```
   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
         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)          -3.41   -11.24     -7.83    1.000e+02   1.000e+02  -1.113e-06
SO2(g)          -5.15    -4.97      0.18    1.000e+02   8.844e+01  -1.156e+01

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

      Elements           Molality       Moles

      C                 1.263e-06   1.113e-06
      S                 1.312e+01   1.156e+01

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

                                    pH  =  -1.268      Charge balance
                                    pe  =   6.718      Adjusted to redox equilibrium
                         Activity of water  =   0.715
                            Ionic strength  =   1.116e+01
                        Mass of water (kg)  =   8.809e-01
                 Total alkalinity (eq/kg)  =  -3.745e+01
                        Total CO2 (mol/kg)  =   1.263e-06
```

```
                        Temperature (°C)  =  25.00
                  Electrical balance (eq)  =   1.307e-12
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                               Iterations  = 113
                                  Total H  = 1.110507e+02
                                  Total O  = 7.863994e+01
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	9.266e+00	1.852e+01	0.967	1.268	0.301	0.00
OH-	2.920e-16	3.719e-16	-15.535	-15.430	0.105	(0)
H2O	5.553e+01	7.148e-01	1.744	-0.146	0.000	18.07
C(-2)	0.000e+00					
C2H4	0.000e+00	0.000e+00	-83.727	-83.727	0.000	(0)
C(-3)	3.638e-26					
C2H6	1.819e-26	1.819e-26	-25.740	-25.740	0.000	(0)
C(-4)	2.243e-27					
CH4	2.243e-27	2.243e-27	-26.649	-26.649	0.000	(0)
C(2)	2.146e-21					
CO	2.146e-21	2.146e-21	-20.668	-20.668	0.000	(0)
C(4)	1.263e-06					
CO2	1.263e-06	1.343e-05	-5.899	-4.872	1.026	(0)
HCO3-	1.615e-13	2.234e-13	-12.792	-12.651	0.141	(0)
CO3-2	2.635e-24	5.351e-25	-23.579	-24.272	-0.692	(0)
H(0)	1.878e-15					
H2	9.389e-16	9.978e-15	-15.027	-14.001	1.026	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-65.512	-64.486	1.026	(0)
S(-2)	6.988e-03					
H2S	6.931e-03	6.931e-03	-2.159	-2.159	0.000	(0)
S5-2	1.137e-05	1.763e-06	-4.944	-5.754	-0.809	(0)
S4-2	4.197e-10	6.510e-11	-9.377	-10.186	-0.809	(0)
HS-	2.875e-11	3.661e-11	-10.541	-10.436	0.105	(0)
S3-2	9.409e-15	1.460e-15	-14.026	-14.836	-0.809	(0)
S2-2	1.250e-19	1.939e-20	-18.903	-19.712	-0.809	(0)
S-2	9.224e-25	2.344e-25	-24.035	-24.630	-0.595	(0)
S(2)	7.154e-05					
HS2O3-	3.417e-05	4.727e-05	-4.466	-4.325	0.141	(0)
S2O3-2	1.594e-06	2.472e-07	-5.798	-6.607	-0.809	(0)
S(3)	1.312e-23					
S2O4-2	6.560e-24	1.667e-24	-23.183	-23.778	-0.595	(0)
S(4)	7.481e+00					
S4O6-2	1.870e+00	2.901e-01	0.272	-0.537	-0.809	(0)
SO2	1.062e-05	1.062e-05	-4.974	-4.974	0.000	(0)
H2SO3	9.564e-06	9.564e-06	-5.019	-5.019	0.000	(0)
HSO3-	3.895e-09	5.388e-09	-8.410	-8.269	0.141	(0)
S5O6-2	4.918e-11	7.629e-12	-10.308	-11.118	-0.809	(0)
SO3-2	8.402e-17	1.707e-17	-16.076	-16.768	-0.692	(0)
S3O6-2	9.391e-19	1.457e-19	-18.027	-18.837	-0.809	(0)
S2O6-2	3.793e-21	5.883e-22	-20.421	-21.230	-0.809	(0)
S(5)	7.741e-21					
S2O5-2	3.870e-21	6.004e-22	-20.412	-21.222	-0.809	(0)
S(6)	5.632e+00					
HSO4-	5.474e+00	7.572e+00	0.738	0.879	0.141	(0)
H2SO4	1.323e-01	1.323e-01	-0.878	-0.878	0.000	(0)
SO4-2	2.609e-02	4.047e-03	-1.583	-2.393	-0.809	(0)
S(7)	0.000e+00					
S2O8-2	0.000e+00	0.000e+00	-55.993	-56.802	-0.809	(0)
S(8)	0.000e+00					
HSO5-	0.000e+00	0.000e+00	-50.770	-50.629	0.141	(0)

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

Phase	SI**	log IAP	log K(298 K, 1 atm)	
C	-10.90	53.25	64.15	C
C(g)	-128.52	53.25	181.77	C
CH4(g)	-23.81	-26.65	-2.84	CH4
CO(g)	-17.67	-20.67	-3.00	CO
CO2(g)	-3.41	-11.24	-7.83	CO2
H2(g)	-10.90	-14.00	-3.10	H2
H2O(g)	-1.73	-0.15	1.59	H2O
H2S(g)	-1.18	-9.17	-7.99	H2S
Ice	-0.28	-0.15	0.14	H2O
O2(g)	-61.59	-64.49	-2.89	O2
S	3.84	-41.27	-45.11	S
S2(g)	-6.20	-13.39	-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.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.27 Seconds.
