```
   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
      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  -8.160e-07
NO2(g)          -5.15     3.20      8.35    1.000e+02   6.871e+01  -3.129e+01

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

      Elements           Molality       Moles

      C                 1.053e-06   8.160e-07
      N                 4.040e+01   3.129e+01

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

                                       pH  =  -1.416      Charge balance
                                       pe  =  23.055      Adjusted to redox equilibrium
                          Activity of water  =   0.177
                             Ionic strength  =   1.203e+01
                          Mass of water (kg)  =   7.746e-01
                 Total alkalinity (eq/kg)  =  -3.231e+01
                          Total CO2 (mol/kg)  =   1.053e-06
                            Temperature (°C)  =  25.00
                   Electrical balance (eq)  =  -3.352e-11
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                                  Iterations  =  33
                                     Total H  = 1.110507e+02
                                     Total O  = 1.181095e+02
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.203e+01	2.607e+01	1.080	1.416	0.336	0.00
OH-	4.770e-17	6.553e-17	-16.321	-16.184	0.138	(0)
H2O	5.553e+01	1.773e-01	1.744	-0.751	0.000	18.07
C(-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-275.568	-275.568	0.000	(0)
C(-3)	0.000e+00					
C2H6	0.000e+00	0.000e+00	-249.958	-249.958	0.000	(0)
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-154.947	-154.947	0.000	(0)
C(2)	0.000e+00					
CO	0.000e+00	0.000e+00	-52.440	-52.440	0.000	(0)
C(4)	1.053e-06					
CO2	1.053e-06	1.343e-05	-5.977	-4.872	1.105	(0)
HCO3-	2.635e-14	3.937e-14	-13.579	-13.405	0.174	(0)
CO3-2	3.089e-25	6.700e-26	-24.510	-25.174	-0.664	(0)
H(0)	0.000e+00					
H2	0.000e+00	0.000e+00	-47.483	-46.378	1.105	(0)
N(-03)	0.000e+00					
HN3	0.000e+00	0.000e+00	-72.269	-72.269	0.000	(0)
N3-	0.000e+00	0.000e+00	-78.562	-78.388	0.174	(0)
N(-3)	0.000e+00					
NH4+	0.000e+00	0.000e+00	-47.723	-47.690	0.033	(0)
NH3	0.000e+00	0.000e+00	-58.346	-58.346	0.000	(0)
N(0)	8.086e+00					
N2	4.043e+00	4.043e+00	0.607	0.607	0.000	(0)
N(3)	1.145e-09					
HNO2	1.145e-09	1.145e-09	-8.941	-8.941	0.000	(0)
NO2-	2.082e-14	2.574e-14	-13.682	-13.589	0.092	(0)
N(5)	3.231e+01					
HNO3	2.028e+01	2.028e+01	1.307	1.307	0.000	(0)
NO3-	1.203e+01	1.487e+01	1.080	1.172	0.092	(0)
O(0)	1.792e-02					
O2	8.960e-03	1.142e-01	-2.048	-0.942	1.105	(0)

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

Phase	SI**	log IAP	log K(298 K, 1 atm)	
C	-74.44	-10.30	64.15	C
C(g)	-192.06	-10.30	181.77	C
CH4(g)	-152.10	-154.95	-2.84	CH4
CO(g)	-49.44	-52.44	-3.00	CO
CO2(g)	-3.41	-11.24	-7.83	CO2
H2(g)	-43.28	-46.38	-3.10	H2
H2O(g)	-2.34	-0.75	1.59	H2O
Ice	-0.89	-0.75	0.14	H2O
N2(g)	3.79	0.61	-3.18	N2
NH3(g)	-60.14	-58.35	1.80	NH3
NO(g)	-12.30	-11.56	0.74	NO
NO2(g)	-5.15	3.20	8.35	NO2
O2(g)	1.95	-0.94	-2.89	O2

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

End of simulation.

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Reading input data for simulation 2.
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End of Run after 0.26 Seconds.
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