   -3.10  H2
  H2O(g)           -1.59     -0.00    1.59  H2O
  Ice              -0.14     -0.00    0.14  H2O
  O2(g)           -39.07    -41.96   -2.89  O2

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

-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying smaller step size, pe step size 10, 5 ...

WARNING: Maximum iterations exceeded, 200

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying reduced tolerance 1e-16 ...

WARNING: Maximum iterations exceeded, 200

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying increased tolerance 1e-14 ...

WARNING: Maximum iterations exceeded, 200

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying diagonal scaling ...

WARNING: Maximum iterations exceeded, 200

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying diagonal scaling and reduced tolerance 1e-16 ...

WARNING: Maximum iterations exceeded, 200
```

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying scaling pure_phase columns 1e-10 ...

WARNING: Maximum iterations exceeded, 200

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying scaling pure_phase columns and diagonal scale 1e-10 ...

WARNING: Maximum iterations exceeded, 200

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying increased scaling 1e-09 ...

WARNING: Maximum iterations exceeded, 200

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Skipping optimize equations for first 5 iterations ...

WARNING: Maximum iterations exceeded, 100

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Adding inequality to make concentrations greater than zero.

WARNING: Maximum iterations exceeded, 100

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying reduced tolerance 1e-17 ...

WARNING: Maximum iterations exceeded, 200

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying reduced tolerance 1e-18 ...

WARNING: Maximum iterations exceeded, 200

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: The program has failed to converge to a numerical solution.

The following equations were not satisfied:
ERROR: Ca has not converged. Total: 6.901962e+01 Calculated: 7.019413e+01 Residual: -1.174515e+00

ERROR: S has not converged. Total: 1.000000e+02 Calculated: 1.036891e+02 Residual: -3.689147e+00

ERROR: Mu Ionic strength has not converged. Residual: -1.807823e+00

ERROR: A(H2O) Activity of water has not converged. Residual: 1.855386e-01

ERROR: pH Charge balance has not converged. Residual: 1.889538e+00

ERROR: Hydrogen Mass of hydrogen has not converged. Residual: -3.434445e+01

ERROR: Oxygen Mass of oxygen has not converged. Residual: 8.856744e+00

ERROR: Calcite Pure phase has not converged. Residual: -5.737553e+00

Using solution 1.

Using pure phase assemblage 1.

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

Phase	SI	log IAP	log K(T, P)	Moles in assemblage Initial	Final	Delta
CO2(g)	-3.77	-11.59	-7.83	1.000e+02	1.692e+02	6.917e+01
Calcite	2.49	4.32	1.82	1.000e+03	9.310e+02	-6.902e+01
SO2(g)	-17.29	-17.12	0.18	1.000e+02	0	-1.000e+02

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

Elements	Molality	Moles
C	2.131e-03	2.450e-03
Ca	6.105e+01	7.019e+01
S	9.018e+01	1.037e+02

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

pH	= 12.326	Charge balance
pe	= -4.357	Adjusted to redox equilibrium
Activity of water	= 0.000	
Ionic strength	= 2.584e+01	
Mass of water (kg)	= 1.150e+00	
Total alkalinity (eq/kg)	= 1.436e+01	
Total CO2 (mol/kg)	= 2.131e-03	
Temperature (°C)	= 25.00	
Electrical balance (eq)	= -1.890e+00	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -5.99	
Iterations	= 201	
Total H	= 1.276816e+02	
Total O	= 3.153837e+02	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	9.174e-13	4.392e-12	-12.037	-11.357	0.680	(0)
H+	5.977e-14	4.721e-13	-13.224	-12.326	0.898	0.00
H2O	5.553e+01	2.152e-10	1.744	-9.667	0.000	18.07
C(-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-76.574	-76.574	0.000	(0)
C(-3)	4.757e-24					
C2H6	2.379e-24	2.379e-24	-23.624	-23.624	0.000	(0)
C(-4)	7.777e-29					
CH4	7.777e-29	7.777e-29	-28.109	-28.109	0.000	(0)
C(2)	2.883e-17					
CO	2.883e-17	2.883e-17	-16.540	-16.540	0.000	(0)
C(4)	2.131e-03					
CaCO3	2.131e-03	2.131e-03	-2.671	-2.671	0.000	(0)
CO3-2	1.579e-07	1.091e-07	-6.802	-6.962	-0.161	(0)
CO2	2.584e-08	5.906e-06	-7.588	-5.229	2.359	(0)
CaHCO3+	2.202e-08	1.159e-07	-7.657	-6.936	0.721	(0)
HCO3-	2.205e-10	1.161e-09	-9.657	-8.935	0.721	(0)
Ca	6.105e+01					
CaSO4	5.461e+01	5.461e+01	1.737	1.737	0.000	(0)
Ca+2	6.443e+00	8.430e+00	0.809	0.926	0.117	(0)
CaCO3	2.131e-03	2.131e-03	-2.671	-2.671	0.000	(0)
CaHCO3+	2.202e-08	1.159e-07	-7.657	-6.936	0.721	(0)
CaOH+	1.031e-10	5.428e-10	-9.987	-9.265	0.721	(0)
H(0)	8.026e-22					
H2	4.013e-22	9.173e-20	-21.397	-19.037	2.359	(0)
O(0)	0.000e+00					

O2	0.000e+00	0.000e+00	-75.814	-73.455	2.359	(0)
S(-2)	3.549e+01					
S5-2	6.793e+00	3.456e+00	0.832	0.539	-0.293	(0)
S4-2	3.724e-01	1.895e-01	-0.429	-0.722	-0.293	(0)
S3-2	1.240e-02	6.309e-03	-1.907	-2.200	-0.293	(0)
S2-2	2.446e-04	1.245e-04	-3.612	-3.905	-0.293	(0)
S-2	2.516e-06	2.234e-06	-5.599	-5.651	-0.052	(0)
HS-	1.858e-06	8.892e-06	-5.731	-5.051	0.680	(0)
H2S	4.291e-11	4.291e-11	-10.367	-10.367	0.000	(0)
S(2)	2.190e-04					
S2O3-2	1.095e-04	5.571e-05	-3.961	-4.254	-0.293	(0)
HS2O3-	5.159e-17	2.716e-16	-16.287	-15.566	0.721	(0)
S(3)	2.772e-26					
S2O4-2	1.386e-26	1.230e-26	-25.858	-25.910	-0.052	(0)
S(4)	8.268e-12					
SO3-2	8.268e-12	5.711e-12	-11.083	-11.243	-0.161	(0)
HSO3-	8.729e-18	4.595e-17	-17.059	-16.338	0.721	(0)
SO2	7.671e-18	7.671e-18	-17.115	-17.115	0.000	(0)
S4O6-2	2.046e-18	1.041e-18	-17.689	-17.982	-0.293	(0)
H2SO3	2.079e-27	2.079e-27	-26.682	-26.682	0.000	(0)
S5O6-2	3.624e-32	1.844e-32	-31.441	-31.734	-0.293	(0)
S2O6-2	9.149e-33	4.655e-33	-32.039	-32.332	-0.293	(0)
S3O6-2	1.526e-33	7.764e-34	-32.817	-33.110	-0.293	(0)
S(5)	5.702e-28					
S2O5-2	2.851e-28	1.451e-28	-27.545	-27.838	-0.293	(0)
S(6)	5.469e+01					
CaSO4	5.461e+01	5.461e+01	1.737	1.737	0.000	(0)
SO4-2	8.715e-02	4.435e-02	-1.060	-1.353	-0.293	(0)
HSO4-	4.017e-13	2.115e-12	-12.396	-11.675	0.721	(0)
H2SO4	9.420e-28	9.420e-28	-27.026	-27.026	0.000	(0)
S(7)	0.000e+00					
S2O8-2	0.000e+00	0.000e+00	-76.580	-76.874	-0.293	(0)
S(8)	0.000e+00					
HSO5-	0.000e+00	0.000e+00	-68.389	-67.667	0.721	(0)

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

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Anhydrite	3.92	-0.43	-4.35	CaSO4
Aragonite	2.35	4.32	1.97	CaCO3
Bassanite	-1.55	-5.26	-3.71	CaSO4:0.5H2O
C	-2.28	61.86	64.15	C
C(g)	-119.90	61.86	181.77	C
Ca	-87.19	52.64	139.83	Ca
Ca(g)	-112.43	52.64	165.07	Ca
Calcite	2.49	4.32	1.82	CaCO3
CaSO4:0.5H2O(beta)	-1.73	-5.26	-3.54	CaSO4:0.5H2O
CH4(g)	-25.27	-28.11	-2.84	CH4
CO(g)	-13.54	-16.54	-3.00	CO
CO2(g)	-3.77	-11.59	-7.83	CO2
Gypsum	-15.23	-19.76	-4.53	CaSO4:2H2O
H2(g)	-15.94	-19.04	-3.10	H2
H2O(g)	-11.25	-9.67	1.59	H2O
H2S(g)	-9.38	-17.38	-7.99	H2S
Ice	-9.81	-9.67	0.14	H2O
Lime	-16.66	15.91	32.57	CaO
Monohydrocalcite	-8.03	-5.35	2.68	CaCO3:H2O
O2(g)	-70.56	-73.46	-2.89	O2
Portlandite	-16.30	6.24	22.55	Ca(OH)2
S	0.67	-44.44	-45.11	S
S2(g)	-12.55	-19.73	-7.19	S2
SO2(g)	-17.29	-17.12	0.18	SO2

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

```
ERROR: Numerical method failed on all combinations of convergence parameters,
cell/soln/mix 1
------------------------------
End of Run after 0.411 Seconds.
------------------------------
```