```
   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
          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 ...

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)          -13.17   -21.00     -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
Portlandite      -0.00    22.55     22.55    1.000e+03   8.107e+02  -1.893e+02
SO2(g)          -23.50   -23.32      0.18    1.000e+02           0  -1.000e+02

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

      Elements           Molality       Moles

      C                 9.857e-06   4.157e-05
      Ca                2.118e+01   8.934e+01
      S                 2.371e+01   1.000e+02

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

                                    pH  =  11.449      Charge balance
                                    pe  =  -8.779      Adjusted to redox equilibrium
```

Activity of water	= 0.532
Ionic strength	= 1.277e+01
Mass of water (kg)	= 4.217e+00
Total alkalinity (eq/kg)	= 6.808e+00
Total CO2 (mol/kg)	= 6.877e-06
Temperature (°C)	= 25.00
Electrical balance (eq)	= 6.262e-13
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 0.00
Iterations	= 50
Total H	= 4.897349e+02
Total O	= 5.342097e+02

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	9.830e-04	1.441e-03	-3.007	-2.841	0.166	(0)
H+	1.532e-12	3.556e-12	-11.815	-11.449	0.366	0.00
H2O	5.553e+01	5.319e-01	1.744	-0.274	0.000	18.07
C(-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-69.373	-69.373	0.000	(0)
C(-3)	2.981e-06					
C2H6	1.490e-06	1.490e-06	-5.827	-5.827	0.000	(0)
C(-4)	1.223e-14					
CH4	1.223e-14	1.223e-14	-13.913	-13.913	0.000	(0)
C(2)	1.823e-25					
CO	1.823e-25	1.823e-25	-24.739	-24.739	0.000	(0)
C(4)	6.877e-06					
CaCO3	6.867e-06	6.867e-06	-5.163	-5.163	0.000	(0)
CO3-2	8.198e-09	1.882e-09	-8.086	-8.725	-0.639	(0)
CaHCO3+	1.764e-09	2.815e-09	-8.754	-8.551	0.203	(0)
HCO3-	9.455e-11	1.509e-10	-10.024	-9.821	0.203	(0)
CO2	1.573e-16	2.340e-15	-15.803	-14.631	1.172	(0)
Ca	2.118e+01					
CaSO4	1.735e+01	1.735e+01	1.239	1.239	0.000	(0)
Ca+2	3.816e+00	1.574e+00	0.582	0.197	-0.385	(0)
CaOH+	2.084e-02	3.326e-02	-1.681	-1.478	0.203	(0)
CaCO3	6.867e-06	6.867e-06	-5.163	-5.163	0.000	(0)
CaHCO3+	1.764e-09	2.815e-09	-8.754	-8.551	0.203	(0)
H(0)	4.868e-10					
H2	2.434e-10	3.620e-09	-9.614	-8.441	1.172	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-77.034	-75.862	1.172	(0)
S(-2)	5.931e+00					
HS-	5.050e+00	7.403e+00	0.703	0.869	0.166	(0)
S-2	8.553e-01	2.468e-01	-0.068	-0.608	-0.540	(0)
S2-2	1.255e-02	2.186e-03	-1.901	-2.660	-0.759	(0)
H2S	2.691e-04	2.691e-04	-3.570	-3.570	0.000	(0)
S3-2	1.011e-04	1.761e-05	-3.995	-4.754	-0.759	(0)
S4-2	4.825e-07	8.406e-08	-6.316	-7.075	-0.759	(0)
S5-2	1.399e-09	2.437e-10	-8.854	-9.613	-0.759	(0)
S(2)	2.760e-06					
S2O3-2	1.380e-06	2.404e-07	-5.860	-6.619	-0.759	(0)
HS2O3-	5.533e-18	8.829e-18	-17.257	-17.054	0.203	(0)
S(3)	2.305e-29					
S2O4-2	1.152e-29	3.326e-30	-28.938	-29.478	-0.540	(0)
S(4)	6.755e-10					
SO3-2	6.755e-10	1.551e-10	-9.170	-9.809	-0.639	(0)
HSO3-	5.891e-15	9.401e-15	-14.230	-14.027	0.203	(0)
SO2	4.783e-24	4.783e-24	-23.320	-23.320	0.000	(0)
H2SO3	3.205e-24	3.205e-24	-23.494	-23.494	0.000	(0)
S4O6-2	1.601e-31	2.790e-32	-30.796	-31.554	-0.759	(0)
S2O6-2	2.834e-38	4.937e-39	-37.548	-38.307	-0.759	(0)
S3O6-2	0.000e+00	0.000e+00	-42.124	-42.883	-0.759	(0)
S5O6-2	0.000e+00	0.000e+00	-48.346	-49.105	-0.759	(0)

```
S(5)          2.820e-32
   S2O5-2          1.410e-32   2.457e-33   -31.851   -32.610    -0.759     (0)
S(6)          1.778e+01
   CaSO4           1.735e+01   1.735e+01     1.239     1.239     0.000     (0)
   SO4-2           4.330e-01   7.543e-02    -0.364    -1.122    -0.759     (0)
   HSO4-           1.698e-11   2.710e-11   -10.770   -10.567     0.203     (0)
   H2SO4           9.092e-26   9.092e-26   -25.041   -25.041     0.000     (0)
S(7)          0.000e+00
   S2O8-2          0.000e+00   0.000e+00   -84.496   -85.255    -0.759     (0)
S(8)          0.000e+00
   HSO5-           0.000e+00   0.000e+00   -67.966   -67.763     0.203     (0)

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

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

  Anhydrite          3.42     -0.93   -4.35  CaSO4
  Aragonite         -0.15      1.82    1.97  CaCO3
  Bassanite          2.64     -1.06   -3.71  CaSO4:0.5H2O
  C                 -9.28     54.87   64.15  C
  C(g)            -126.90     54.87  181.77  C
  Ca               -79.08     60.75  139.83  Ca
  Ca(g)           -104.32     60.75  165.07  Ca
  Calcite            0.00      1.82    1.82  CaCO3
  CaSO4:0.5H2O(beta)   2.47     -1.06   -3.54  CaSO4:0.5H2O
  CH4(g)          -11.07    -13.91   -2.84  CH4
  CO(g)           -21.74    -24.74   -3.00  CO
  CO2(g)          -13.17    -21.00   -7.83  CO2
  Gypsum            3.06     -1.47   -4.53  CaSO4:2H2O
  H2(g)            -5.34     -8.44   -3.10  H2
  H2O(g)           -1.86     -0.27    1.59  H2O
  H2S(g)           -2.59    -10.58   -7.99  H2S
  Ice              -0.41     -0.27    0.14  H2O
  Lime             -9.75     22.82   32.57  CaO
  Monohydrocalcite  -1.13      1.55    2.68  CaCO3:H2O
  O2(g)           -72.97    -75.86   -2.89  O2
  Portlandite      -0.00     22.55   22.55  Ca(OH)2
  S                -3.13    -48.24  -45.11  S
  S2(g)           -20.14    -27.33   -7.19  S2
  SO2(g)          -23.50    -23.32    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 0.286 Seconds.
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