```
   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
      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:                    Ca has not converged. Total: 8.771799e+00      Calculated:
4.553890e+01      Residual: -3.676711e+01

ERROR:                     N has not converged. Total: 1.000000e+02      Calculated:
1.114308e+02      Residual: -1.143078e+01

ERROR:                    Mu Ionic strength has not converged.     Residual: -6.120566e-02

ERROR:                A(H2O) Activity of water has not converged.  Residual: 6.147328e-01

ERROR:                    pH Charge balance has not converged.     Residual: -8.819823e-02

ERROR:              Hydrogen Mass of hydrogen has not converged.   Residual: 2.533069e+02

ERROR:                Oxygen Mass of oxygen has not converged.     Residual: -1.325796e+02

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)	-8.59	-16.42	-7.83	1.000e+02	1.400e+02	4.000e+01
Calcite	-0.96	0.86	1.82	1.000e+03	9.912e+02	-8.772e+00
NO2(g)	-12.36	-4.01	8.35	1.000e+02	0	-1.000e+02

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

Elements	Molality	Moles
C	7.539e-07	8.344e-07
Ca	4.115e+01	4.554e+01
N	1.007e+02	1.114e+02

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

pH	= 19.847	Charge balance
pe	= 10.475	Adjusted to redox equilibrium
Activity of water	= 0.000	
Ionic strength	= 4.115e+01	
Mass of water (kg)	= 1.107e+00	
Total alkalinity (eq/kg)	= 1.508e-06	
Total CO2 (mol/kg)	= 7.539e-07	
Temperature (°C)	= 25.00	
Electrical balance (eq)	= 8.820e-02	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 0.10	
Iterations	= 201	
Total H	= 1.229029e+02	
Total O	= 3.344203e+02	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	5.314e-18	1.050e-16	-17.275	-15.979	1.296	(0)
H+	4.270e-22	1.423e-20	-21.370	-19.847	1.523	0.00
H2O	5.553e+01	1.551e-22	1.744	-21.809	0.000	18.07
C(-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-305.890	-305.890	0.000	(0)
C(-3)	0.000e+00					
C2H6	0.000e+00	0.000e+00	-297.646	-297.646	0.000	(0)
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-187.473	-187.473	0.000	(0)
C(2)	0.000e+00					
CO	0.000e+00	0.000e+00	-53.929	-53.929	0.000	(0)
C(4)	7.539e-07					
CaCO3	7.534e-07	7.534e-07	-6.123	-6.123	0.000	(0)
CO3-2	4.741e-10	1.295e-09	-9.324	-8.888	0.436	(0)
CO2	1.581e-14	8.840e-11	-13.801	-10.054	3.748	(0)
CaHCO3+	5.657e-20	1.236e-18	-19.247	-17.908	1.339	(0)
HCO3-	1.901e-20	4.153e-19	-19.721	-18.382	1.339	(0)
Ca	4.115e+01					
CaNO3+	4.110e+01	8.979e+02	1.614	2.953	1.339	(0)
Ca+2	4.719e-02	2.511e-01	-1.326	-0.600	0.726	(0)
CaCO3	7.534e-07	7.534e-07	-6.123	-6.123	0.000	(0)
CaOH+	1.769e-17	3.865e-16	-16.752	-15.413	1.339	(0)
CaHCO3+	5.657e-20	1.236e-18	-19.247	-17.908	1.339	(0)
H(0)	0.000e+00					
H2	0.000e+00	0.000e+00	-67.491	-63.743	3.748	(0)
N(-03)	0.000e+00					
N3-	0.000e+00	0.000e+00	-66.609	-65.269	1.339	(0)
HN3	0.000e+00	0.000e+00	-80.414	-80.414	0.000	(0)

N(-3)	0.000e+00					
NH3	0.000e+00	0.000e+00	-84.215	-84.215	0.000	(0)
NH4+	0.000e+00	0.000e+00	-95.986	-94.821	1.164	(0)
N(0)	1.847e+01					
N2	9.235e+00	9.235e+00	0.965	0.965	0.000	(0)
N(3)	3.508e-10					
NO2-	3.508e-10	6.086e-09	-9.455	-8.216	1.239	(0)
HNO2	1.478e-25	1.478e-25	-24.830	-24.830	0.000	(0)
N(5)	8.221e+01					
NO3-	4.111e+01	7.134e+02	1.614	2.853	1.239	(0)
CaNO3+	4.110e+01	8.979e+02	1.614	2.953	1.339	(0)
HNO3	5.310e-19	5.310e-19	-18.275	-18.275	0.000	(0)
O(0)	1.680e-12					
O2	8.400e-13	4.698e-09	-12.076	-8.328	3.748	(0)

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

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Aragonite	-1.11	0.86	1.97	CaCO3
C	-72.24	-8.09	64.15	C
C(g)	-189.86	-8.09	181.77	C
Ca	-118.38	21.45	139.83	Ca
Ca(g)	-143.62	21.45	165.07	Ca
Calcite	-0.96	0.86	1.82	CaCO3
CH4(g)	-184.63	-187.47	-2.84	CH4
CO(g)	-50.93	-53.93	-3.00	CO
CO2(g)	-8.59	-16.42	-7.83	CO2
H2(g)	-60.64	-63.74	-3.10	H2
H2O(g)	-23.40	-21.81	1.59	H2O
Ice	-21.95	-21.81	0.14	H2O
Lime	-15.29	17.28	32.57	CaO
Monohydrocalcite	-23.62	-20.94	2.68	CaCO3:H2O
N2(g)	4.14	0.97	-3.18	N2
NH3(g)	-86.01	-84.21	1.80	NH3
NO(g)	-15.81	-15.08	0.74	NO
NO2(g)	-12.36	-4.01	8.35	NO2
O2(g)	-5.44	-8.33	-2.89	O2
Portlandite	-27.07	-4.53	22.55	Ca(OH)2

**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 0.4 Seconds.
