```
   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
          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.

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  -5.466e-10
NO2(g)          -5.15     3.20      8.35    1.000e+02   8.166e+01  -1.834e+01
SO2(g)          -5.15    -4.97      0.18    1.000e+02   7.554e+01  -2.446e+01

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

      Elements           Molality       Moles

      C                 7.011e-10   5.466e-10
      N                 2.353e+01   1.834e+01
      S                 3.138e+01   2.446e+01

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

                                    pH  =  -3.260      Charge balance
                                    pe  =  40.766      Adjusted to redox equilibrium
                       Activity of water  =   0.000
                          Ionic strength  =   4.704e+01
                       Mass of water (kg)  =   7.796e-01
                 Total alkalinity (eq/kg)  =  -3.140e+01
                       Total CO2 (mol/kg)  =   7.011e-10
                         Temperature (°C)  =  25.00
                  Electrical balance (eq)  =  -7.051e-14
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
```

Iterations = 53
Total H = 1.110507e+02
Total O = 1.411356e+02

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	3.136e+01	1.000e+03	1.496	3.260	1.764	0.00
H2O	5.553e+01	2.503e-33	1.744	-32.602	0.000	18.07
OH-	0.000e+00	0.000e+00	-51.412	-49.878	1.534	(0)
C(-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-338.573	-338.573	0.000	(0)
C(-3)	0.000e+00					
C2H6	0.000e+00	0.000e+00	-344.698	-344.698	0.000	(0)
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-218.184	-218.184	0.000	(0)
C(2)	0.000e+00					
CO	0.000e+00	0.000e+00	-52.324	-52.324	0.000	(0)
C(4)	7.011e-10					
CO2	7.011e-10	1.343e-05	-9.154	-4.872	4.282	(0)
HCO3-	0.000e+00	0.000e+00	-48.678	-47.099	1.579	(0)
CO3-2	0.000e+00	0.000e+00	-61.382	-60.712	0.670	(0)
H(0)	0.000e+00					
H2	0.000e+00	0.000e+00	-82.395	-78.112	4.282	(0)
N(-03)	0.000e+00					
HN3	0.000e+00	0.000e+00	-87.440	-87.440	0.000	(0)
N3-	0.000e+00	0.000e+00	-96.982	-95.403	1.579	(0)
N(-3)	0.000e+00					
NH4+	0.000e+00	0.000e+00	-94.616	-93.216	1.400	(0)
NH3	0.000e+00	0.000e+00	-105.716	-105.716	0.000	(0)
NH4SO4-	0.000e+00	0.000e+00	-110.272	-108.694	1.579	(0)
N(0)	2.353e+01					
N2	1.176e+01	1.176e+01	1.071	1.071	0.000	(0)
N(3)	1.555e-25					
HNO2	1.555e-25	1.555e-25	-24.808	-24.808	0.000	(0)
NO2-	1.669e-33	5.004e-32	-32.778	-31.301	1.477	(0)
N(5)	2.109e-15					
HNO3	2.108e-15	2.108e-15	-14.676	-14.676	0.000	(0)
NO3-	7.385e-19	2.214e-17	-18.132	-16.655	1.477	(0)
O(0)	6.992e-06					
O2	3.496e-06	6.694e-02	-5.456	-1.174	4.282	(0)
S(-2)	0.000e+00					
H2S	0.000e+00	0.000e+00	-129.582	-129.582	0.000	(0)
HS-	0.000e+00	0.000e+00	-141.386	-139.852	1.534	(0)
S-2	0.000e+00	0.000e+00	-156.824	-156.038	0.786	(0)
S2-2	0.000e+00	0.000e+00	-214.960	-214.432	0.528	(0)
S3-2	0.000e+00	0.000e+00	-273.395	-272.867	0.528	(0)
S4-2	0.000e+00	0.000e+00	-332.057	-331.529	0.528	(0)
S5-2	0.000e+00	0.000e+00	-390.936	-390.407	0.528	(0)
S(2)	0.000e+00					
HS2O3-	0.000e+00	0.000e+00	-103.664	-102.085	1.579	(0)
S2O3-2	0.000e+00	0.000e+00	-106.888	-106.359	0.528	(0)
S(3)	0.000e+00					
S2O4-2	0.000e+00	0.000e+00	-92.660	-91.875	0.786	(0)
S(4)	1.062e-05					
SO2	1.062e-05	1.062e-05	-4.974	-4.974	0.000	(0)
S2O6-2	2.858e-27	9.647e-27	-26.544	-26.016	0.528	(0)
H2SO3	3.349e-38	3.349e-38	-37.475	-37.475	0.000	(0)
HSO3-	0.000e+00	0.000e+00	-44.295	-42.717	1.579	(0)
SO3-2	0.000e+00	0.000e+00	-53.879	-53.209	0.670	(0)
S3O6-2	0.000e+00	0.000e+00	-87.462	-86.933	0.528	(0)
S4O6-2	0.000e+00	0.000e+00	-132.474	-131.945	0.528	(0)
S5O6-2	0.000e+00	0.000e+00	-206.365	-205.837	0.528	(0)
S(5)	0.000e+00					

```
   S2O5-2          0.000e+00   0.000e+00   -58.191   -57.662     0.528     (0)
S(6)          2.129e-02
   H2SO4           2.096e-02   2.096e-02    -1.679    -1.679     0.000     (0)
   HSO4-           3.221e-04   1.221e-02    -3.492    -1.913     1.579     (0)
   SO4-2           1.966e-08   6.637e-08    -7.706    -7.178     0.528     (0)
   NH4SO4-         0.000e+00   0.000e+00  -110.272  -108.694     1.579     (0)
S(7)          3.136e+01
   S2O8-2          1.568e+01   5.293e+01     1.195     1.724     0.528     (0)
S(8)          4.528e-24
   HSO5-           4.528e-24   1.715e-22   -23.344   -21.766     1.579     (0)

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

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

  C                -74.21    -10.06   64.15  C
  C(g)             -191.83   -10.06  181.77  C
  CH4(g)           -215.34   -218.18   -2.84  CH4
  CO(g)             -49.33    -52.32   -3.00  CO
  CO2(g)             -3.41    -11.24   -7.83  CO2
  H2(g)             -75.01    -78.11   -3.10  H2
  H2O(g)            -34.19    -32.60    1.59  H2O
  H2S(g)           -128.60   -136.59   -7.99  H2S
  Ice               -32.74    -32.60    0.14  H2O
  N2(g)               4.25      1.07   -3.18  N2
  NH3(g)           -107.51   -105.72    1.80  NH3
  NO(g)             -12.18    -11.45    0.74  NO
  NO2(g)             -5.15      3.20    8.35  NO2
  O2(g)               1.72     -1.17   -2.89  O2
  S                 -59.47   -104.58  -45.11  S
  S2(g)            -132.83   -140.01   -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.

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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 0.27 Seconds.
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