```
   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
          Portlandite 0 1000
          CO2(g)    -3.408822658 100
          NO2(g)    -5.149185348 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: Mass of water is less than 1e-10 kilogram.
The aqueous phase may not be stable relative to given masses of minerals.
WARNING: Numerical method failed with this set of convergence parameters.

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

WARNING: Mass of water is less than 1e-10 kilogram.
The aqueous phase may not be stable relative to given masses of minerals.
WARNING: Numerical method failed with this set of convergence parameters.

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

WARNING: Mass of water is less than 1e-10 kilogram.
The aqueous phase may not be stable relative to given masses of minerals.
WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying diagonal scaling ...

WARNING: Mass of water is less than 1e-10 kilogram.
The aqueous phase may not be stable relative to given masses of minerals.
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 ...

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)	-13.15	-20.98	-7.83	1.000e+02	0	-1.000e+02
Calcite	0.00	1.82	1.82	1.000e+03	1.100e+03	1.000e+02
NO2(g)	-15.97	-7.62	8.35	1.000e+02	0	-1.000e+02
Portlandite	0.00	22.55	22.55	1.000e+03	8.600e+02	-1.400e+02

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

Elements	Molality	Moles
C	6.928e-06	2.440e-05
Ca	1.136e+01	4.002e+01
N	2.840e+01	1.000e+02

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

pH	= 11.858	Charge balance
pe	= 6.846	Adjusted to redox equilibrium
Activity of water	= 0.556	
Ionic strength	= 1.246e+01	
Mass of water (kg)	= 3.521e+00	
Total alkalinity (eq/kg)	= 1.072e-02	
Total CO2 (mol/kg)	= 6.928e-06	
Temperature (°C)	= 25.00	
Electrical balance (eq)	= -4.449e-11	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -0.00	
Iterations	= 33	
Total H	= 3.910884e+02	
Total O	= 4.355631e+02	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	2.708e-03	3.861e-03	-2.567	-2.413	0.154	(0)
H+	6.155e-13	1.387e-12	-12.211	-11.858	0.353	0.00
H2O	5.553e+01	5.561e-01	1.744	-0.255	0.000	18.07
C(-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-261.812	-261.812	0.000	(0)
C(-3)	0.000e+00					
C2H6	0.000e+00	0.000e+00	-230.333	-230.333	0.000	(0)
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-142.199	-142.199	0.000	(0)
C(2)	0.000e+00					
CO	0.000e+00	0.000e+00	-56.806	-56.806	0.000	(0)
C(4)	6.928e-06					
CaCO3	6.867e-06	6.867e-06	-5.163	-5.163	0.000	(0)

```
   CO3-2           6.032e-08   1.352e-08    -7.220    -7.869    -0.650     (0)
   CaHCO3+         7.077e-10   1.098e-09    -9.150    -8.959     0.191     (0)
   HCO3-           2.724e-10   4.227e-10    -9.565    -9.374     0.191     (0)
   CO2             1.756e-16   2.446e-15   -15.755   -14.612     1.144     (0)
Ca              1.136e+01
   CaNO3+          1.081e+01   1.677e+01     1.034     1.225     0.191     (0)
   Ca+2            5.456e-01   2.192e-01    -0.263    -0.659    -0.396     (0)
   CaOH+           7.999e-03   1.241e-02    -2.097    -1.906     0.191     (0)
   CaCO3           6.867e-06   6.867e-06    -5.163    -5.163     0.000     (0)
   CaHCO3+         7.077e-10   1.098e-09    -9.150    -8.959     0.191     (0)
H(0)            0.000e+00
   H2              0.000e+00   0.000e+00   -41.652   -40.508     1.144     (0)
N(-03)          0.000e+00
   N3-             0.000e+00   0.000e+00   -62.600   -62.409     0.191     (0)
   HN3             0.000e+00   0.000e+00   -69.564   -69.564     0.000     (0)
N(-3)           0.000e+00
   NH3             0.000e+00   0.000e+00   -49.618   -49.618     0.000     (0)
   NH4+            0.000e+00   0.000e+00   -52.284   -52.236     0.048     (0)
N(0)            5.680e+00
   N2              2.840e+00   2.840e+00     0.453     0.453     0.000     (0)
N(3)            4.871e-09
   NO2-            4.871e-09   6.245e-09    -8.312    -8.204     0.108     (0)
   HNO2            1.479e-17   1.479e-17   -16.830   -16.830     0.000     (0)
N(5)            2.272e+01
   NO3-            1.191e+01   1.527e+01     1.076     1.184     0.108     (0)
   CaNO3+          1.081e+01   1.677e+01     1.034     1.225     0.191     (0)
   HNO3            1.108e-12   1.108e-12   -11.956   -11.956     0.000     (0)
O(0)            2.935e-13
   O2              1.467e-13   2.044e-12   -12.833   -11.690     1.144     (0)

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

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

  Aragonite         -0.15      1.82    1.97  CaCO3
  C                -73.43     -9.29   64.15  C
  C(g)            -191.05     -9.29  181.77  C
  Ca              -111.19     28.65  139.83  Ca
  Ca(g)           -136.43     28.65  165.07  Ca
  Calcite           0.00      1.82    1.82  CaCO3
  CH4(g)          -139.36   -142.20   -2.84  CH4
  CO(g)            -53.81    -56.81   -3.00  CO
  CO2(g)           -13.15    -20.98   -7.83  CO2
  H2(g)            -37.41    -40.51   -3.10  H2
  H2O(g)            -1.84     -0.25    1.59  H2O
  Ice               -0.39     -0.25    0.14  H2O
  Lime              -9.77     22.80   32.57  CaO
  Monohydrocalcite  -1.11      1.57    2.68  CaCO3:H2O
  N2(g)              3.63      0.45   -3.18  N2
  NH3(g)           -51.41    -49.62    1.80  NH3
  NO(g)            -17.75    -17.01    0.74  NO
  NO2(g)           -15.97     -7.62    8.35  NO2
  O2(g)             -8.80    -11.69   -2.89  O2
  Portlandite        0.00     22.55   22.55  Ca(OH)2

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

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End of simulation.
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Reading input data for simulation 2.
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End of Run after 0.47 Seconds.
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```