```
   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
          NO2(g)    -5.149185348 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: Mu Ionic strength has not converged. Residual: 4.278832e-14

ERROR: A(H2O) Activity of water has not converged. Residual: -9.879523e-01

ERROR: pH Charge balance has not converged. Residual: 6.692130e-15

Using solution 1.
Using pure phase assemblage 1.

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

				Moles in assemblage		
Phase	SI	log IAP	log K(T, P)	Initial	Final	Delta
CO2(g)	-3.41	-11.24	-7.83	1.000e+02	1.000e+02	-1.343e-05
Calcite	-91.66	-89.83	1.82	1.000e+03	1.000e+03	1.000e-10
NO2(g)	-5.15	3.20	8.35	1.000e+02	9.953e+01	-4.724e-01
SO2(g)	-5.15	-4.97	0.18	1.000e+02	1.000e+02	-1.062e-05

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

Elements	Molality	Moles
C	1.343e-05	1.343e-05
Ca	1.000e-22	1.000e-22
N	4.724e-01	4.724e-01
S	1.062e-05	1.062e-05

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

pH	=	26.112	Charge balance
pe	=	49.714	Adjusted to redox equilibrium
Activity of water	=	0.000	
Ionic strength	=	4.949e-14	
Mass of water (kg)	=	1.000e+00	
Total alkalinity (eq/kg)	=	-2.124e-05	
Total CO2 (mol/kg)	=	1.343e-05	
Temperature (°C)	=	25.00	
Electrical balance (eq)	=	-6.703e-15	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	-100.00	
Iterations	=	201	
Total H	=	1.110507e+02	
Total O	=	5.647026e+01	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	7.720e-27	7.720e-27	-26.112	-26.112	-0.000	0.00
H2O	5.553e+01	0.000e+00	1.744	-108.818	0.000	18.07
OH-	0.000e+00	0.000e+00	-96.722	-96.722	-0.000	(0)
C(-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-493.552	-493.552	0.000	(0)
C(-3)	0.000e+00					
C2H6	0.000e+00	0.000e+00	-576.317	-576.317	0.000	(0)
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-372.314	-372.314	0.000	(0)
C(2)	0.000e+00					
CO	0.000e+00	0.000e+00	-52.748	-52.748	0.000	(0)
C(4)	1.343e-05					
CO2	1.343e-05	1.343e-05	-4.872	-4.872	0.000	(0)
CO3-2	0.000e+00	0.000e+00	-78.184	-78.184	-0.000	(0)
HCO3-	0.000e+00	0.000e+00	-93.943	-93.943	-0.000	(0)
CaCO3	0.000e+00	0.000e+00	-96.819	-96.819	0.000	(0)
CaHCO3+	0.000e+00	0.000e+00	-114.870	-114.870	-0.000	(0)
Ca	1.000e-22					
Ca+2	1.000e-22	1.000e-22	-22.000	-22.000	-0.000	(0)
CaSO4	0.000e+00	0.000e+00	-44.061	-44.061	0.000	(0)
CaNO3+	0.000e+00	0.000e+00	-46.478	-46.478	-0.000	(0)
CaCO3	0.000e+00	0.000e+00	-96.819	-96.819	0.000	(0)
CaHCO3+	0.000e+00	0.000e+00	-114.870	-114.870	-0.000	(0)
CaOH+	0.000e+00	0.000e+00	-117.556	-117.556	-0.000	(0)
H(0)	0.000e+00					
H2	0.000e+00	0.000e+00	-154.753	-154.753	0.000	(0)
N(-03)	0.000e+00					
N3-	0.000e+00	0.000e+00	-106.897	-106.897	-0.000	(0)
HN3	0.000e+00	0.000e+00	-128.307	-128.307	0.000	(0)
N(-3)	0.000e+00					
NH3	0.000e+00	0.000e+00	-221.526	-221.526	0.000	(0)
NH4+	0.000e+00	0.000e+00	-238.398	-238.398	-0.000	(0)
NH4SO4-	0.000e+00	0.000e+00	-270.923	-270.923	-0.000	(0)
N(0)	4.724e-01					
N2	2.362e-01	2.362e-01	-0.627	-0.627	0.000	(0)

N(3)	0.000e+00					
NO2-	0.000e+00	0.000e+00	-40.249	-40.249	-0.000	(0)
HNO2	0.000e+00	0.000e+00	-63.129	-63.129	0.000	(0)
N(5)	6.631e-26					
NO3-	6.631e-26	6.631e-26	-25.178	-25.178	-0.000	(0)
CaNO3+	0.000e+00	0.000e+00	-46.478	-46.478	-0.000	(0)
HNO3	0.000e+00	0.000e+00	-52.572	-52.572	0.000	(0)
O(0)	9.449e-01					
O2	4.724e-01	4.724e-01	-0.326	-0.326	0.000	(0)
S(-2)	0.000e+00					
S-2	0.000e+00	0.000e+00	-174.782	-174.782	-0.000	(0)
HS-	0.000e+00	0.000e+00	-187.969	-187.969	-0.000	(0)
H2S	0.000e+00	0.000e+00	-207.072	-207.072	0.000	(0)
S2-2	0.000e+00	0.000e+00	-234.025	-234.025	-0.000	(0)
S3-2	0.000e+00	0.000e+00	-293.308	-293.308	-0.000	(0)
S4-2	0.000e+00	0.000e+00	-352.819	-352.819	-0.000	(0)
S5-2	0.000e+00	0.000e+00	-412.546	-412.546	-0.000	(0)
S(2)	0.000e+00					
S2O3-2	0.000e+00	0.000e+00	-124.679	-124.679	-0.000	(0)
HS2O3-	0.000e+00	0.000e+00	-149.778	-149.778	-0.000	(0)
S(3)	0.000e+00					
S2O4-2	0.000e+00	0.000e+00	-109.770	-109.770	-0.000	(0)
S(4)	1.062e-05					
SO2	1.062e-05	1.062e-05	-4.974	-4.974	0.000	(0)
S2O6-2	0.000e+00	0.000e+00	-43.063	-43.063	-0.000	(0)
SO3-2	0.000e+00	0.000e+00	-70.680	-70.680	-0.000	(0)
HSO3-	0.000e+00	0.000e+00	-89.561	-89.561	-0.000	(0)
S3O6-2	0.000e+00	0.000e+00	-104.829	-104.829	-0.000	(0)
H2SO3	0.000e+00	0.000e+00	-113.692	-113.692	0.000	(0)
S4O6-2	0.000e+00	0.000e+00	-150.690	-150.690	-0.000	(0)
S5O6-2	0.000e+00	0.000e+00	-225.430	-225.430	-0.000	(0)
S(5)	0.000e+00					
S2O5-2	0.000e+00	0.000e+00	-75.134	-75.134	-0.000	(0)
S(6)	5.954e-25					
SO4-2	5.954e-25	5.954e-25	-24.225	-24.225	-0.000	(0)
CaSO4	0.000e+00	0.000e+00	-44.061	-44.061	0.000	(0)
HSO4-	0.000e+00	0.000e+00	-48.333	-48.333	-0.000	(0)
H2SO4	0.000e+00	0.000e+00	-77.471	-77.471	0.000	(0)
NH4SO4-	0.000e+00	0.000e+00	-270.923	-270.923	-0.000	(0)
S(7)	6.703e-15					
S2O8-2	3.351e-15	3.351e-15	-14.475	-14.475	-0.000	(0)
S(8)	0.000e+00					
HSO5-	0.000e+00	0.000e+00	-67.761	-67.761	-0.000	(0)

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

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Anhydrite	-41.88	-46.23	-4.35	CaSO4
Aragonite	-91.80	-89.83	1.97	CaCO3
Bassanite	-96.93	-100.63	-3.71	CaSO4:0.5H2O
C	-75.06	-10.91	64.15	C
C(g)	-192.68	-10.91	181.77	C
Ca	-218.26	-78.43	139.83	Ca
Ca(g)	-243.50	-78.43	165.07	Ca
Calcite	-91.66	-89.83	1.82	CaCO3
CaSO4:0.5H2O(beta)	-97.10	-100.63	-3.54	CaSO4:0.5H2O
CH4(g)	-369.47	-372.31	-2.84	CH4
CO(g)	-49.75	-52.75	-3.00	CO
CO2(g)	-3.41	-11.24	-7.83	CO2
Gypsum	-259.33	-263.86	-4.53	CaSO4:2H2O
H2(g)	-151.65	-154.75	-3.10	H2
H2O(g)	-110.40	-108.82	1.59	H2O
H2S(g)	-206.09	-214.08	-7.99	H2S
Ice	-108.96	-108.82	0.14	H2O
Lime	-111.16	-78.59	32.57	CaO

```
  Monohydrocalcite-201.33   -198.65    2.68  CaCO3:H2O
  N2(g)              2.55     -0.63   -3.18  N2
  NH3(g)          -223.32   -221.53    1.80  NH3
  NO(g)            -12.61    -11.87    0.74  NO
  NO2(g)            -5.15      3.20    8.35  NO2
  O2(g)              2.57     -0.33   -2.89  O2
  Portlandite     -209.96   -187.41   22.55  Ca(OH)2
  S                -60.32   -105.43  -45.11  S
  S2(g)           -134.52   -141.71   -7.19  S2
  SO2(g)            -5.15     -4.97    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 0.49 Seconds.
------------------------------
```