```
   Input file: C:\Users\weissd2k\OneDrive - Imperial College London\3 Teaching\Lectures
\60055 Contaminant Transport\Resources\PHREEQC\examples\ex9.pqi
  Output file: C:\Users\weissd2k\OneDrive - Imperial College London\3 Teaching\Lectures
\60055 Contaminant Transport\Resources\PHREEQC\examples\ex9.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.7.3-15968\database
\phreeqc.dat

------------------
Reading data base.
------------------

      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 (x86)\USGS\Phreeqc Interactive 3.7.3-15968\database
\phreeqc.dat
      TITLE Example 9.--Kinetically controlled oxidation of ferrous
                        iron. Decoupled valence states of iron.
      SOLUTION_MASTER_SPECIES
      Fe_di               Fe_di+2    0.0     Fe_di              55.847
      Fe_tri              Fe_tri+3   0.0     Fe_tri             55.847
      SOLUTION_SPECIES
      Fe_di+2 = Fe_di+2
              log_k   0.0
      Fe_tri+3 = Fe_tri+3
              log_k   0.0
      Fe_di+2 + H2O = Fe_diOH+ + H+
              log_k   -9.5
              delta_h 13.20   kcal
      Fe_di+2 + Cl- = Fe_diCl+
              log_k   0.14
      Fe_di+2 + CO3-2 = Fe_diCO3
              log_k   4.38
      Fe_di+2 + HCO3- = Fe_diHCO3+
              log_k   2.0
      Fe_di+2 + SO4-2 = Fe_diSO4
              log_k   2.25
              delta_h 3.230   kcal
      Fe_di+2 + HSO4- = Fe_diHSO4+
              log_k   1.08
      Fe_di+2 + 2HS- = Fe_di(HS)2
              log_k   8.95
      Fe_di+2 + 3HS- = Fe_di(HS)3-
              log_k   10.987
      Fe_di+2 + HPO4-2 = Fe_diHPO4
              log_k   3.6
      Fe_di+2 + H2PO4- = Fe_diH2PO4+
              log_k   2.7
      Fe_di+2 + F- = Fe_diF+
              log_k   1.0
      Fe_tri+3 + H2O = Fe_triOH+2 + H+
              log_k   -2.19
              delta_h 10.4    kcal
      Fe_tri+3 + 2 H2O = Fe_tri(OH)2+ + 2 H+
              log_k   -5.67
              delta_h 17.1    kcal
      Fe_tri+3 + 3 H2O = Fe_tri(OH)3 + 3 H+
              log_k   -12.56
```

```
              delta_h 24.8    kcal
      Fe_tri+3 + 4 H2O = Fe_tri(OH)4- + 4 H+
              log_k   -21.6
              delta_h 31.9    kcal
      2 Fe_tri+3 + 2 H2O = Fe_tri2(OH)2+4 + 2 H+
              log_k   -2.95
              delta_h 13.5    kcal
      3 Fe_tri+3 + 4 H2O = Fe_tri3(OH)4+5 + 4 H+
              log_k   -6.3
              delta_h 14.3    kcal
      Fe_tri+3 + Cl- = Fe_triCl+2
              log_k   1.48
              delta_h 5.6     kcal
      Fe_tri+3 + 2 Cl- = Fe_triCl2+
              log_k   2.13
      Fe_tri+3 + 3 Cl- = Fe_triCl3
              log_k   1.13
      Fe_tri+3 + SO4-2 = Fe_triSO4+
              log_k   4.04
              delta_h 3.91    kcal
      Fe_tri+3 + HSO4- = Fe_triHSO4+2
              log_k   2.48
      Fe_tri+3 + 2 SO4-2 = Fe_tri(SO4)2-
              log_k   5.38
              delta_h 4.60    kcal
      Fe_tri+3 + HPO4-2 = Fe_triHPO4+
              log_k   5.43
              delta_h 5.76    kcal
      Fe_tri+3 + H2PO4- = Fe_triH2PO4+2
              log_k   5.43
      Fe_tri+3 + F- = Fe_triF+2
              log_k   6.2
              delta_h 2.7     kcal
      Fe_tri+3 + 2 F- = Fe_triF2+
              log_k   10.8
              delta_h 4.8     kcal
      Fe_tri+3 + 3 F- = Fe_triF3
              log_k   14.0
              delta_h 5.4     kcal
      PHASES
      Goethite
              Fe_triOOH + 3 H+ = Fe_tri+3 + 2 H2O
              log_k   -1.0
      END
-----
TITLE
-----

 Example 9.--Kinetically controlled oxidation of ferrous
                 iron. Decoupled valence states of iron.

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 2.
------------------------------------

      SOLUTION 1
              pH  7.0
              pe 10.0  O2(g) -0.67
              Fe_di  0.1
              Na  10.
              Cl  10.  charge
      EQUILIBRIUM_PHASES 1
              O2(g)           -0.67
      RATES
```

```
      Fe_di_ox
        start
        10  Fe_di = TOT("Fe_di")
        20  if (Fe_di <= 0) then goto 200
        30  p_o2 = SR("O2(g)")
        40  moles = (2.91e-9 + 1.33e12 * (ACT("OH-"))^2 * p_o2) * Fe_di * TIME
        200 SAVE moles
        end
      KINETICS 1
      Fe_di_ox
              formula  Fe_di  -1.0  Fe_tri  1.0
              steps 100 400 3100 10800 21600 5.04e4 8.64e4 1.728e5 1.728e5 1.728e5 1.728e5
              step_divide 1e-4
      INCREMENTAL_REACTIONS true
      SELECTED_OUTPUT
              file ex9.sel
              reset false
      USER_PUNCH
              headings Days  Fe(2)  Fe(3)  pH  si_goethite
        10 PUNCH SIM_TIME / 3600 / 24, TOT("Fe_di")*1e6, TOT("Fe_tri")*1e6, -LA("H+"),
SI("Goethite")
      USER_GRAPH Example 9
              -headings _time_ Fe(2) Fe(3) pH
              -chart_title "Oxidation of Ferrous Iron"
              -axis_titles "Time, in days" "Micromole per kilogram water" "pH"
              -axis_scale secondary_y_axis 4.0 7.0 1.0 0.5
        -start
        10 GRAPH_X TOTAL_TIME / 3600 / 24
        20 GRAPH_Y TOT("Fe_di")*1e6, TOT("Fe_tri")*1e6
        30 GRAPH_SY -LA("H+")
        -end
      END
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

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

      Elements           Molality       Moles

      Cl                1.020e-02   1.020e-02  Charge balance
      Fe_di             1.000e-04   1.000e-04
      Na                1.000e-02   1.000e-02

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

                                       pH  =   7.000
                                       pe  =  13.629      Equilibrium with O2(g)
      Specific Conductance (µS/cm,  25°C)  = 1192
                           Density (g/cm³)  =   0.99747
                                Volume (L)  =   1.00315
                        Activity of water  =   1.000
                  Ionic strength (mol/kgw)  =   1.030e-02
                       Mass of water (kg)  =   1.000e+00
                  Total alkalinity (eq/kg)  =   2.313e-07
                          Temperature (°C)  =  25.00
                   Electrical balance (eq)  =   3.500e-18
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                                Iterations  =   9
                                   Total H  = 1.110124e+02
                                   Total O  = 5.550676e+01

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

                                                Log       Log       Log    mole V
   Species          Molality    Activity  Molality  Activity     Gamma    cm³/mol
```

```
   OH-             1.126e-07   1.012e-07    -6.949    -6.995    -0.046     -4.03
   H+              1.096e-07   1.000e-07    -6.960    -7.000    -0.040      0.00
   H2O             5.551e+01   9.997e-01     1.744    -0.000     0.000     18.07
Cl             1.020e-02
   Cl-             1.020e-02   9.174e-03    -1.991    -2.037    -0.046     18.14
   Fe_diCl+        9.148e-07   8.240e-07    -6.039    -6.084    -0.045     (0)
Fe_di          1.000e-04
   Fe_di+2         9.886e-05   6.507e-05    -4.005    -4.187    -0.182     (0)
   Fe_diCl+        9.148e-07   8.240e-07    -6.039    -6.084    -0.045     (0)
   Fe_diOH+        2.284e-07   2.057e-07    -6.641    -6.687    -0.045     (0)
H(0)           0.000e+00
   H2              0.000e+00   0.000e+00   -44.410   -44.409     0.001     28.61
Na             1.000e-02
   Na+             1.000e-02   9.022e-03    -2.000    -2.045    -0.045     -1.38
   NaOH            9.106e-20   9.128e-20   -19.041   -19.040     0.001     (0)
O(0)           5.465e-04
   O2              2.732e-04   2.739e-04    -3.563    -3.562     0.001     30.40

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

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

  H2(g)           -41.31    -44.41    -3.10  H2
  H2O(g)           -1.50     -0.00     1.50  H2O
  Halite           -5.65     -4.08     1.57  NaCl
  O2(g)            -0.67     -3.56    -2.89  O2   Pressure   0.2 atm, phi 1.000

**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: Negative moles in solution 1 for Fe_tri, -6.101497e-06. Recovering...
WARNING: Negative moles in solution 1 for Fe_tri, -1.392301e-06. Recovering...
Using solution 1.
Using pure phase assemblage 1.
Using kinetics 1.

Kinetics 1.

      Time step: 100 seconds  (Incremented time: 100 seconds)

      Rate name       Delta Moles Total Moles   Reactant        Coefficient

      Fe_di_ox         -1.066e-06   1.000e+00   Fe_di                   -1
                                                Fe_tri                   1

-------------------------------Phase assemblage-------------------------------

                                                          Moles in assemblage
Phase               SI  log IAP  log K(T, P)   Initial       Final       Delta

O2(g)           -0.67    -3.56     -2.89    1.000e+01   1.000e+01  -2.665e-07

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

      Elements           Molality       Moles

      Cl                1.020e-02   1.020e-02
      Fe_di             9.893e-05   9.893e-05
      Fe_tri            1.066e-06   1.066e-06
      Na                1.000e-02   1.000e-02
```

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

pH	= 6.044	Charge balance
pe	= 14.585	Adjusted to redox equilibrium
Specific Conductance (µS/cm, 25°C)	= 1192	
Density (g/cm³)	= 0.99747	
Volume (L)	= 1.00315	
Activity of water	= 1.000	
Ionic strength (mol/kgw)	= 1.030e-02	
Mass of water (kg)	= 1.000e+00	
Total alkalinity (eq/kg)	= 1.297e-06	
Temperature (°C)	= 25.00	
Electrical balance (eq)	= 7.978e-16	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 0.00	
Iterations	= 208 (195 overall)	
Total H	= 1.110124e+02	
Total O	= 5.550676e+01	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	9.895e-07	9.029e-07	-6.005	-6.044	-0.040	0.00
OH-	1.247e-08	1.121e-08	-7.904	-7.951	-0.046	-4.03
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.07
Cl	1.020e-02					
Cl-	1.020e-02	9.174e-03	-1.991	-2.037	-0.046	18.14
Fe_diCl+	9.069e-07	8.169e-07	-6.042	-6.088	-0.045	(0)
Fe_triCl+2	1.362e-13	8.965e-14	-12.866	-13.047	-0.182	(0)
Fe_triCl2+	4.079e-15	3.674e-15	-14.389	-14.435	-0.045	(0)
Fe_triCl3	3.362e-18	3.370e-18	-17.473	-17.472	0.001	(0)
Fe_di	9.893e-05					
Fe_di+2	9.800e-05	6.450e-05	-4.009	-4.190	-0.182	(0)
Fe_diCl+	9.069e-07	8.169e-07	-6.042	-6.088	-0.045	(0)
Fe_diOH+	2.507e-08	2.259e-08	-7.601	-7.646	-0.045	(0)
Fe_tri	1.066e-06					
Fe_tri(OH)2+	9.416e-07	8.481e-07	-6.026	-6.072	-0.045	(0)
Fe_tri(OH)3	1.207e-07	1.210e-07	-6.918	-6.917	0.001	(0)
Fe_triOH+2	3.514e-09	2.313e-09	-8.454	-8.636	-0.182	(0)
Fe_tri(OH)4-	1.356e-10	1.221e-10	-9.868	-9.913	-0.045	(0)
Fe_tri+3	8.292e-13	3.236e-13	-12.081	-12.490	-0.409	(0)
Fe_triCl+2	1.362e-13	8.965e-14	-12.866	-13.047	-0.182	(0)
Fe_triCl2+	4.079e-15	3.674e-15	-14.389	-14.435	-0.045	(0)
Fe_tri2(OH)2+4	7.673e-16	1.440e-16	-15.115	-15.842	-0.727	(0)
Fe_triCl3	3.362e-18	3.370e-18	-17.473	-17.472	0.001	(0)
Fe_tri3(OH)4+5	3.484e-19	2.552e-20	-18.458	-19.593	-1.135	(0)
H(0)	0.000e+00					
H2	0.000e+00	0.000e+00	-44.410	-44.409	0.001	28.61
Na	1.000e-02					
Na+	1.000e-02	9.022e-03	-2.000	-2.045	-0.045	-1.38
NaOH	1.009e-20	1.011e-20	-19.996	-19.995	0.001	(0)
O(0)	5.465e-04					
O2	2.732e-04	2.739e-04	-3.563	-3.562	0.001	30.40

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

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Goethite	6.64	5.64	-1.00	Fe_triOOH
H2(g)	-41.31	-44.41	-3.10	H2
H2O(g)	-1.50	-0.00	1.50	H2O
Halite	-5.65	-4.08	1.57	NaCl
O2(g)	-0.67	-3.56	-2.89	O2 Pressure 0.2 atm, phi 1.000

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

Reaction step 2.

Using solution 1.
Using pure phase assemblage 1.
Using kinetics 1.

Kinetics 1.

Time step: 400 seconds (Incremented time: 500 seconds)

Rate name	Delta Moles	Total Moles	Reactant	Coefficient
Fe_di_ox	-7.416e-07	1.000e+00	Fe_di	-1
			Fe_tri	1

----------Phase assemblage----------

Phase	SI	log IAP	log K(T, P)	Moles in assemblage Initial	Final	Delta
O2(g)	-0.67	-3.56	-2.89	1.000e+01	1.000e+01	-1.854e-07

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

Elements	Molality	Moles
Cl	1.020e-02	1.020e-02
Fe_di	9.819e-05	9.819e-05
Fe_tri	1.808e-06	1.808e-06
Na	1.000e-02	1.000e-02

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

pH	= 5.807	Charge balance
pe	= 14.823	Adjusted to redox equilibrium
Specific Conductance (µS/cm, 25°C)	= 1192	
Density (g/cm³)	= 0.99747	
Volume (L)	= 1.00315	
Activity of water	= 1.000	
Ionic strength (mol/kgw)	= 1.030e-02	
Mass of water (kg)	= 1.000e+00	
Total alkalinity (eq/kg)	= 2.039e-06	
Temperature (°C)	= 25.00	
Electrical balance (eq)	= 8.026e-16	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 0.00	
Iterations	= 27	
Total H	= 1.110124e+02	
Total O	= 5.550676e+01	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.711e-06	1.561e-06	-5.767	-5.807	-0.040	0.00
OH-	7.211e-09	6.481e-09	-8.142	-8.188	-0.046	-4.03
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.07
Cl	1.020e-02					
Cl-	1.020e-02	9.174e-03	-1.991	-2.037	-0.046	18.14
Fe_diCl+	9.002e-07	8.108e-07	-6.046	-6.091	-0.045	(0)
Fe_triCl+2	7.235e-13	4.762e-13	-12.141	-12.322	-0.182	(0)
Fe_triCl2+	2.167e-14	1.951e-14	-13.664	-13.710	-0.045	(0)
Fe_triCl3	1.786e-17	1.790e-17	-16.748	-16.747	0.001	(0)
Fe_di	9.819e-05					
Fe_di+2	9.728e-05	6.403e-05	-4.012	-4.194	-0.182	(0)
Fe_diCl+	9.002e-07	8.108e-07	-6.046	-6.091	-0.045	(0)
Fe_diOH+	1.439e-08	1.296e-08	-7.842	-7.887	-0.045	(0)
Fe_tri	1.808e-06					

```
   Fe_tri(OH)2+    1.673e-06   1.507e-06    -5.777    -5.822    -0.045      (0)
   Fe_tri(OH)3     1.240e-07   1.243e-07    -6.907    -6.906     0.001      (0)
   Fe_triOH+2      1.080e-08   7.106e-09    -7.967    -8.148    -0.182      (0)
   Fe_tri(OH)4-    8.057e-11   7.257e-11   -10.094   -10.139    -0.045      (0)
   Fe_tri+3        4.405e-12   1.719e-12   -11.356   -11.765    -0.409      (0)
   Fe_triCl+2      7.235e-13   4.762e-13   -12.141   -12.322    -0.182      (0)
   Fe_triCl2+      2.167e-14   1.951e-14   -13.664   -13.710    -0.045      (0)
   Fe_tri2(OH)2+4   7.241e-15   1.359e-15   -14.140   -14.867    -0.727      (0)
   Fe_triCl3       1.786e-17   1.790e-17   -16.748   -16.747     0.001      (0)
   Fe_tri3(OH)4+5   5.841e-18   4.278e-19   -17.234   -18.369    -1.135      (0)
H(0)           0.000e+00
   H2              0.000e+00   0.000e+00   -44.410   -44.409     0.001     28.61
Na             1.000e-02
   Na+             1.000e-02   9.022e-03    -2.000    -2.045    -0.045     -1.38
   NaOH            5.833e-21   5.847e-21   -20.234   -20.233     0.001      (0)
O(0)           5.465e-04
   O2              2.732e-04   2.739e-04    -3.563    -3.562     0.001     30.40

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

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

  Goethite          6.65      5.65   -1.00  Fe_triOOH
  H2(g)           -41.31    -44.41   -3.10  H2
  H2O(g)           -1.50     -0.00    1.50  H2O
  Halite           -5.65     -4.08    1.57  NaCl
  O2(g)            -0.67     -3.56   -2.89  O2   Pressure   0.2 atm, phi 1.000

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

Reaction step 3.

Using solution 1.
Using pure phase assemblage 1.
Using kinetics 1.

Kinetics 1.

      Time step: 3100 seconds  (Incremented time: 3600 seconds)

      Rate name       Delta Moles Total Moles   Reactant        Coefficient

      Fe_di_ox         -1.626e-06   1.000e+00   Fe_di                   -1
                                                Fe_tri                   1

-------------------------------Phase assemblage-------------------------------

                                                          Moles in assemblage
Phase               SI  log IAP  log K(T, P)   Initial       Final       Delta

O2(g)            -0.67    -3.56     -2.89    1.000e+01   1.000e+01  -4.065e-07

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

      Elements           Molality       Moles

      Cl                1.020e-02   1.020e-02
      Fe_di             9.657e-05   9.657e-05
      Fe_tri            3.433e-06   3.433e-06
      Na                1.000e-02   1.000e-02

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

                                    pH  =   5.522      Charge balance
                                    pe  =  15.108      Adjusted to redox equilibrium
      Specific Conductance (µS/cm,  25°C)  = 1193
                         Density (g/cm³)   =   0.99747
```

```
                                Volume (L)  =   1.00315
                          Activity of water  =   1.000
                   Ionic strength (mol/kgw)  =   1.029e-02
                         Mass of water (kg)  =   1.000e+00
                  Total alkalinity (eq/kg)  =   3.665e-06
                          Temperature (°C)  =  25.00
                   Electrical balance (eq)  =   8.914e-16
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                                Iterations  =  67
                                   Total H  = 1.110124e+02
                                   Total O  = 5.550677e+01

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

                                                    Log       Log       Log    mole V
   Species          Molality    Activity  Molality  Activity     Gamma    cm³/mol

   H+              3.298e-06   3.009e-06    -5.482    -5.522    -0.040      0.00
   OH-             3.741e-09   3.362e-09    -8.427    -8.473    -0.046     -4.03
   H2O             5.551e+01   9.997e-01     1.744    -0.000     0.000     18.07
Cl             1.020e-02
   Cl-             1.020e-02   9.174e-03    -1.991    -2.037    -0.046     18.14
   Fe_diCl+        8.854e-07   7.975e-07    -6.053    -6.098    -0.045     (0)
   Fe_triCl+2      5.249e-12   3.455e-12   -11.280   -11.462    -0.182     (0)
   Fe_triCl2+      1.572e-13   1.416e-13   -12.804   -12.849    -0.045     (0)
   Fe_triCl3       1.296e-16   1.299e-16   -15.887   -15.886     0.001     (0)
Fe_di          9.657e-05
   Fe_di+2         9.567e-05   6.298e-05    -4.019    -4.201    -0.182     (0)
   Fe_diCl+        8.854e-07   7.975e-07    -6.053    -6.098    -0.045     (0)
   Fe_diOH+        7.345e-09   6.616e-09    -8.134    -8.179    -0.045     (0)
Fe_tri         3.433e-06
   Fe_tri(OH)2+    3.267e-06   2.943e-06    -5.486    -5.531    -0.045     (0)
   Fe_tri(OH)3     1.256e-07   1.259e-07    -6.901    -6.900     0.001     (0)
   Fe_triOH+2      4.064e-08   2.675e-08    -7.391    -7.573    -0.182     (0)
   Fe_tri(OH)4-    4.236e-11   3.815e-11   -10.373   -10.418    -0.045     (0)
   Fe_tri+3        3.196e-11   1.247e-11   -10.495   -10.904    -0.409     (0)
   Fe_triCl+2      5.249e-12   3.455e-12   -11.280   -11.462    -0.182     (0)
   Fe_triCl2+      1.572e-13   1.416e-13   -12.804   -12.849    -0.045     (0)
   Fe_tri2(OH)2+4  1.026e-13   1.926e-14   -12.989   -13.715    -0.727     (0)
   Fe_tri3(OH)4+5  1.616e-16   1.184e-17   -15.791   -16.927    -1.135     (0)
   Fe_triCl3       1.296e-16   1.299e-16   -15.887   -15.886     0.001     (0)
H(0)           0.000e+00
   H2              0.000e+00   0.000e+00   -44.410   -44.409     0.001     28.61
Na             1.000e-02
   Na+             1.000e-02   9.022e-03    -2.000    -2.045    -0.045     -1.38
   NaOH            3.026e-21   3.034e-21   -20.519   -20.518     0.001     (0)
O(0)           5.465e-04
   O2              2.732e-04   2.739e-04    -3.563    -3.562     0.001     30.40

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

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

  Goethite           6.66      5.66   -1.00  Fe_triOOH
  H2(g)            -41.31    -44.41   -3.10  H2
  H2O(g)            -1.50     -0.00    1.50  H2O
  Halite            -5.65     -4.08    1.57  NaCl
  O2(g)             -0.67     -3.56   -2.89  O2   Pressure   0.2 atm, phi 1.000

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

Reaction step 4.

Using solution 1.
Using pure phase assemblage 1.
Using kinetics 1.
```

Kinetics 1.

Time step: 10800 seconds (Incremented time: 14400 seconds)

Rate name	Delta Moles	Total Moles	Reactant	Coefficient
Fe_di_ox	-1.967e-06	1.000e+00	Fe_di	-1
			Fe_tri	1

----------Phase assemblage----------

Phase	SI	log IAP	log K(T, P)	Moles in assemblage Initial	Final	Delta
O2(g)	-0.67	-3.56	-2.89	1.000e+01	1.000e+01	-4.919e-07

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

Elements	Molality	Moles
Cl	1.020e-02	1.020e-02
Fe_di	9.460e-05	9.460e-05
Fe_tri	5.400e-06	5.400e-06
Na	1.000e-02	1.000e-02

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

pH	= 5.324	Charge balance
pe	= 15.306	Adjusted to redox equilibrium
Specific Conductance (µS/cm, 25°C)	= 1194	
Density (g/cm³)	= 0.99747	
Volume (L)	= 1.00315	
Activity of water	= 1.000	
Ionic strength (mol/kgw)	= 1.029e-02	
Mass of water (kg)	= 1.000e+00	
Total alkalinity (eq/kg)	= 5.632e-06	
Temperature (°C)	= 25.00	
Electrical balance (eq)	= 6.865e-15	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 0.00	
Iterations	= 26	
Total H	= 1.110124e+02	
Total O	= 5.550677e+01	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	5.200e-06	4.745e-06	-5.284	-5.324	-0.040	0.00
OH-	2.373e-09	2.132e-09	-8.625	-8.671	-0.046	-4.03
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.07
Cl	1.020e-02					
Cl-	1.020e-02	9.174e-03	-1.991	-2.037	-0.046	18.14
Fe_diCl+	8.674e-07	7.813e-07	-6.062	-6.107	-0.045	(0)
Fe_triCl+2	2.066e-11	1.360e-11	-10.685	-10.866	-0.182	(0)
Fe_triCl2+	6.189e-13	5.574e-13	-12.208	-12.254	-0.045	(0)
Fe_triCl3	5.102e-16	5.114e-16	-15.292	-15.291	0.001	(0)
Fe_di	9.460e-05					
Fe_di+2	9.373e-05	6.170e-05	-4.028	-4.210	-0.182	(0)
Fe_diCl+	8.674e-07	7.813e-07	-6.062	-6.107	-0.045	(0)
Fe_diOH+	4.563e-09	4.110e-09	-8.341	-8.386	-0.045	(0)
Fe_tri	5.400e-06					
Fe_tri(OH)2+	5.172e-06	4.659e-06	-5.286	-5.332	-0.045	(0)
Fe_tri(OH)3	1.262e-07	1.265e-07	-6.899	-6.898	0.001	(0)
Fe_triOH+2	1.015e-07	6.678e-08	-6.994	-7.175	-0.182	(0)
Fe_tri+3	1.258e-10	4.910e-11	-9.900	-10.309	-0.409	(0)
Fe_tri(OH)4-	2.697e-11	2.430e-11	-10.569	-10.614	-0.045	(0)
Fe_triCl+2	2.066e-11	1.360e-11	-10.685	-10.866	-0.182	(0)

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   Fe_tri2(OH)2+4   6.394e-13   1.200e-13   -12.194   -12.921    -0.726     (0)
   Fe_triCl2+       6.189e-13   5.574e-13   -12.208   -12.254    -0.045     (0)
   Fe_tri3(OH)4+5   1.595e-15   1.169e-16   -14.797   -15.932    -1.135     (0)
   Fe_triCl3        5.102e-16   5.114e-16   -15.292   -15.291     0.001     (0)
H(0)           0.000e+00
   H2               0.000e+00   0.000e+00   -44.410   -44.409     0.001     28.61
Na             1.000e-02
   Na+              1.000e-02   9.022e-03    -2.000    -2.045    -0.045     -1.38
   NaOH             1.919e-21   1.924e-21   -20.717   -20.716     0.001     (0)
O(0)           5.465e-04
   O2               2.732e-04   2.739e-04    -3.563    -3.562     0.001     30.40

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

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

  Goethite           6.66      5.66   -1.00  Fe_triOOH
  H2(g)            -41.31    -44.41   -3.10  H2
  H2O(g)            -1.50     -0.00    1.50  H2O
  Halite            -5.65     -4.08    1.57  NaCl
  O2(g)             -0.67     -3.56   -2.89  O2   Pressure   0.2 atm, phi 1.000

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

Reaction step 5.

Using solution 1.
Using pure phase assemblage 1.
Using kinetics 1.

Kinetics 1.

      Time step: 21600 seconds  (Incremented time: 36000 seconds)

      Rate name       Delta Moles Total Moles   Reactant        Coefficient

      Fe_di_ox         -1.889e-06   1.000e+00   Fe_di                    -1
                                                Fe_tri                    1

-------------------------------Phase assemblage-------------------------------

                                                          Moles in assemblage
Phase               SI  log IAP  log K(T, P)   Initial       Final       Delta

O2(g)           -0.67    -3.56     -2.89    1.000e+01   1.000e+01  -4.723e-07

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

      Elements           Molality       Moles

      Cl                1.020e-02   1.020e-02
      Fe_di             9.271e-05   9.271e-05
      Fe_tri            7.289e-06   7.289e-06
      Na                1.000e-02   1.000e-02

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

                                    pH  =   5.194      Charge balance
                                    pe  =  15.435      Adjusted to redox equilibrium
      Specific Conductance (µS/cm,  25°C)  = 1194
                         Density (g/cm³)  =   0.99747
                              Volume (L)  =   1.00315
                     Activity of water    =   1.000
                Ionic strength (mol/kgw)  =   1.029e-02
                     Mass of water (kg)   =   1.000e+00
                Total alkalinity (eq/kg)  =   7.520e-06
                       Temperature (°C)   =  25.00
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                  Electrical balance (eq)  =   6.866e-15
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                                Iterations  =  24
                                   Total H  = 1.110124e+02
                                   Total O  = 5.550677e+01

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

                                                  Log       Log       Log    mole V
   Species          Molality    Activity  Molality  Activity     Gamma    cm³/mol

   H+              7.004e-06   6.391e-06    -5.155    -5.194    -0.040      0.00
   OH-             1.762e-09   1.583e-09    -8.754    -8.800    -0.046     -4.03
   H2O             5.551e+01   9.997e-01     1.744    -0.000     0.000     18.07
Cl             1.020e-02
   Cl-             1.020e-02   9.174e-03    -1.991    -2.037    -0.046     18.14
   Fe_diCl+        8.501e-07   7.658e-07    -6.071    -6.116    -0.045     (0)
   Fe_triCl+2      5.057e-11   3.329e-11   -10.296   -10.478    -0.182     (0)
   Fe_triCl2+      1.514e-12   1.364e-12   -11.820   -11.865    -0.045     (0)
   Fe_triCl3       1.249e-15   1.252e-15   -14.904   -14.903     0.001     (0)
Fe_di          9.271e-05
   Fe_di+2         9.186e-05   6.047e-05    -4.037    -4.218    -0.182     (0)
   Fe_diCl+        8.501e-07   7.658e-07    -6.071    -6.116    -0.045     (0)
   Fe_diOH+        3.321e-09   2.991e-09    -8.479    -8.524    -0.045     (0)
Fe_tri         7.289e-06
   Fe_tri(OH)2+    6.978e-06   6.285e-06    -5.156    -5.202    -0.045     (0)
   Fe_triOH+2      1.843e-07   1.213e-07    -6.734    -6.916    -0.182     (0)
   Fe_tri(OH)3     1.264e-07   1.267e-07    -6.898    -6.897     0.001     (0)
   Fe_tri+3        3.078e-10   1.201e-10    -9.512    -9.920    -0.409     (0)
   Fe_triCl+2      5.057e-11   3.329e-11   -10.296   -10.478    -0.182     (0)
   Fe_tri(OH)4-    2.006e-11   1.807e-11   -10.698   -10.743    -0.045     (0)
   Fe_tri2(OH)2+4   2.111e-12   3.963e-13   -11.676   -12.402    -0.726     (0)
   Fe_triCl2+      1.514e-12   1.364e-12   -11.820   -11.865    -0.045     (0)
   Fe_tri3(OH)4+5   7.101e-15   5.204e-16   -14.149   -15.284    -1.135     (0)
   Fe_triCl3       1.249e-15   1.252e-15   -14.904   -14.903     0.001     (0)
H(0)           0.000e+00
   H2              0.000e+00   0.000e+00   -44.410   -44.409     0.001     28.61
Na             1.000e-02
   Na+             1.000e-02   9.022e-03    -2.000    -2.045    -0.045     -1.38
   NaOH            1.425e-21   1.428e-21   -20.846   -20.845     0.001     (0)
O(0)           5.465e-04
   O2              2.732e-04   2.739e-04    -3.563    -3.562     0.001     30.40

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

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

  Goethite           6.66      5.66   -1.00  Fe_triOOH
  H2(g)           -41.31    -44.41   -3.10  H2
  H2O(g)           -1.50     -0.00    1.50  H2O
  Halite           -5.65     -4.08    1.57  NaCl
  O2(g)            -0.67     -3.56   -2.89  O2   Pressure   0.2 atm, phi 1.000

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

Reaction step 6.

Using solution 1.
Using pure phase assemblage 1.
Using kinetics 1.

Kinetics 1.

      Time step: 50400 seconds  (Incremented time: 86400 seconds)

      Rate name       Delta Moles Total Moles   Reactant        Coefficient
```

Fe_di_ox	-2.424e-06	1.000e+00	Fe_di -1 Fe_tri 1

Phase assemblage

Phase	SI	log IAP	log K(T, P)	Moles in assemblage: Initial	Final	Delta
O2(g)	-0.67	-3.56	-2.89	1.000e+01	1.000e+01	-6.060e-07

Solution composition

Elements	Molality	Moles
Cl	1.020e-02	1.020e-02
Fe_di	9.029e-05	9.029e-05
Fe_tri	9.712e-06	9.712e-06
Na	1.000e-02	1.000e-02

Description of solution

pH	= 5.072	Charge balance
pe	= 15.557	Adjusted to redox equilibrium
Specific Conductance (µS/cm, 25°C)	= 1195	
Density (g/cm³)	= 0.99747	
Volume (L)	= 1.00315	
Activity of water	= 1.000	
Ionic strength (mol/kgw)	= 1.029e-02	
Mass of water (kg)	= 1.000e+00	
Total alkalinity (eq/kg)	= 9.944e-06	
Temperature (°C)	= 25.00	
Electrical balance (eq)	= 6.880e-15	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 0.00	
Iterations	= 24	
Total H	= 1.110124e+02	
Total O	= 5.550677e+01	

Distribution of species

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	9.285e-06	8.472e-06	-5.032	-5.072	-0.040	0.00
OH-	1.329e-09	1.194e-09	-8.877	-8.923	-0.046	-4.03
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.07
Cl	**1.020e-02**					
Cl-	1.020e-02	9.174e-03	-1.991	-2.037	-0.046	18.14
Fe_diCl+	8.280e-07	7.458e-07	-6.082	-6.127	-0.045	(0)
Fe_triCl+2	1.180e-10	7.765e-11	-9.928	-10.110	-0.182	(0)
Fe_triCl2+	3.533e-12	3.182e-12	-11.452	-11.497	-0.045	(0)
Fe_triCl3	2.912e-15	2.919e-15	-14.536	-14.535	0.001	(0)
Fe_di	**9.029e-05**					
Fe_di+2	8.946e-05	5.889e-05	-4.048	-4.230	-0.182	(0)
Fe_diCl+	8.280e-07	7.458e-07	-6.082	-6.127	-0.045	(0)
Fe_diOH+	2.439e-09	2.197e-09	-8.613	-8.658	-0.045	(0)
Fe_tri	**9.712e-06**					
Fe_tri(OH)2+	9.261e-06	8.342e-06	-5.033	-5.079	-0.045	(0)
Fe_triOH+2	3.243e-07	2.135e-07	-6.489	-6.671	-0.182	(0)
Fe_tri(OH)3	1.265e-07	1.268e-07	-6.898	-6.897	0.001	(0)
Fe_tri+3	7.180e-10	2.803e-10	-9.144	-9.552	-0.409	(0)
Fe_triCl+2	1.180e-10	7.765e-11	-9.928	-10.110	-0.182	(0)
Fe_tri(OH)4-	1.515e-11	1.364e-11	-10.820	-10.865	-0.045	(0)
Fe_tri2(OH)2+4	6.533e-12	1.227e-12	-11.185	-11.911	-0.726	(0)
Fe_triCl2+	3.533e-12	3.182e-12	-11.452	-11.497	-0.045	(0)
Fe_tri3(OH)4+5	2.917e-14	2.138e-15	-13.535	-14.670	-1.135	(0)
Fe_triCl3	2.912e-15	2.919e-15	-14.536	-14.535	0.001	(0)
H(0)	**0.000e+00**					
H2	0.000e+00	0.000e+00	-44.410	-44.409	0.001	28.61

```
Na            1.000e-02
   Na+             1.000e-02   9.022e-03    -2.000    -2.045    -0.045     -1.38
   NaOH            1.075e-21   1.077e-21   -20.969   -20.968     0.001     (0)
O(0)          5.465e-04
   O2              2.732e-04   2.739e-04    -3.563    -3.562     0.001     30.40

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

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

  Goethite           6.66      5.66   -1.00  Fe_triOOH
  H2(g)            -41.31    -44.41   -3.10  H2
  H2O(g)            -1.50     -0.00    1.50  H2O
  Halite            -5.65     -4.08    1.57  NaCl
  O2(g)             -0.67     -3.56   -2.89  O2   Pressure   0.2 atm, phi 1.000

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

Reaction step 7.

Using solution 1.
Using pure phase assemblage 1.
Using kinetics 1.

Kinetics 1.

      Time step: 86400 seconds  (Incremented time: 172800 seconds)

      Rate name       Delta Moles Total Moles   Reactant        Coefficient

      Fe_di_ox         -2.479e-06   1.000e+00   Fe_di                   -1
                                                Fe_tri                   1

-------------------------------Phase assemblage-------------------------------

                                                          Moles in assemblage
Phase               SI  log IAP  log K(T, P)   Initial       Final       Delta

O2(g)            -0.67    -3.56     -2.89    1.000e+01   1.000e+01  -6.200e-07

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

      Elements           Molality       Moles

      Cl                1.020e-02   1.020e-02
      Fe_di             8.781e-05   8.781e-05
      Fe_tri            1.219e-05   1.219e-05
      Na                1.000e-02   1.000e-02

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

                                    pH  =   4.976      Charge balance
                                    pe  =  15.653      Adjusted to redox equilibrium
      Specific Conductance (µS/cm,  25°C)  = 1196
                         Density (g/cm³)  =   0.99747
                              Volume (L)  =   1.00314
                     Activity of water  =   1.000
                Ionic strength (mol/kgw)  =   1.029e-02
                     Mass of water (kg)  =   1.000e+00
                Total alkalinity (eq/kg)  =   1.242e-05
                       Temperature (°C)  =  25.00
                 Electrical balance (eq)  =   6.873e-15
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                               Iterations  =  23
                                  Total H  = 1.110124e+02
                                  Total O  = 5.550677e+01
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.158e-05	1.057e-05	-4.936	-4.976	-0.040	0.00
OH-	1.065e-09	9.574e-10	-8.973	-9.019	-0.046	-4.03
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.07
Cl	1.020e-02					
Cl-	1.020e-02	9.175e-03	-1.991	-2.037	-0.046	18.14
Fe_diCl+	8.053e-07	7.253e-07	-6.094	-6.139	-0.045	(0)
Fe_triCl+2	2.291e-10	1.508e-10	-9.640	-9.822	-0.182	(0)
Fe_triCl2+	6.860e-12	6.180e-12	-11.164	-11.209	-0.045	(0)
Fe_triCl3	5.656e-15	5.669e-15	-14.247	-14.246	0.001	(0)
Fe_di	8.781e-05					
Fe_di+2	8.700e-05	5.727e-05	-4.060	-4.242	-0.182	(0)
Fe_diCl+	8.053e-07	7.253e-07	-6.094	-6.139	-0.045	(0)
Fe_diOH+	1.902e-09	1.713e-09	-8.721	-8.766	-0.045	(0)
Fe_tri	1.219e-05					
Fe_tri(OH)2+	1.156e-05	1.041e-05	-4.937	-4.982	-0.045	(0)
Fe_triOH+2	5.049e-07	3.324e-07	-6.297	-6.478	-0.182	(0)
Fe_tri(OH)3	1.266e-07	1.269e-07	-6.898	-6.897	0.001	(0)
Fe_tri+3	1.394e-09	5.442e-10	-8.856	-9.264	-0.409	(0)
Fe_triCl+2	2.291e-10	1.508e-10	-9.640	-9.822	-0.182	(0)
Fe_tri2(OH)2+4	1.583e-11	2.974e-12	-10.800	-11.527	-0.726	(0)
Fe_tri(OH)4-	1.215e-11	1.095e-11	-10.915	-10.961	-0.045	(0)
Fe_triCl2+	6.860e-12	6.180e-12	-11.164	-11.209	-0.045	(0)
Fe_tri3(OH)4+5	8.822e-14	6.469e-15	-13.054	-14.189	-1.135	(0)
Fe_triCl3	5.656e-15	5.669e-15	-14.247	-14.246	0.001	(0)
H(0)	0.000e+00					
H2	0.000e+00	0.000e+00	-44.410	-44.409	0.001	28.61
Na	1.000e-02					
Na+	1.000e-02	9.022e-03	-2.000	-2.045	-0.045	-1.38
NaOH	8.618e-22	8.638e-22	-21.065	-21.064	0.001	(0)
O(0)	5.465e-04					
O2	2.732e-04	2.739e-04	-3.563	-3.562	0.001	30.40

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

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Goethite	6.66	5.66	-1.00	Fe_triOOH
H2(g)	-41.31	-44.41	-3.10	H2
H2O(g)	-1.50	-0.00	1.50	H2O
Halite	-5.65	-4.08	1.57	NaCl
O2(g)	-0.67	-3.56	-2.89	O2 Pressure 0.2 atm, phi 1.000

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

Reaction step 8.

Using solution 1.
Using pure phase assemblage 1.
Using kinetics 1.

Kinetics 1.

Time step: 172800 seconds (Incremented time: 345600 seconds)

Rate name	Delta Moles	Total Moles	Reactant	Coefficient
Fe_di_ox	-3.110e-06	1.000e+00	Fe_di	-1
			Fe_tri	1

----------Phase assemblage----------

Moles in assemblage

Phase	SI	log IAP	log K(T, P)	Initial	Final	Delta
O2(g)	-0.67	-3.56	-2.89	1.000e+01	1.000e+01	-7.777e-07

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

Elements	Molality	Moles
Cl	1.020e-02	1.020e-02
Fe_di	8.470e-05	8.470e-05
Fe_tri	1.530e-05	1.530e-05
Na	1.000e-02	1.000e-02

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

pH	= 4.881	Charge balance
pe	= 15.748	Adjusted to redox equilibrium
Specific Conductance (µS/cm, 25°C)	= 1197	
Density (g/cm³)	= 0.99747	
Volume (L)	= 1.00314	
Activity of water	= 1.000	
Ionic strength (mol/kgw)	= 1.028e-02	
Mass of water (kg)	= 1.000e+00	
Total alkalinity (eq/kg)	= 1.553e-05	
Temperature (°C)	= 25.00	
Electrical balance (eq)	= 6.871e-15	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 0.00	
Iterations	= 23	
Total H	= 1.110124e+02	
Total O	= 5.550677e+01	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.441e-05	1.315e-05	-4.841	-4.881	-0.040	0.00
OH-	8.561e-10	7.695e-10	-9.067	-9.114	-0.046	-4.03
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.07
Cl	1.020e-02					
Cl-	1.020e-02	9.175e-03	-1.991	-2.037	-0.046	18.14
Fe_diCl+	7.768e-07	6.997e-07	-6.110	-6.155	-0.045	(0)
Fe_triCl+2	4.415e-10	2.907e-10	-9.355	-9.537	-0.182	(0)
Fe_triCl2+	1.322e-11	1.191e-11	-10.879	-10.924	-0.045	(0)
Fe_triCl3	1.090e-14	1.093e-14	-13.962	-13.961	0.001	(0)
Fe_di	8.470e-05					
Fe_di+2	8.392e-05	5.525e-05	-4.076	-4.258	-0.182	(0)
Fe_diCl+	7.768e-07	6.997e-07	-6.110	-6.155	-0.045	(0)
Fe_diOH+	1.475e-09	1.328e-09	-8.831	-8.877	-0.045	(0)
Fe_tri	1.530e-05					
Fe_tri(OH)2+	1.439e-05	1.296e-05	-4.842	-4.887	-0.045	(0)
Fe_triOH+2	7.821e-07	5.149e-07	-6.107	-6.288	-0.182	(0)
Fe_tri(OH)3	1.266e-07	1.269e-07	-6.897	-6.896	0.001	(0)
Fe_tri+3	2.687e-09	1.049e-09	-8.571	-8.979	-0.408	(0)
Fe_triCl+2	4.415e-10	2.907e-10	-9.355	-9.537	-0.182	(0)
Fe_tri2(OH)2+4	3.799e-11	7.136e-12	-10.420	-11.147	-0.726	(0)
Fe_triCl2+	1.322e-11	1.191e-11	-10.879	-10.924	-0.045	(0)
Fe_tri(OH)4-	9.771e-12	8.802e-12	-11.010	-11.055	-0.045	(0)
Fe_tri3(OH)4+5	2.635e-13	1.933e-14	-12.579	-13.714	-1.135	(0)
Fe_triCl3	1.090e-14	1.093e-14	-13.962	-13.961	0.001	(0)
H(0)	0.000e+00					
H2	0.000e+00	0.000e+00	-44.410	-44.409	0.001	28.61
Na	1.000e-02					
Na+	1.000e-02	9.022e-03	-2.000	-2.045	-0.045	-1.38
NaOH	6.926e-22	6.942e-22	-21.160	-21.158	0.001	(0)
O(0)	5.465e-04					
O2	2.732e-04	2.739e-04	-3.563	-3.562	0.001	30.40

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

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Goethite	6.66	5.66	-1.00	Fe_triOOH
H2(g)	-41.31	-44.41	-3.10	H2
H2O(g)	-1.50	-0.00	1.50	H2O
Halite	-5.65	-4.08	1.57	NaCl
O2(g)	-0.67	-3.56	-2.89	O2 Pressure 0.2 atm, phi 1.000

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

Reaction step 9.

Using solution 1.
Using pure phase assemblage 1.
Using kinetics 1.

Kinetics 1.

Time step: 172800 seconds (Incremented time: 518400 seconds)

Rate name	Delta Moles	Total Moles	Reactant	Coefficient
Fe_di_ox	-2.172e-06	1.000e+00	Fe_di	-1
			Fe_tri	1

-------------------------------Phase assemblage-------------------------------

Phase	SI	log IAP	log K(T, P)	Moles in assemblage: Initial	Final	Delta
O2(g)	-0.67	-3.56	-2.89	1.000e+01	1.000e+01	-5.431e-07

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

Elements	Molality	Moles
Cl	1.020e-02	1.020e-02
Fe_di	8.253e-05	8.253e-05
Fe_tri	1.747e-05	1.747e-05
Na	1.000e-02	1.000e-02

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

pH	= 4.826	Charge balance
pe	= 15.803	Adjusted to redox equilibrium
Specific Conductance (µS/cm, 25°C)	= 1197	
Density (g/cm³)	= 0.99747	
Volume (L)	= 1.00314	
Activity of water	= 1.000	
Ionic strength (mol/kgw)	= 1.028e-02	
Mass of water (kg)	= 1.000e+00	
Total alkalinity (eq/kg)	= 1.771e-05	
Temperature (°C)	= 25.00	
Electrical balance (eq)	= 5.313e-14	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 0.00	
Iterations	= 20	
Total H	= 1.110124e+02	
Total O	= 5.550677e+01	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.635e-05	1.492e-05	-4.786	-4.826	-0.040	0.00

```
   OH-              7.543e-10   6.780e-10    -9.122    -9.169    -0.046     -4.03
   H2O              5.551e+01   9.996e-01     1.744    -0.000     0.000     18.07
Cl              1.020e-02
   Cl-              1.020e-02   9.175e-03    -1.991    -2.037    -0.046     18.14
   Fe_diCl+         7.569e-07   6.818e-07    -6.121    -6.166    -0.045     (0)
   Fe_triCl+2       6.454e-10   4.249e-10    -9.190    -9.372    -0.182     (0)
   Fe_triCl2+       1.933e-11   1.742e-11   -10.714   -10.759    -0.045     (0)
   Fe_triCl3        1.594e-14   1.598e-14   -13.798   -13.796     0.001     (0)
Fe_di           8.253e-05
   Fe_di+2          8.177e-05   5.383e-05    -4.087    -4.269    -0.182     (0)
   Fe_diCl+         7.569e-07   6.818e-07    -6.121    -6.166    -0.045     (0)
   Fe_diOH+         1.266e-09   1.140e-09    -8.898    -8.943    -0.045     (0)
Fe_tri          1.747e-05
   Fe_tri(OH)2+     1.633e-05   1.471e-05    -4.787    -4.832    -0.045     (0)
   Fe_triOH+2       1.008e-06   6.633e-07    -5.997    -6.178    -0.182     (0)
   Fe_tri(OH)3      1.267e-07   1.270e-07    -6.897    -6.896     0.001     (0)
   Fe_tri+3         3.928e-09   1.534e-09    -8.406    -8.814    -0.408     (0)
   Fe_triCl+2       6.454e-10   4.249e-10    -9.190    -9.372    -0.182     (0)
   Fe_tri2(OH)2+4   6.303e-11   1.184e-11   -10.200   -10.927    -0.726     (0)
   Fe_triCl2+       1.933e-11   1.742e-11   -10.714   -10.759    -0.045     (0)
   Fe_tri(OH)4-     8.612e-12   7.758e-12   -11.065   -11.110    -0.045     (0)
   Fe_tri3(OH)4+5   4.963e-13   3.641e-14   -12.304   -13.439    -1.135     (0)
   Fe_triCl3        1.594e-14   1.598e-14   -13.798   -13.796     0.001     (0)
H(0)            0.000e+00
   H2               0.000e+00   0.000e+00   -44.410   -44.409     0.001     28.61
Na              1.000e-02
   Na+              1.000e-02   9.022e-03    -2.000    -2.045    -0.045     -1.38
   NaOH             6.103e-22   6.117e-22   -21.214   -21.213     0.001     (0)
O(0)            5.465e-04
   O2               2.732e-04   2.739e-04    -3.563    -3.562     0.001     30.40

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

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

  Goethite           6.66      5.66   -1.00  Fe_triOOH
  H2(g)            -41.31    -44.41   -3.10  H2
  H2O(g)            -1.50     -0.00    1.50  H2O
  Halite            -5.65     -4.08    1.57  NaCl
  O2(g)             -0.67     -3.56   -2.89  O2   Pressure   0.2 atm, phi 1.000

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

Reaction step 10.

Using solution 1.
Using pure phase assemblage 1.
Using kinetics 1.

Kinetics 1.

      Time step: 172800 seconds  (Incremented time: 691200 seconds)

      Rate name       Delta Moles Total Moles   Reactant        Coefficient

      Fe_di_ox         -1.723e-06   1.000e+00   Fe_di                    -1
                                                Fe_tri                    1

--------------------------------Phase assemblage--------------------------------

                                                          Moles in assemblage
Phase               SI  log IAP  log K(T, P)   Initial       Final       Delta

O2(g)            -0.67    -3.56     -2.89    1.000e+01   1.000e+01  -4.308e-07

------------------------------Solution composition------------------------------
```

Elements	Molality	Moles
Cl	1.020e-02	1.020e-02
Fe_di	8.080e-05	8.080e-05
Fe_tri	1.920e-05	1.920e-05
Na	1.000e-02	1.000e-02

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

pH	= 4.787	Charge balance
pe	= 15.842	Adjusted to redox equilibrium
Specific Conductance (µS/cm, 25°C)	= 1198	
Density (g/cm³)	= 0.99747	
Volume (L)	= 1.00314	
Activity of water	= 1.000	
Ionic strength (mol/kgw)	= 1.028e-02	
Mass of water (kg)	= 1.000e+00	
Total alkalinity (eq/kg)	= 1.943e-05	
Temperature (°C)	= 25.00	
Electrical balance (eq)	= 5.622e-14	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 0.00	
Iterations	= 20	
Total H	= 1.110124e+02	
Total O	= 5.550677e+01	

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.788e-05	1.631e-05	-4.748	-4.787	-0.040	0.00
OH-	6.901e-10	6.203e-10	-9.161	-9.207	-0.046	-4.03
H2O	5.551e+01	9.996e-01	1.744	-0.000	0.000	18.07
Cl	1.020e-02					
Cl-	1.020e-02	9.175e-03	-1.991	-2.037	-0.046	18.14
Fe_diCl+	7.411e-07	6.676e-07	-6.130	-6.175	-0.045	(0)
Fe_triCl+2	8.433e-10	5.552e-10	-9.074	-9.256	-0.182	(0)
Fe_triCl2+	2.526e-11	2.275e-11	-10.598	-10.643	-0.045	(0)
Fe_triCl3	2.083e-14	2.088e-14	-13.681	-13.680	0.001	(0)
Fe_di	8.080e-05					
Fe_di+2	8.006e-05	5.271e-05	-4.097	-4.278	-0.182	(0)
Fe_diCl+	7.411e-07	6.676e-07	-6.130	-6.175	-0.045	(0)
Fe_diOH+	1.134e-09	1.021e-09	-8.945	-8.991	-0.045	(0)
Fe_tri	1.920e-05					
Fe_tri(OH)2+	1.786e-05	1.609e-05	-4.748	-4.794	-0.045	(0)
Fe_triOH+2	1.204e-06	7.928e-07	-5.919	-6.101	-0.182	(0)
Fe_tri(OH)3	1.267e-07	1.270e-07	-6.897	-6.896	0.001	(0)
Fe_tri+3	5.132e-09	2.004e-09	-8.290	-8.698	-0.408	(0)
Fe_triCl+2	8.433e-10	5.552e-10	-9.074	-9.256	-0.182	(0)
Fe_tri2(OH)2+4	9.004e-11	1.692e-11	-10.046	-10.772	-0.726	(0)
Fe_triCl2+	2.526e-11	2.275e-11	-10.598	-10.643	-0.045	(0)
Fe_tri(OH)4-	7.880e-12	7.098e-12	-11.103	-11.149	-0.045	(0)
Fe_tri3(OH)4+5	7.750e-13	5.687e-14	-12.111	-13.245	-1.134	(0)
Fe_triCl3	2.083e-14	2.088e-14	-13.681	-13.680	0.001	(0)
H(0)	0.000e+00					
H2	0.000e+00	0.000e+00	-44.410	-44.409	0.001	28.61
Na	1.000e-02					
Na+	1.000e-02	9.022e-03	-2.000	-2.045	-0.045	-1.38
NaOH	5.583e-22	5.596e-22	-21.253	-21.252	0.001	(0)
O(0)	5.465e-04					
O2	2.732e-04	2.739e-04	-3.563	-3.562	0.001	30.40

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

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Goethite	6.66	5.66	-1.00	Fe_triOOH
H2(g)	-41.31	-44.41	-3.10	H2

```
  H2O(g)           -1.50     -0.00    1.50  H2O
  Halite           -5.65     -4.08    1.57  NaCl
  O2(g)            -0.67     -3.56   -2.89  O2   Pressure   0.2 atm, phi 1.000

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

Reaction step 11.

Using solution 1.
Using pure phase assemblage 1.
Using kinetics 1.

Kinetics 1.

      Time step: 172800 seconds  (Incremented time: 864000 seconds)

      Rate name       Delta Moles Total Moles   Reactant        Coefficient

      Fe_di_ox         -1.451e-06   1.000e+00   Fe_di                   -1
                                                Fe_tri                   1

-------------------------------Phase assemblage--------------------------------

                                                          Moles in assemblage
Phase               SI  log IAP  log K(T, P)   Initial       Final       Delta

O2(g)            -0.67    -3.56     -2.89    1.000e+01   1.000e+01  -3.627e-07

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

      Elements           Molality       Moles

      Cl                1.020e-02   1.020e-02
      Fe_di             7.935e-05   7.935e-05
      Fe_tri            2.065e-05   2.065e-05
      Na                1.000e-02   1.000e-02

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

                                       pH  =   4.758      Charge balance
                                       pe  =  15.872      Adjusted to redox equilibrium
      Specific Conductance (µS/cm,  25°C)  = 1198
                           Density (g/cm³)  =   0.99747
                                Volume (L)  =   1.00314
                        Activity of water  =   1.000
                  Ionic strength (mol/kgw)  =   1.028e-02
                       Mass of water (kg)  =   1.000e+00
                  Total alkalinity (eq/kg)  =   2.088e-05
                          Temperature (°C)  =  25.00
                   Electrical balance (eq)  =   5.666e-14
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                                Iterations  =  20
                                   Total H  = 1.110124e+02
                                   Total O  = 5.550677e+01

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

                                                 Log       Log       Log    mole V
   Species          Molality    Activity  Molality  Activity     Gamma    cm³/mol

   H+              1.915e-05   1.747e-05    -4.718    -4.758    -0.040      0.00
   OH-             6.443e-10   5.791e-10    -9.191    -9.237    -0.046     -4.03
   H2O             5.551e+01   9.996e-01     1.744    -0.000     0.000     18.07
Cl            1.020e-02
   Cl-             1.020e-02   9.175e-03    -1.991    -2.037    -0.046     18.14
   Fe_diCl+        7.278e-07   6.556e-07    -6.138    -6.183    -0.045     (0)
   Fe_triCl+2      1.036e-09   6.823e-10    -8.985    -9.166    -0.182     (0)
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   Fe_triCl2+      3.104e-11   2.796e-11   -10.508   -10.553    -0.045     (0)
   Fe_triCl3       2.559e-14   2.565e-14   -13.592   -13.591     0.001     (0)
Fe_di         7.935e-05
   Fe_di+2         7.862e-05   5.177e-05    -4.104    -4.286    -0.182     (0)
   Fe_diCl+        7.278e-07   6.556e-07    -6.138    -6.183    -0.045     (0)
   Fe_diOH+        1.040e-09   9.366e-10    -8.983    -9.028    -0.045     (0)
Fe_tri        2.065e-05
   Fe_tri(OH)2+    1.913e-05   1.723e-05    -4.718    -4.764    -0.045     (0)
   Fe_triOH+2      1.382e-06   9.096e-07    -5.860    -6.041    -0.182     (0)
   Fe_tri(OH)3     1.267e-07   1.270e-07    -6.897    -6.896     0.001     (0)
   Fe_tri+3        6.306e-09   2.462e-09    -8.200    -8.609    -0.408     (0)
   Fe_triCl+2      1.036e-09   6.823e-10    -8.985    -9.166    -0.182     (0)
   Fe_tri2(OH)2+4   1.185e-10   2.227e-11    -9.926   -10.652    -0.726     (0)
   Fe_triCl2+      3.104e-11   2.796e-11   -10.508   -10.553    -0.045     (0)
   Fe_tri(OH)4-    7.358e-12   6.628e-12   -11.133   -11.179    -0.045     (0)
   Fe_tri3(OH)4+5   1.093e-12   8.019e-14   -11.961   -13.096    -1.134     (0)
   Fe_triCl3       2.559e-14   2.565e-14   -13.592   -13.591     0.001     (0)
H(0)          0.000e+00
   H2              0.000e+00   0.000e+00   -44.410   -44.409     0.001     28.61
Na            1.000e-02
   Na+             1.000e-02   9.022e-03    -2.000    -2.045    -0.045     -1.38
   NaOH            5.213e-22   5.225e-22   -21.283   -21.282     0.001     (0)
O(0)          5.465e-04
   O2              2.732e-04   2.739e-04    -3.563    -3.562     0.001     30.40

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

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

  Goethite           6.66      5.66   -1.00  Fe_triOOH
  H2(g)           -41.31    -44.41   -3.10  H2
  H2O(g)           -1.50     -0.00    1.50  H2O
  Halite           -5.65     -4.08    1.57  NaCl
  O2(g)            -0.67     -3.56   -2.89  O2   Pressure   0.2 atm, phi 1.000

**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 3.
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End of Run after 0.462 Seconds.
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