```
   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
          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: 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: 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 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--------------------------------

                                                        Moles in assemblage
Phase               SI  log IAP  log K(T, P)   Initial       Final       Delta

CO2(g)          -13.29   -21.12     -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)          -16.43    -8.08      8.35    1.000e+02           0  -1.000e+02
Portlandite       0.00    22.55     22.55    1.000e+03   7.800e+02  -2.200e+02
SO2(g)          -55.38   -55.21      0.18    1.000e+02           0  -1.000e+02

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

      Elements           Molality       Moles

      C                 6.907e-06   3.427e-05
      Ca                2.419e+01   1.200e+02
      N                 2.015e+01   1.000e+02
      S                 2.015e+01   1.000e+02

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

                                       pH  =  11.877      Charge balance
                                       pe  =   6.745      Adjusted to redox equilibrium
                          Activity of water  =   0.398
                             Ionic strength  =   1.056e+01
                         Mass of water (kg)  =   4.962e+00
                 Total alkalinity (eq/kg)  =   1.506e-02
                         Total CO2 (mol/kg)  =   6.907e-06
                           Temperature (°C)  =  25.00
                  Electrical balance (eq)  =  -1.908e-11
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                                 Iterations  =  26
                                    Total H  = 5.511253e+02
                                    Total O  = 7.956001e+02

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

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

   OH-             2.390e-03   2.887e-03    -2.622    -2.539     0.082     (0)
   H+              7.029e-13   1.328e-12   -12.153   -11.877     0.276      0.00
   H2O             5.553e+01   3.979e-01     1.744    -0.400     0.000     18.07
C(-2)         0.000e+00
   C2H4            0.000e+00   0.000e+00  -260.543  -260.543     0.000     (0)
C(-3)         0.000e+00
   C2H6            0.000e+00   0.000e+00  -228.901  -228.901     0.000     (0)
C(-4)         0.000e+00
   CH4             0.000e+00   0.000e+00  -141.402  -141.402     0.000     (0)
C(2)          0.000e+00
```

| | | | | | | |
|---|---|---|---|---|---|---|
| CO | 0.000e+00 | 0.000e+00 | -56.643 | -56.643 | 0.000 | (0) |
| C(4) | 6.907e-06 | | | | | |
| CaCO3 | 6.867e-06 | 6.867e-06 | -5.163 | -5.163 | 0.000 | (0) |
| CO3-2 | 3.891e-08 | 7.557e-09 | -7.410 | -8.122 | -0.712 | (0) |
| CaHCO3+ | 8.014e-10 | 1.051e-09 | -9.096 | -8.978 | 0.118 | (0) |
| HCO3- | 1.725e-10 | 2.262e-10 | -9.763 | -9.646 | 0.118 | (0) |
| CO2 | 1.870e-16 | 1.751e-15 | -15.728 | -14.757 | 0.971 | (0) |
| Ca | 2.419e+01 | | | | | |
| CaSO4 | 1.804e+01 | 1.804e+01 | 1.256 | 1.256 | 0.000 | (0) |
| CaNO3+ | 5.001e+00 | 6.558e+00 | 0.699 | 0.817 | 0.118 | (0) |
| Ca+2 | 1.142e+00 | 3.921e-01 | 0.058 | -0.407 | -0.464 | (0) |
| CaOH+ | 1.266e-02 | 1.660e-02 | -1.898 | -1.780 | 0.118 | (0) |
| CaCO3 | 6.867e-06 | 6.867e-06 | -5.163 | -5.163 | 0.000 | (0) |
| CaHCO3+ | 8.014e-10 | 1.051e-09 | -9.096 | -8.978 | 0.118 | (0) |
| H(0) | 0.000e+00 | | | | | |
| H2 | 0.000e+00 | 0.000e+00 | -41.316 | -40.345 | 0.971 | (0) |
| N(-03) | 0.000e+00 | | | | | |
| N3- | 0.000e+00 | 0.000e+00 | -61.934 | -61.816 | 0.118 | (0) |
| HN3 | 0.000e+00 | 0.000e+00 | -68.990 | -68.990 | 0.000 | (0) |
| N(-3) | 0.000e+00 | | | | | |
| NH3 | 0.000e+00 | 0.000e+00 | -49.209 | -49.209 | 0.000 | (0) |
| NH4+ | 0.000e+00 | 0.000e+00 | -51.826 | -51.846 | -0.020 | (0) |
| NH4SO4- | 0.000e+00 | 0.000e+00 | -60.766 | -60.648 | 0.118 | (0) |
| N(0) | 1.209e+01 | | | | | |
| N2 | 6.046e+00 | 6.046e+00 | 0.781 | 0.781 | 0.000 | (0) |
| N(3) | 2.546e-09 | | | | | |
| NO2- | 2.546e-09 | 2.777e-09 | -8.594 | -8.556 | 0.038 | (0) |
| HNO2 | 6.292e-18 | 6.292e-18 | -17.201 | -17.201 | 0.000 | (0) |
| N(5) | 8.061e+00 | | | | | |
| CaNO3+ | 5.001e+00 | 6.558e+00 | 0.699 | 0.817 | 0.118 | (0) |
| NO3- | 3.060e+00 | 3.337e+00 | 0.486 | 0.523 | 0.038 | (0) |
| HNO3 | 2.318e-13 | 2.318e-13 | -12.635 | -12.635 | 0.000 | (0) |
| O(0) | 1.055e-13 | | | | | |
| O2 | 5.277e-14 | 4.940e-13 | -13.278 | -12.306 | 0.971 | (0) |
| S(-2) | 0.000e+00 | | | | | |
| HS- | 0.000e+00 | 0.000e+00 | -126.131 | -126.049 | 0.082 | (0) |
| S-2 | 0.000e+00 | 0.000e+00 | -126.483 | -127.098 | -0.615 | (0) |
| H2S | 0.000e+00 | 0.000e+00 | -130.916 | -130.916 | 0.000 | (0) |
| S2-2 | 0.000e+00 | 0.000e+00 | -223.765 | -224.593 | -0.828 | (0) |
| S3-2 | 0.000e+00 | 0.000e+00 | -321.301 | -322.129 | -0.828 | (0) |
| S4-2 | 0.000e+00 | 0.000e+00 | -419.065 | -419.892 | -0.828 | (0) |
| S5-2 | 0.000e+00 | 0.000e+00 | -517.045 | -517.872 | -0.828 | (0) |
| S(2) | 0.000e+00 | | | | | |
| S2O3-2 | 0.000e+00 | 0.000e+00 | -132.391 | -133.218 | -0.828 | (0) |
| HS2O3- | 0.000e+00 | 0.000e+00 | -144.199 | -144.081 | 0.118 | (0) |
| S(3) | 0.000e+00 | | | | | |
| S2O4-2 | 0.000e+00 | 0.000e+00 | -123.684 | -124.300 | -0.615 | (0) |
| S(4) | 0.000e+00 | | | | | |
| SO3-2 | 0.000e+00 | 0.000e+00 | -40.255 | -40.967 | -0.712 | (0) |
| HSO3- | 0.000e+00 | 0.000e+00 | -45.729 | -45.612 | 0.118 | (0) |
| SO2 | 0.000e+00 | 0.000e+00 | -55.207 | -55.207 | 0.000 | (0) |
| H2SO3 | 0.000e+00 | 0.000e+00 | -55.507 | -55.507 | 0.000 | (0) |
| S2O6-2 | 0.000e+00 | 0.000e+00 | -68.745 | -69.573 | -0.828 | (0) |
| S3O6-2 | 0.000e+00 | 0.000e+00 | -168.764 | -169.592 | -0.828 | (0) |
| S4O6-2 | 0.000e+00 | 0.000e+00 | -252.878 | -253.705 | -0.828 | (0) |
| S5O6-2 | 0.000e+00 | 0.000e+00 | -365.870 | -366.698 | -0.828 | (0) |
| S(5) | 0.000e+00 | | | | | |
| S2O5-2 | 0.000e+00 | 0.000e+00 | -94.826 | -95.654 | -0.828 | (0) |
| S(6) | 2.015e+01 | | | | | |
| CaSO4 | 1.804e+01 | 1.804e+01 | 1.256 | 1.256 | 0.000 | (0) |
| SO4-2 | 2.117e+00 | 3.149e-01 | 0.326 | -0.502 | -0.828 | (0) |
| HSO4- | 3.221e-11 | 4.224e-11 | -10.492 | -10.374 | 0.118 | (0) |
| H2SO4 | 5.291e-26 | 5.291e-26 | -25.276 | -25.276 | 0.000 | (0) |
| NH4SO4- | 0.000e+00 | 0.000e+00 | -60.766 | -60.648 | 0.118 | (0) |
| S(7) | 0.000e+00 | | | | | |
| S2O8-2 | 0.000e+00 | 0.000e+00 | -52.138 | -52.965 | -0.828 | (0) |

```
S(8)          1.230e-36
   HSO5-           1.230e-36   1.613e-36   -35.910   -35.792     0.118     (0)

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

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

  Anhydrite          3.44     -0.91   -4.35  CaSO4
  Aragonite         -0.15      1.82    1.97  CaCO3
  Bassanite          2.60     -1.11   -3.71  CaSO4:0.5H2O
  C                -72.96     -8.82   64.15  C
  C(g)            -190.58     -8.82  181.77  C
  Ca              -110.73     29.10  139.83  Ca
  Ca(g)           -135.97     29.10  165.07  Ca
  Calcite           -0.00      1.82    1.82  CaCO3
  CaSO4:0.5H2O(beta)   2.43     -1.11   -3.54  CaSO4:0.5H2O
  CH4(g)          -138.56   -141.40   -2.84  CH4
  CO(g)            -53.65    -56.64   -3.00  CO
  CO2(g)           -13.29    -21.12   -7.83  CO2
  Gypsum             2.82     -1.71   -4.53  CaSO4:2H2O
  H2(g)            -37.24    -40.35   -3.10  H2
  H2O(g)            -1.99     -0.40    1.59  H2O
  H2S(g)          -129.93   -137.93   -7.99  H2S
  Ice               -0.54     -0.40    0.14  H2O
  Lime              -9.62     22.95   32.57  CaO
  Monohydrocalcite  -1.25      1.42    2.68  CaCO3:H2O
  N2(g)              3.96      0.78   -3.18  N2
  NH3(g)           -51.01    -49.21    1.80  NH3
  NO(g)            -17.89    -17.16    0.74  NO
  NO2(g)           -16.43     -8.08    8.35  NO2
  O2(g)             -9.41    -12.31   -2.89  O2
  Portlandite        0.00     22.55   22.55  Ca(OH)2
  S                -98.57   -143.68  -45.11  S
  S2(g)           -211.03   -218.22   -7.19  S2
  SO2(g)           -55.38    -55.21    0.18  SO2

**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.
------------------------------------

------------------------------
End of Run after 0.38 Seconds.
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```