```
   Input file: F:\Doutoramento\artigos originais\Furnas springs - modelling\Phreeqc
\Especiação\Speciation1_L.pqi
  Output file: F:\Doutoramento\artigos originais\Furnas springs - modelling\Phreeqc
\Especiação\Speciation1_L.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
      Solution 1 # Ref  LF1   Caldeira da Lagoa
      temp  89.4
      pH    4.1
      pe    2.922
      redox pe
      units mg/l
      Alkalinity 25 as Ca.5CO3.5
      Cl    34.4
      S(6)  70.7
      Na    105.2
      Mg    3.1
      K     22.7
      Ca    14.2
      Si    191.44 as SiO2
      Al    1.0256
      END
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

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

      Elements           Molality       Moles

      Al                 3.803e-05   3.803e-05
      Alkalinity         2.841e-04   2.841e-04
      Ca                 3.545e-04   3.545e-04
      Cl                 9.708e-04   9.708e-04
      K                  5.808e-04   5.808e-04
      Mg                 1.276e-04   1.276e-04
      Na                 4.578e-03   4.578e-03
      S(6)               7.363e-04   7.363e-04
      Si                 3.188e-03   3.188e-03

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

                                     pH  =   4.100
                                     pe  =   2.922
      Specific Conductance (µS/cm,  89°C)  = 1271
                          Density (g/cm³)  =   0.96649
```

Volume (L)	1.03787
Activity of water	0.999
Ionic strength (mol/kgw)	5.444e-03
Mass of water (kg)	1.000e+00
Total carbon (mol/kg)	5.744e-02
Total CO2 (mol/kg)	5.744e-02
Temperature (°C)	89.40
Electrical balance (eq)	3.510e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|)	40.16
Iterations	9
Total H	1.110257e+02
Total O	5.563719e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	8.613e-05	7.943e-05	-4.065	-4.100	-0.035	0.00
OH-	5.294e-09	4.832e-09	-8.276	-8.316	-0.040	-5.09
H2O	5.551e+01	9.988e-01	1.744	-0.001	0.000	18.66
Al	3.803e-05					
Al(OH)2+	2.514e-05	2.304e-05	-4.600	-4.638	-0.038	(0)
AlOH+2	6.864e-06	4.839e-06	-5.163	-5.315	-0.152	-30.78
AlSO4+	2.942e-06	2.691e-06	-5.531	-5.570	-0.039	(0)
Al+3	1.981e-06	9.557e-07	-5.703	-6.020	-0.317	-47.55
Al(OH)3	9.092e-07	9.103e-07	-6.041	-6.041	0.001	(0)
Al(OH)4-	1.392e-07	1.273e-07	-6.856	-6.895	-0.039	(0)
Al(SO4)2-	5.333e-08	4.878e-08	-7.273	-7.312	-0.039	(0)
AlHSO4+2	7.365e-11	5.134e-11	-10.133	-10.290	-0.157	(0)
C(4)	5.744e-02					
CO2	5.660e-02	5.667e-02	-1.247	-1.247	0.001	38.06
HCO3-	3.276e-04	3.002e-04	-3.485	-3.523	-0.038	25.28
(CO2)2	2.578e-04	2.581e-04	-3.589	-3.588	0.001	76.12
CaHCO3+	1.522e-06	1.396e-06	-5.818	-5.855	-0.037	10.62
NaHCO3	5.215e-07	5.222e-07	-6.283	-6.282	0.001	1.80
MgHCO3+	4.932e-07	4.506e-07	-6.307	-6.346	-0.039	5.72
CaCO3	7.063e-10	7.071e-10	-9.151	-9.150	0.001	-14.46
CO3-2	3.937e-10	2.775e-10	-9.405	-9.557	-0.152	-10.93
NaCO3-	3.413e-10	3.119e-10	-9.467	-9.506	-0.039	-1.66
MgCO3	4.953e-11	4.959e-11	-10.305	-10.305	0.001	-17.08
Ca	3.545e-04					
Ca+2	3.257e-04	2.294e-04	-3.487	-3.639	-0.152	-19.04
CaSO4	2.716e-05	2.720e-05	-4.566	-4.565	0.001	8.76
CaHCO3+	1.522e-06	1.396e-06	-5.818	-5.855	-0.037	10.62
CaHSO4+	5.621e-08	5.136e-08	-7.250	-7.289	-0.039	(0)
CaCO3	7.063e-10	7.071e-10	-9.151	-9.150	0.001	-14.46
CaOH+	5.238e-13	4.786e-13	-12.281	-12.320	-0.039	(0)
Cl	9.708e-04					
Cl-	9.708e-04	8.865e-04	-3.013	-3.052	-0.039	16.93
H(0)	7.542e-18					
H2	3.771e-18	3.776e-18	-17.424	-17.423	0.001	28.57
K	5.808e-04					
K+	5.762e-04	5.261e-04	-3.239	-3.279	-0.040	10.05
KSO4-	4.556e-06	4.175e-06	-5.341	-5.379	-0.038	33.65
Mg	1.276e-04					
Mg+2	9.848e-05	6.965e-05	-4.007	-4.157	-0.150	-24.41
MgSO4	2.859e-05	2.863e-05	-4.544	-4.543	0.001	7.10
MgHCO3+	4.932e-07	4.506e-07	-6.307	-6.346	-0.039	5.72
MgOH+	4.135e-10	3.796e-10	-9.384	-9.421	-0.037	(0)
MgCO3	4.953e-11	4.959e-11	-10.305	-10.305	0.001	-17.08
Na	4.578e-03					
Na+	4.563e-03	4.175e-03	-2.341	-2.379	-0.039	0.26
NaSO4-	1.432e-05	1.312e-05	-4.844	-4.882	-0.038	8.01
NaHCO3	5.215e-07	5.222e-07	-6.283	-6.282	0.001	1.80
NaCO3-	3.413e-10	3.119e-10	-9.467	-9.506	-0.039	-1.66
NaOH	2.015e-21	2.017e-21	-20.696	-20.695	0.001	(0)
O(0)	0.000e+00					

```
   O2              0.000e+00   0.000e+00   -40.444   -40.443     0.001     33.52
S(6)          7.363e-04
   SO4-2           6.382e-04   4.482e-04    -3.195    -3.348    -0.153     14.36
   MgSO4           2.859e-05   2.863e-05    -4.544    -4.543     0.001      7.10
   CaSO4           2.716e-05   2.720e-05    -4.566    -4.565     0.001      8.76
   HSO4-           2.038e-05   1.863e-05    -4.691    -4.730    -0.039     41.14
   NaSO4-          1.432e-05   1.312e-05    -4.844    -4.882    -0.038      8.01
   KSO4-           4.556e-06   4.175e-06    -5.341    -5.379    -0.038     33.65
   AlSO4+          2.942e-06   2.691e-06    -5.531    -5.570    -0.039     (0)
   CaHSO4+         5.621e-08   5.136e-08    -7.250    -7.289    -0.039     (0)
   Al(SO4)2-       5.333e-08   4.878e-08    -7.273    -7.312    -0.039     (0)
   AlHSO4+2        7.365e-11   5.134e-11   -10.133   -10.290    -0.157     (0)
Si            3.188e-03
   H4SiO4          3.188e-03   3.192e-03    -2.497    -2.496     0.001     49.10
   H3SiO4-         2.999e-08   2.741e-08    -7.523    -7.562    -0.039     27.01
   H2SiO4-2        5.874e-16   4.141e-16   -15.231   -15.383    -0.152     (0)

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

  Phase               SI** log IAP   log K(362 K,   1 atm)

  Al(OH)3(a)       -1.07      6.28     7.35  Al(OH)3
  Albite           -2.13    -16.76   -14.63  NaAlSi3O8
  Alunite           4.50     -3.44    -7.94  KAl3(SO4)2(OH)6
  Anhydrite        -1.88     -6.99    -5.11  CaSO4
  Anorthite        -4.21    -22.42   -18.21  CaAl2Si2O8
  Aragonite        -4.19    -13.20    -9.01  CaCO3
  Ca-Montmorillonite   3.41    -34.02  -37.43  Ca0.165Al2.33Si3.67O10(OH)2
  Calcite          -3.80    -13.20    -9.39  CaCO3
  Chalcedony        0.44     -2.49    -2.94  SiO2
  Chlorite(14A)   -23.37     25.28    48.66  Mg5Al2Si3O10(OH)8
  Chrysotile      -18.45      7.14    25.59  Mg3Si2O5(OH)4
  CO2(g)            0.69     -1.25    -1.94  CO2
  Dolomite         -7.88    -26.91   -19.03  CaMg(CO3)2
  Gibbsite          1.14      6.28     5.14  Al(OH)3
  Gypsum           -2.20     -6.99    -4.79  CaSO4:2H2O
  H2(g)           -14.31    -17.42    -3.12  H2
  H2O(g)           -0.17     -0.00     0.17  H2O
  Halite           -7.04     -5.43     1.61  NaCl
  Illite            0.63    -32.52   -33.15  K0.6Mg0.25Al2.3Si3.5O10(OH)2
  K-feldspar       -1.10    -17.66   -16.56  KAlSi3O8
  K-mica            7.20     12.17     4.97  KAl3Si3O10(OH)2
  Kaolinite         4.73      7.57     2.84  Al2Si2O5(OH)4
  O2(g)           -37.33    -40.44    -3.11  O2
  Quartz            0.71     -2.49    -3.20  SiO2
  Sepiolite       -13.77      0.60    14.37  Mg2Si3O7.5OH:3H2O
  Sepiolite(d)    -18.06      0.60    18.66  Mg2Si3O7.5OH:3H2O
  SiO2(a)          -0.22     -2.49    -2.28  SiO2
  Sylvite          -7.50     -6.33     1.16  KCl
  Talc            -13.22      2.15    15.36  Mg3Si4O10(OH)2

**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 0.222 Seconds.
--------------------------------
```

```
   Input file: F:\Doutoramento\artigos originais\Furnas springs - modelling\Phreeqc
\Especiação\Speciation2_L.pqi
  Output file: F:\Doutoramento\artigos originais\Furnas springs - modelling\Phreeqc
\Especiação\Speciation2_L.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
      Solution 2        # LF2 Nascente Ponte
      temp        21
      pH          5.5
      pe          4
      redox       pe
      units mg/l
      Alkalinity  200.9 as Ca.5CO3.5
      Cl          22.9
      S(6)        14.7
      Na          55.8
      Mg          3.4
      K           28.5
      Ca          10.5
      END
----------------------------------------
Beginning of initial solution calculations.
----------------------------------------

Initial solution 2.

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

      Elements           Molality       Moles

      Alkalinity        2.282e-03   2.282e-03
      Ca                2.621e-04   2.621e-04
      Cl                6.461e-04   6.461e-04
      K                 7.291e-04   7.291e-04
      Mg                1.399e-04   1.399e-04
      Na                2.428e-03   2.428e-03
      S(6)              1.531e-04   1.531e-04

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

                                       pH  =   5.500
                                       pe  =   4.000
      Specific Conductance (µS/cm,  21°C)  = 339
                           Density (g/cm³)  =   0.99836
                                Volume (L)  =   1.00262
                        Activity of water  =   1.000
                  Ionic strength (mol/kgw)  =   4.109e-03
                       Mass of water (kg)  =   1.000e+00
```

```
                  Total carbon (mol/kg)  =   1.825e-02
                     Total CO2 (mol/kg)  =   1.825e-02
                       Temperature (°C)  =  21.00
                Electrical balance (eq)  =   7.263e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  10.15
                               Iterations  =  11
                                  Total H  = 1.110147e+02
                                  Total O  = 5.554561e+01
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	3.368e-06	3.162e-06	-5.473	-5.500	-0.027	0.00
OH-	2.513e-09	2.344e-09	-8.600	-8.630	-0.030	-4.25
H2O	5.551e+01	9.996e-01	1.744	-0.000	0.000	18.05
C(4)	1.825e-02					
CO2	1.596e-02	1.597e-02	-1.797	-1.797	0.000	34.24
HCO3-	2.275e-03	2.127e-03	-2.643	-2.672	-0.029	24.40
CaHCO3+	5.248e-06	4.911e-06	-5.280	-5.309	-0.029	9.54
(CO2)2	4.086e-06	4.090e-06	-5.389	-5.388	0.000	68.47
NaHCO3	2.769e-06	2.772e-06	-5.558	-5.557	0.000	1.80
MgHCO3+	2.710e-06	2.529e-06	-5.567	-5.597	-0.030	5.38
CO3-2	3.791e-08	2.898e-08	-7.421	-7.538	-0.117	-5.51
CaCO3	8.731e-09	8.740e-09	-8.059	-8.059	0.000	-14.61
MgCO3	2.683e-09	2.685e-09	-8.571	-8.571	0.000	-17.08
NaCO3-	1.067e-09	9.959e-10	-8.972	-9.002	-0.030	-1.38
Ca	2.621e-04					
Ca+2	2.531e-04	1.934e-04	-3.597	-3.714	-0.117	-18.09
CaHCO3+	5.248e-06	4.911e-06	-5.280	-5.309	-0.029	9.54
CaSO4	3.688e-06	3.692e-06	-5.433	-5.433	0.000	7.34
CaCO3	8.731e-09	8.740e-09	-8.059	-8.059	0.000	-14.61
CaHSO4+	7.777e-11	7.260e-11	-10.109	-10.139	-0.030	(0)
CaOH+	1.087e-11	1.015e-11	-10.964	-10.994	-0.030	(0)
Cl	6.461e-04					
Cl-	6.461e-04	6.029e-04	-3.190	-3.220	-0.030	17.97
H(0)	1.473e-22					
H2	7.364e-23	7.371e-23	-22.133	-22.132	0.000	28.61
K	7.291e-04					
K+	7.286e-04	6.797e-04	-3.138	-3.168	-0.030	8.90
KSO4-	5.266e-07	4.924e-07	-6.279	-6.308	-0.029	34.02
Mg	1.399e-04					
Mg+2	1.348e-04	1.033e-04	-3.870	-3.986	-0.116	-21.57
MgHCO3+	2.710e-06	2.529e-06	-5.567	-5.597	-0.030	5.38
MgSO4	2.411e-06	2.413e-06	-5.618	-5.617	0.000	5.68
MgCO3	2.683e-09	2.685e-09	-8.571	-8.571	0.000	-17.08
MgOH+	8.778e-11	8.219e-11	-10.057	-10.085	-0.029	(0)
Na	2.428e-03					
Na+	2.424e-03	2.264e-03	-2.615	-2.645	-0.030	-1.65
NaHCO3	2.769e-06	2.772e-06	-5.558	-5.557	0.000	1.80
NaSO4-	1.309e-06	1.224e-06	-5.883	-5.912	-0.029	14.12
NaCO3-	1.067e-09	9.959e-10	-8.972	-9.002	-0.030	-1.38
NaOH	5.302e-22	5.307e-22	-21.276	-21.275	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-49.424	-49.424	0.000	30.07
S(6)	1.531e-04					
SO4-2	1.451e-04	1.107e-04	-3.838	-3.956	-0.118	14.07
CaSO4	3.688e-06	3.692e-06	-5.433	-5.433	0.000	7.34
MgSO4	2.411e-06	2.413e-06	-5.618	-5.617	0.000	5.68
NaSO4-	1.309e-06	1.224e-06	-5.883	-5.912	-0.029	14.12
KSO4-	5.266e-07	4.924e-07	-6.279	-6.308	-0.029	34.02
HSO4-	3.345e-08	3.122e-08	-7.476	-7.506	-0.030	40.02
CaHSO4+	7.777e-11	7.260e-11	-10.109	-10.139	-0.030	(0)

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

Phase	SI**	log IAP	log K(294 K, 1 atm)

```
  Anhydrite        -3.44     -7.67   -4.23  CaSO4
  Aragonite        -2.94    -11.25   -8.31  CaCO3
  Calcite          -2.80    -11.25   -8.45  CaCO3
  CO2(g)           -0.38     -1.80   -1.42  CO2
  Dolomite         -5.76    -22.78  -17.02  CaMg(CO3)2
  Gypsum           -3.09     -7.67   -4.58  CaSO4:2H2O
  H2(g)           -19.04    -22.13   -3.09  H2
  H2O(g)           -1.61     -0.00    1.61  H2O
  Halite           -7.43     -5.86    1.57  NaCl
  O2(g)           -46.56    -49.42   -2.86  O2
  Sylvite          -7.27     -6.39    0.88  KCl

**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.
-----------------------------------

      Solution 3  #LF3  Miguel Henriques
      temp        20.7
      pH          5.4
      pe          4
      redox       pe
      units mg/l
      Alkalinity  157.2 as Ca.5CO3.5
      Cl          22.1
      S(6)        10.3
      Na          57.1
      Mg          3.3
      K           29.2
      Ca          10.4
      END
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 3.

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

      Elements           Molality       Moles

      Alkalinity        1.786e-03   1.786e-03
      Ca                2.596e-04   2.596e-04
      Cl                6.235e-04   6.235e-04
      K                 7.470e-04   7.470e-04
      Mg                1.358e-04   1.358e-04
      Na                2.484e-03   2.484e-03
      S(6)              1.073e-04   1.073e-04

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

                                    pH  =   5.400
                                    pe  =   4.000
      Specific Conductance (µS/cm,  21°C)  = 315
                         Density (g/cm³)  =   0.99840
                              Volume (L)  =   1.00254
                     Activity of water    =   1.000
                Ionic strength (mol/kgw)  =   3.795e-03
                     Mass of water (kg)   =   1.000e+00
                Total carbon (mol/kg)     =   1.764e-02
                   Total CO2 (mol/kg)     =   1.764e-02
```

```
                    Temperature (°C)  =  20.70
                Electrical balance (eq)  =   1.398e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  21.13
                             Iterations  =  10
                                Total H  = 1.110142e+02
                                Total O  = 5.554371e+01
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	4.231e-06	3.981e-06	-5.374	-5.400	-0.026	0.00
OH-	1.944e-09	1.818e-09	-8.711	-8.740	-0.029	-4.26
H2O	5.551e+01	9.996e-01	1.744	-0.000	0.000	18.05
C(4)	1.764e-02					
CO2	1.584e-02	1.585e-02	-1.800	-1.800	0.000	34.22
HCO3-	1.782e-03	1.670e-03	-2.749	-2.777	-0.028	24.37
CaHCO3+	4.122e-06	3.867e-06	-5.385	-5.413	-0.028	9.52
(CO2)2	3.985e-06	3.988e-06	-5.400	-5.399	0.000	68.44
NaHCO3	2.235e-06	2.237e-06	-5.651	-5.650	0.000	1.80
MgHCO3+	2.096e-06	1.961e-06	-5.679	-5.708	-0.029	5.37
CO3-2	2.326e-08	1.795e-08	-7.633	-7.746	-0.113	-5.55
CaCO3	5.426e-09	5.431e-09	-8.266	-8.265	0.000	-14.61
MgCO3	1.636e-09	1.637e-09	-8.786	-8.786	0.000	-17.08
NaCO3-	6.659e-10	6.232e-10	-9.177	-9.205	-0.029	-1.42
Ca	2.596e-04					
Ca+2	2.528e-04	1.950e-04	-3.597	-3.710	-0.113	-18.10
CaHCO3+	4.122e-06	3.867e-06	-5.385	-5.413	-0.028	9.52
CaSO4	2.624e-06	2.626e-06	-5.581	-5.581	0.000	7.33
CaCO3	5.426e-09	5.431e-09	-8.266	-8.265	0.000	-14.61
CaHSO4+	6.919e-11	6.475e-11	-10.160	-10.189	-0.029	(0)
CaOH+	8.684e-12	8.127e-12	-11.061	-11.090	-0.029	(0)
Cl	6.235e-04					
Cl-	6.235e-04	5.833e-04	-3.205	-3.234	-0.029	17.96
H(0)	2.342e-22					
H2	1.171e-22	1.172e-22	-21.932	-21.931	0.000	28.61
K	7.470e-04					
K+	7.466e-04	6.983e-04	-3.127	-3.156	-0.029	8.89
KSO4-	3.795e-07	3.557e-07	-6.421	-6.449	-0.028	34.01
Mg	1.358e-04					
Mg+2	1.320e-04	1.021e-04	-3.879	-3.991	-0.112	-21.57
MgHCO3+	2.096e-06	1.961e-06	-5.679	-5.708	-0.029	5.37
MgSO4	1.672e-06	1.674e-06	-5.777	-5.776	0.000	5.66
MgCO3	1.636e-09	1.637e-09	-8.786	-8.786	0.000	-17.08
MgOH+	6.689e-11	6.277e-11	-10.175	-10.202	-0.028	(0)
Na	2.484e-03					
Na+	2.481e-03	2.324e-03	-2.605	-2.634	-0.029	-1.67
NaHCO3	2.235e-06	2.237e-06	-5.651	-5.650	0.000	1.80
NaSO4-	9.456e-07	8.863e-07	-6.024	-6.052	-0.028	14.10
NaCO3-	6.659e-10	6.232e-10	-9.177	-9.205	-0.029	-1.42
NaOH	4.220e-22	4.224e-22	-21.375	-21.374	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-49.926	-49.926	0.000	30.05
S(6)	1.073e-04					
SO4-2	1.016e-04	7.824e-05	-3.993	-4.107	-0.113	14.02
CaSO4	2.624e-06	2.626e-06	-5.581	-5.581	0.000	7.33
MgSO4	1.672e-06	1.674e-06	-5.777	-5.776	0.000	5.66
NaSO4-	9.456e-07	8.863e-07	-6.024	-6.052	-0.028	14.10
KSO4-	3.795e-07	3.557e-07	-6.421	-6.449	-0.028	34.01
HSO4-	2.951e-08	2.762e-08	-7.530	-7.559	-0.029	39.99
CaHSO4+	6.919e-11	6.475e-11	-10.160	-10.189	-0.029	(0)

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

Phase	SI**	log IAP	log K(293 K, 1 atm)	
Anhydrite	-3.59	-7.82	-4.23	CaSO4

Aragonite	-3.15	-11.46	-8.31	CaCO3
Calcite	-3.00	-11.46	-8.45	CaCO3
CO2(g)	-0.38	-1.80	-1.42	CO2
Dolomite	-6.18	-23.19	-17.01	CaMg(CO3)2
Gypsum	-3.23	-7.82	-4.58	CaSO4:2H2O
H2(g)	-18.84	-21.93	-3.09	H2
H2O(g)	-1.62	-0.00	1.62	H2O
Halite	-7.43	-5.87	1.57	NaCl
O2(g)	-47.07	-49.93	-2.86	O2
Sylvite	-7.27	-6.39	0.88	KCl

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

End of simulation.

Reading input data for simulation 3.

```
      Solution 4  #LF4 Name   Água Prata
      temp        21.4
      pH          5.1
      pe          4
      redox       pe
      units mg/l
      Alkalinity  110.1 as Ca.5CO3.5
      Cl          25.2
      S(6)        16.7
      Na          45.4
      Mg          3.2
      K           25.4
      Ca          10.4
      END
```

Beginning of initial solution calculations.

Initial solution 4.

---Solution composition---

Elements	Molality	Moles
Alkalinity	1.251e-03	1.251e-03
Ca	2.595e-04	2.595e-04
Cl	7.110e-04	7.110e-04
K	6.497e-04	6.497e-04
Mg	1.317e-04	1.317e-04
Na	1.975e-03	1.975e-03
S(6)	1.739e-04	1.739e-04

---Description of solution---

```
                                    pH  =   5.100
                                    pe  =   4.000
      Specific Conductance (µS/cm,  21°C)  = 287
                          Density (g/cm³)  =   0.99828
                               Volume (L)  =   1.00290
                      Activity of water  =   1.000
                 Ionic strength (mol/kgw)  =   3.390e-03
                       Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)  =   2.336e-02
                     Total CO2 (mol/kg)  =   2.336e-02
                       Temperature (°C)  =  21.40
                 Electrical balance (eq)  =   1.098e-03
```

Percent error, 100*(Cat-|An|)/(Cat+|An|) = 19.30
Iterations = 10
Total H = 1.110137e+02
Total O = 5.555489e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	8.418e-06	7.943e-06	-5.075	-5.100	-0.025	0.00
OH-	1.026e-09	9.630e-10	-8.989	-9.016	-0.028	-4.23
H2O	5.551e+01	9.995e-01	1.744	-0.000	0.000	18.05
C(4)	2.336e-02					
CO2	2.208e-02	2.210e-02	-1.656	-1.656	0.000	34.26
HCO3-	1.254e-03	1.179e-03	-2.902	-2.929	-0.027	24.43
(CO2)2	7.934e-06	7.940e-06	-5.101	-5.100	0.000	68.51
CaHCO3+	2.968e-06	2.792e-06	-5.528	-5.554	-0.026	9.55
MgHCO3+	1.445e-06	1.357e-06	-5.840	-5.868	-0.027	5.39
NaHCO3	1.253e-06	1.254e-06	-5.902	-5.902	0.000	1.80
CO3-2	8.251e-09	6.449e-09	-8.083	-8.191	-0.107	-5.49
CaCO3	1.994e-09	1.995e-09	-8.700	-8.700	0.000	-14.61
MgCO3	5.808e-10	5.813e-10	-9.236	-9.236	0.000	-17.09
NaCO3-	1.973e-10	1.852e-10	-9.705	-9.732	-0.027	-1.35
Ca	2.595e-04					
Ca+2	2.522e-04	1.970e-04	-3.598	-3.705	-0.107	-18.10
CaSO4	4.381e-06	4.384e-06	-5.358	-5.358	0.000	7.36
CaHCO3+	2.968e-06	2.792e-06	-5.528	-5.554	-0.026	9.55
CaCO3	1.994e-09	1.995e-09	-8.700	-8.700	0.000	-14.61
CaHSO4+	2.319e-10	2.177e-10	-9.635	-9.662	-0.027	(0)
CaOH+	4.382e-12	4.115e-12	-11.358	-11.386	-0.027	(0)
Cl	7.110e-04					
Cl-	7.110e-04	6.673e-04	-3.148	-3.176	-0.028	17.98
H(0)	9.257e-22					
H2	4.628e-22	4.632e-22	-21.335	-21.334	0.000	28.61
K	6.497e-04					
K+	6.492e-04	6.092e-04	-3.188	-3.215	-0.028	8.91
KSO4-	5.494e-07	5.166e-07	-6.260	-6.287	-0.027	34.03
Mg	1.317e-04					
Mg+2	1.275e-04	9.983e-05	-3.895	-4.001	-0.106	-21.60
MgSO4	2.738e-06	2.740e-06	-5.563	-5.562	0.000	5.69
MgHCO3+	1.445e-06	1.357e-06	-5.840	-5.868	-0.027	5.39
MgCO3	5.808e-10	5.813e-10	-9.236	-9.236	0.000	-17.09
MgOH+	3.487e-11	3.282e-11	-10.458	-10.484	-0.026	(0)
Na	1.975e-03					
Na+	1.973e-03	1.853e-03	-2.705	-2.732	-0.027	-1.64
NaHCO3	1.253e-06	1.254e-06	-5.902	-5.902	0.000	1.80
NaSO4-	1.241e-06	1.167e-06	-5.906	-5.933	-0.027	14.06
NaCO3-	1.973e-10	1.852e-10	-9.705	-9.732	-0.027	-1.35
NaOH	1.783e-22	1.785e-22	-21.749	-21.748	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-50.888	-50.888	0.000	30.11
S(6)	1.739e-04					
SO4-2	1.649e-04	1.286e-04	-3.783	-3.891	-0.108	14.11
CaSO4	4.381e-06	4.384e-06	-5.358	-5.358	0.000	7.36
MgSO4	2.738e-06	2.740e-06	-5.563	-5.562	0.000	5.69
NaSO4-	1.241e-06	1.167e-06	-5.906	-5.933	-0.027	14.06
KSO4-	5.494e-07	5.166e-07	-6.260	-6.287	-0.027	34.03
HSO4-	9.790e-08	9.192e-08	-7.009	-7.037	-0.027	40.04
CaHSO4+	2.319e-10	2.177e-10	-9.635	-9.662	-0.027	(0)

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

Phase	SI**	log IAP	log K(294 K, 1 atm)	
Anhydrite	-3.36	-7.60	-4.24	CaSO4
Aragonite	-3.58	-11.90	-8.31	CaCO3
Calcite	-3.44	-11.90	-8.46	CaCO3

```
  CO2(g)           -0.23     -1.66   -1.42  CO2
  Dolomite         -7.06    -24.09  -17.02  CaMg(CO3)2
  Gypsum           -3.01     -7.60   -4.58  CaSO4:2H2O
  H2(g)           -18.24    -21.33   -3.09  H2
  H2O(g)           -1.60     -0.00    1.60  H2O
  Halite           -7.47     -5.91    1.57  NaCl
  O2(g)           -48.02    -50.89   -2.87  O2
  Sylvite          -7.27     -6.39    0.88  KCl

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

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

-----------------------------------
Reading input data for simulation 4.
-----------------------------------

      Solution 5  #LF5  Caldeirão
      temp        73
      pH          6.1
      pe          1.383
      redox       pe
      units mg/l
      Alkalinity  207.5 as Ca.5CO3.5
      Cl          32.7
      S(6)        9.4
      Na          78.9
      Mg          4
      K           17.1
      Ca          10
      Si          153.22 as SiO2
      Al          0.24908
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 5.

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

      Elements           Molality       Moles

      Al                 9.236e-06   9.236e-06
      Alkalinity         2.358e-03   2.358e-03
      Ca                 2.496e-04   2.496e-04
      Cl                 9.228e-04   9.228e-04
      K                  4.375e-04   4.375e-04
      Mg                 1.646e-04   1.646e-04
      Na                 3.434e-03   3.434e-03
      S(6)               9.790e-05   9.790e-05
      Si                 2.551e-03   2.551e-03

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

                                     pH  =   6.100
                                     pe  =   1.383
      Specific Conductance (µS/cm,  73°C)  = 887
                           Density (g/cm³)  =   0.97639
                                Volume (L)  =   1.02490
                        Activity of water  =   1.000
                  Ionic strength (mol/kgw)  =   4.525e-03
                       Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)  =   5.829e-03
                     Total CO2 (mol/kg)  =   5.829e-03
```

Temperature (°C) = 73.00
Electrical balance (eq) = 1.251e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 15.47
Iterations = 8
Total H = 1.110250e+02
Total O = 5.553083e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	8.539e-07	7.943e-07	-6.069	-6.100	-0.031	0.00
OH-	2.548e-07	2.351e-07	-6.594	-6.629	-0.035	-4.30
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.46
Al	9.236e-06					
Al(OH)4-	7.871e-06	7.273e-06	-5.104	-5.138	-0.034	(0)
Al(OH)3	9.353e-07	9.362e-07	-6.029	-6.029	0.000	(0)
Al(OH)2+	4.274e-07	3.955e-07	-6.369	-6.403	-0.034	(0)
AlOH+2	2.302e-09	1.688e-09	-8.638	-8.773	-0.135	-29.79
Al+3	1.510e-11	7.877e-12	-10.821	-11.104	-0.283	-45.85
AlSO4+	2.974e-12	2.748e-12	-11.527	-11.561	-0.034	(0)
Al(SO4)2-	7.357e-15	6.798e-15	-14.133	-14.168	-0.034	(0)
AlHSO4+2	5.239e-19	3.807e-19	-18.281	-18.419	-0.139	(0)
C(4)	5.829e-03					
CO2	3.507e-03	3.510e-03	-2.455	-2.455	0.000	36.95
HCO3-	2.305e-03	2.133e-03	-2.637	-2.671	-0.034	25.72
CaHCO3+	7.296e-06	6.758e-06	-5.137	-5.170	-0.033	10.57
MgHCO3+	4.621e-06	4.267e-06	-5.335	-5.370	-0.035	5.88
NaHCO3	3.005e-06	3.008e-06	-5.522	-5.522	0.000	1.80
(CO2)2	7.554e-07	7.562e-07	-6.122	-6.121	0.000	73.90
CO3-2	2.740e-07	2.009e-07	-6.562	-6.697	-0.135	-7.74
CaCO3	2.384e-07	2.386e-07	-6.623	-6.622	0.000	-14.49
NaCO3-	1.033e-07	9.542e-08	-6.986	-7.020	-0.035	-0.53
MgCO3	4.560e-08	4.565e-08	-7.341	-7.341	0.000	-17.09
Ca	2.496e-04					
Ca+2	2.394e-04	1.754e-04	-3.621	-3.756	-0.135	-18.52
CaHCO3+	7.296e-06	6.758e-06	-5.137	-5.170	-0.033	10.57
CaSO4	2.743e-06	2.745e-06	-5.562	-5.561	0.000	8.57
CaCO3	2.384e-07	2.386e-07	-6.623	-6.622	0.000	-14.49
CaOH+	3.968e-11	3.663e-11	-10.401	-10.436	-0.035	(0)
CaHSO4+	3.827e-11	3.533e-11	-10.417	-10.452	-0.035	(0)
Cl	9.228e-04					
Cl-	9.228e-04	8.517e-04	-3.035	-3.070	-0.035	17.70
H(0)	1.013e-18					
H2	5.067e-19	5.072e-19	-18.295	-18.295	0.000	28.58
K	4.375e-04					
K+	4.371e-04	4.033e-04	-3.359	-3.394	-0.035	9.91
KSO4-	4.067e-07	3.764e-07	-6.391	-6.424	-0.034	34.09
Mg	1.646e-04					
Mg+2	1.549e-04	1.139e-04	-3.810	-3.943	-0.134	-23.61
MgSO4	4.995e-06	5.000e-06	-5.301	-5.301	0.000	6.91
MgHCO3+	4.621e-06	4.267e-06	-5.335	-5.370	-0.035	5.88
MgCO3	4.560e-08	4.565e-08	-7.341	-7.341	0.000	-17.09
MgOH+	2.349e-08	2.177e-08	-7.629	-7.662	-0.033	(0)
Na	3.434e-03					
Na+	3.429e-03	3.169e-03	-2.465	-2.499	-0.034	0.02
NaHCO3	3.005e-06	3.008e-06	-5.522	-5.522	0.000	1.80
NaSO4-	1.440e-06	1.333e-06	-5.842	-5.875	-0.034	10.29
NaCO3-	1.033e-07	9.542e-08	-6.986	-7.020	-0.035	-0.53
NaOH	7.442e-20	7.450e-20	-19.128	-19.128	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-42.448	-42.448	0.000	32.91
S(6)	9.790e-05					
SO4-2	8.830e-05	6.456e-05	-4.054	-4.190	-0.136	15.66
MgSO4	4.995e-06	5.000e-06	-5.301	-5.301	0.000	6.91
CaSO4	2.743e-06	2.745e-06	-5.562	-5.561	0.000	8.57
NaSO4-	1.440e-06	1.333e-06	-5.842	-5.875	-0.034	10.29

```
   KSO4-           4.067e-07   3.764e-07    -6.391    -6.424    -0.034     34.09
   HSO4-           1.815e-08   1.676e-08    -7.741    -7.776    -0.035     41.41
   CaHSO4+         3.827e-11   3.533e-11   -10.417   -10.452    -0.035     (0)
   AlSO4+          2.974e-12   2.748e-12   -11.527   -11.561    -0.034     (0)
   Al(SO4)2-       7.357e-15   6.798e-15   -14.133   -14.168    -0.034     (0)
   AlHSO4+2        5.239e-19   3.807e-19   -18.281   -18.419    -0.139     (0)
Si            2.551e-03
   H4SiO4          2.550e-03   2.552e-03    -2.594    -2.593     0.000     49.60
   H3SiO4-         1.792e-06   1.655e-06    -5.747    -5.781    -0.035     27.66
   H2SiO4-2        2.038e-12   1.494e-12   -11.691   -11.826    -0.135     (0)

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

  Phase               SI** log IAP   log K(346 K,   1 atm)

  Al(OH)3(a)       -0.91      7.20     8.11  Al(OH)3
  Albite           -0.05    -15.42   -15.37  NaAlSi3O8
  Alunite          -1.98     -8.49    -6.51  KAl3(SO4)2(OH)6
  Anhydrite        -3.07     -7.95    -4.88  CaSO4
  Anorthite        -0.68    -19.22   -18.54  CaAl2Si2O8
  Aragonite        -1.66    -10.45    -8.79  CaCO3
  Ca-Montmorillonite   4.79    -34.31   -39.09  Ca0.165Al2.33Si3.67O10(OH)2
  Calcite          -1.37    -10.45    -9.09  CaCO3
  Chalcedony        0.48     -2.59    -3.07  SiO2
  Chlorite(14A)    -5.09     47.90    52.98  Mg5Al2Si3O10(OH)8
  Chrysotile       -7.46     19.58    27.05  Mg3Si2O5(OH)4
  CO2(g)           -0.59     -2.45    -1.86  CO2
  Dolomite         -2.69    -21.09   -18.40  CaMg(CO3)2
  Gibbsite          1.40      7.20     5.79  Al(OH)3
  Gypsum           -3.24     -7.95    -4.70  CaSO4:2H2O
  H2(g)           -15.16    -18.29    -3.13  H2
  H2O(g)           -0.46     -0.00     0.46  H2O
  Halite           -7.17     -5.57     1.60  NaCl
  Illite            3.47    -31.24   -34.71  K0.6Mg0.25Al2.3Si3.5O10(OH)2
  K-feldspar        1.13    -16.31   -17.44  KAlSi3O8
  K-mica            9.85     16.52     6.67  KAl3Si3O10(OH)2
  Kaolinite         5.36      9.21     3.85  Al2Si2O5(OH)4
  O2(g)           -39.35    -42.45    -3.09  O2
  Quartz            0.78     -2.59    -3.37  SiO2
  Sepiolite        -5.94      8.73    14.67  Mg2Si3O7.5OH:3H2O
  Sepiolite(d)     -9.93      8.73    18.66  Mg2Si3O7.5OH:3H2O
  SiO2(a)          -0.22     -2.59    -2.37  SiO2
  Sylvite          -7.57     -6.46     1.11  KCl
  Talc             -2.29     14.40    16.69  Mg3Si4O10(OH)2

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

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

------------------------------------
Reading input data for simulation 5.
------------------------------------

      Solution 6  #LF6  Água Prata 2
      temp        16.6
      pH          5.1
      pe          4
      redox       pe
      units mg/l
      Alkalinity  164.1 as Ca.5CO3.5
      Cl          19.9
      S(6)        9.7
      Na          34.4
      Mg          3.7
      K           19.9
```

```
      Ca          8.2
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 6.

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

      Elements           Molality       Moles

      Alkalinity        1.864e-03   1.864e-03
      Ca                2.046e-04   2.046e-04
      Cl                5.615e-04   5.615e-04
      K                 5.091e-04   5.091e-04
      Mg                1.522e-04   1.522e-04
      Na                1.497e-03   1.497e-03
      S(6)              1.010e-04   1.010e-04

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

                                     pH  =   5.100
                                     pe  =   4.000
      Specific Conductance (µS/cm,  17°C)  = 231
                          Density (g/cm³)  =   0.99936
                               Volume (L)  =   1.00242
                        Activity of water  =   0.999
                  Ionic strength (mol/kgw)  =   3.111e-03
                       Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)  =   3.750e-02
                     Total CO2 (mol/kg)  =   3.750e-02
                       Temperature (°C)  =  16.60
                  Electrical balance (eq)  =   9.188e-05
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   1.72
                                Iterations  =   9
                                   Total H  = 1.110143e+02
                                   Total O  = 5.558350e+01

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

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

   H+              8.396e-06   7.943e-06    -5.076    -5.100    -0.024      0.00
   OH-             6.934e-10   6.525e-10    -9.159    -9.185    -0.026     -4.50
   H2O             5.551e+01   9.993e-01     1.744    -0.000     0.000     18.04
C(4)          3.750e-02
   CO2             3.560e-02   3.562e-02    -1.449    -1.448     0.000     34.01
   HCO3-           1.865e-03   1.759e-03    -2.729    -2.755    -0.026     23.97
   (CO2)2          1.740e-05   1.741e-05    -4.760    -4.759     0.000     68.03
   CaHCO3+         3.214e-06   3.032e-06    -5.493    -5.518    -0.025      9.33
   MgHCO3+         2.487e-06   2.342e-06    -5.604    -5.630    -0.026      5.22
   NaHCO3          1.462e-06   1.463e-06    -5.835    -5.835     0.000      1.80
   CO3-2           1.088e-08   8.599e-09    -7.963    -8.066    -0.102     -6.09
   CaCO3           1.975e-09   1.976e-09    -8.704    -8.704     0.000    -14.63
   MgCO3           8.450e-10   8.456e-10    -9.073    -9.073     0.000    -17.08
   NaCO3-          1.548e-10   1.458e-10    -9.810    -9.836    -0.026     -1.94
Ca            2.046e-04
   Ca+2            1.994e-04   1.576e-04    -3.700    -3.803    -0.102    -18.19
   CaHCO3+         3.214e-06   3.032e-06    -5.493    -5.518    -0.025      9.33
   CaSO4           1.998e-06   1.999e-06    -5.699    -5.699     0.000      7.14
   CaCO3           1.975e-09   1.976e-09    -8.704    -8.704     0.000    -14.63
   CaHSO4+         9.912e-11   9.334e-11   -10.004   -10.030    -0.026      (0)
   CaOH+           3.494e-12   3.290e-12   -11.457   -11.483    -0.026      (0)
Cl            5.615e-04
   Cl-             5.615e-04   5.285e-04    -3.251    -3.277    -0.026     17.78
H(0)          9.730e-22
```

```
   H2              4.865e-22   4.868e-22   -21.313   -21.313     0.000     28.62
K               5.091e-04
   K+              5.088e-04   4.789e-04    -3.293    -3.320    -0.026      8.72
   KSO4-           2.337e-07   2.203e-07    -6.631    -6.657    -0.026     33.86
Mg              1.522e-04
   Mg+2            1.481e-04   1.172e-04    -3.830    -3.931    -0.101    -21.43
   MgHCO3+         2.487e-06   2.342e-06    -5.604    -5.630    -0.026      5.22
   MgSO4           1.674e-06   1.675e-06    -5.776    -5.776     0.000      5.48
   MgCO3           8.450e-10   8.456e-10    -9.073    -9.073     0.000    -17.08
   MgOH+           2.600e-11   2.454e-11   -10.585   -10.610    -0.025     (0)
Na              1.497e-03
   Na+             1.495e-03   1.408e-03    -2.825    -2.851    -0.026     -1.95
   NaHCO3          1.462e-06   1.463e-06    -5.835    -5.835     0.000      1.80
   NaSO4-          5.395e-07   5.087e-07    -6.268    -6.294    -0.026     14.12
   NaCO3-          1.548e-10   1.458e-10    -9.810    -9.836    -0.026     -1.94
   NaOH            9.183e-23   9.190e-23   -22.037   -22.037     0.000     (0)
O(0)            0.000e+00
   O2              0.000e+00   0.000e+00   -52.545   -52.545     0.000     29.67
S(6)            1.010e-04
   SO4-2           9.650e-05   7.614e-05    -4.015    -4.118    -0.103     13.29
   CaSO4           1.998e-06   1.999e-06    -5.699    -5.699     0.000      7.14
   MgSO4           1.674e-06   1.675e-06    -5.776    -5.776     0.000      5.48
   NaSO4-          5.395e-07   5.087e-07    -6.268    -6.294    -0.026     14.12
   KSO4-           2.337e-07   2.203e-07    -6.631    -6.657    -0.026     33.86
   HSO4-           5.232e-08   4.927e-08    -7.281    -7.307    -0.026     39.63
   CaHSO4+         9.912e-11   9.334e-11   -10.004   -10.030    -0.026     (0)

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

  Phase               SI** log IAP   log K(289 K,   1 atm)

  Anhydrite         -3.73     -7.92   -4.19  CaSO4
  Aragonite         -3.58    -11.87   -8.29  CaCO3
  Calcite           -3.44    -11.87   -8.43  CaCO3
  CO2(g)            -0.09     -1.45   -1.36  CO2
  Dolomite          -6.91    -23.86  -16.96  CaMg(CO3)2
  Gypsum            -3.33     -7.92   -4.59  CaSO4:2H2O
  H2(g)            -18.23    -21.31   -3.08  H2
  H2O(g)            -1.73     -0.00    1.73  H2O
  Halite            -7.69     -6.13    1.56  NaCl
  O2(g)            -49.72    -52.54   -2.83  O2
  Sylvite           -7.45     -6.60    0.86  KCl

**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 6.
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      Solution 7 #LF7   Azeda do Rebentão
      temp        15.9
      pH          5.1
      pe          4
      redox       pe
      units mg/l
      Alkalinity  129.6 as Ca.5CO3.5
      Cl          20.9
      S(6)        10.5
      Na          34.1
      Mg          3.8
      K           19.6
      Ca          8.2
      END
```

```
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 7.

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

      Elements           Molality       Moles

      Alkalinity        1.472e-03   1.472e-03
      Ca                2.046e-04   2.046e-04
      Cl                5.896e-04   5.896e-04
      K                 5.014e-04   5.014e-04
      Mg                1.563e-04   1.563e-04
      Na                1.484e-03   1.484e-03
      S(6)              1.093e-04   1.093e-04

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

                                       pH  =   5.100
                                       pe  =   4.000
      Specific Conductance (µS/cm,  16°C)  = 216
                           Density (g/cm³)  =   0.99939
                                Volume (L)  =   1.00205
                        Activity of water  =   0.999
                  Ionic strength (mol/kgw)  =   2.944e-03
                       Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)  =   3.004e-02
                     Total CO2 (mol/kg)  =   3.004e-02
                       Temperature (°C)  =  15.90
                  Electrical balance (eq)  =   4.264e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   8.57
                                 Iterations  =  10
                                    Total H  = 1.110139e+02
                                    Total O  = 5.556822e+01

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

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

   H+             8.385e-06   7.943e-06    -5.076    -5.100    -0.024      0.00
   OH-            6.531e-10   6.156e-10    -9.185    -9.211    -0.026     -4.54
   H2O            5.551e+01   9.994e-01     1.744    -0.000     0.000     18.03
C(4)           3.004e-02
   CO2            2.854e-02   2.856e-02    -1.545    -1.544     0.000     33.98
   HCO3-          1.475e-03   1.393e-03    -2.831    -2.856    -0.025     23.90
   (CO2)2         1.090e-05   1.091e-05    -4.963    -4.962     0.000     67.95
   CaHCO3+        2.524e-06   2.385e-06    -5.598    -5.623    -0.025      9.29
   MgHCO3+        2.033e-06   1.918e-06    -5.692    -5.717    -0.025      5.19
   NaHCO3         1.154e-06   1.155e-06    -5.938    -5.937     0.000      1.80
   CO3-2          8.413e-09   6.690e-09    -8.075    -8.175    -0.100     -6.20
   CaCO3          1.536e-09   1.537e-09    -8.814    -8.813     0.000    -14.63
   MgCO3          6.737e-10   6.742e-10    -9.172    -9.171     0.000    -17.08
   NaCO3-         1.151e-10   1.085e-10    -9.939    -9.965    -0.025     -2.04
Ca             2.046e-04
   Ca+2           1.999e-04   1.589e-04    -3.699    -3.799    -0.100    -18.21
   CaHCO3+        2.524e-06   2.385e-06    -5.598    -5.623    -0.025      9.29
   CaSO4          2.182e-06   2.183e-06    -5.661    -5.661     0.000      7.11
   CaCO3          1.536e-09   1.537e-09    -8.814    -8.813     0.000    -14.63
   CaHSO4+        1.071e-10   1.011e-10    -9.970    -9.995    -0.025     (0)
   CaOH+          3.519e-12   3.319e-12   -11.454   -11.479    -0.025     (0)
Cl             5.896e-04
   Cl-            5.896e-04   5.559e-04    -3.229    -3.255    -0.026     17.74
H(0)           9.802e-22
   H2             4.901e-22   4.904e-22   -21.310   -21.309     0.000     28.62
K              5.014e-04
```

```
   K+              5.011e-04   4.724e-04    -3.300    -3.326    -0.026      8.69
   KSO4-           2.473e-07   2.336e-07    -6.607    -6.632    -0.025     33.83
Mg             1.563e-04
   Mg+2            1.525e-04   1.214e-04    -3.817    -3.916    -0.099    -21.41
   MgHCO3+         2.033e-06   1.918e-06    -5.692    -5.717    -0.025      5.19
   MgSO4           1.852e-06   1.853e-06    -5.732    -5.732     0.000      5.44
   MgCO3           6.737e-10   6.742e-10    -9.172    -9.171     0.000    -17.08
   MgOH+           2.515e-11   2.377e-11   -10.600   -10.624    -0.024      (0)
Na             1.484e-03
   Na+             1.482e-03   1.398e-03    -2.829    -2.854    -0.025     -2.00
   NaHCO3          1.154e-06   1.155e-06    -5.938    -5.937     0.000      1.80
   NaSO4-          5.796e-07   5.473e-07    -6.237    -6.262    -0.025     14.12
   NaCO3-          1.151e-10   1.085e-10    -9.939    -9.965    -0.025     -2.04
   NaOH            8.603e-23   8.609e-23   -22.065   -22.065     0.000      (0)
O(0)           0.000e+00
   O2              0.000e+00   0.000e+00   -52.791   -52.791     0.000     29.60
S(6)           1.093e-04
   SO4-2           1.044e-04   8.288e-05    -3.981    -4.082    -0.100     13.15
   CaSO4           2.182e-06   2.183e-06    -5.661    -5.661     0.000      7.11
   MgSO4           1.852e-06   1.853e-06    -5.732    -5.732     0.000      5.44
   NaSO4-          5.796e-07   5.473e-07    -6.237    -6.262    -0.025     14.12
   KSO4-           2.473e-07   2.336e-07    -6.607    -6.632    -0.025     33.83
   HSO4-           5.607e-08   5.289e-08    -7.251    -7.277    -0.025     39.56
   CaHSO4+         1.071e-10   1.011e-10    -9.970    -9.995    -0.025      (0)

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

  Phase               SI** log IAP   log K(289 K,   1 atm)

  Anhydrite        -3.70     -7.88   -4.18  CaSO4
  Aragonite        -3.69    -11.97   -8.28  CaCO3
  Calcite          -3.55    -11.97   -8.43  CaCO3
  CO2(g)           -0.19     -1.54   -1.35  CO2
  Dolomite         -7.12    -24.06  -16.95  CaMg(CO3)2
  Gypsum           -3.29     -7.88   -4.59  CaSO4:2H2O
  H2(g)           -18.23    -21.31   -3.08  H2
  H2O(g)           -1.74     -0.00    1.74  H2O
  Halite           -7.67     -6.11    1.56  NaCl
  O2(g)           -49.97    -52.79   -2.82  O2
  Sylvite          -7.43     -6.58    0.85  KCl

**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 7.
------------------------------------

      Solution 8  #LF8  Água Santa
      temp        91.9
      pH          7.3
      pe          4
      redox       pe
      units mg/l
      Alkalinity  324.7 as Ca.5CO3.5
      Cl          60
      S(6)        13.2
      Na          172.2
      Mg          0.9
      K           19.6
      Ca          6.7
      END
----------------------------------------
Beginning of initial solution calculations.
```

Initial solution 8.

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

Elements	Molality	Moles
Alkalinity	3.690e-03	3.690e-03
Ca	1.673e-04	1.673e-04
Cl	1.693e-03	1.693e-03
K	5.016e-04	5.016e-04
Mg	3.704e-05	3.704e-05
Na	7.495e-03	7.495e-03
S(6)	1.375e-04	1.375e-04

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

pH	= 7.300
pe	= 4.000
Specific Conductance (µS/cm, 92°C)	= 1861
Density (g/cm³)	= 0.96438
Volume (L)	= 1.03746
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 7.297e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 4.055e-03
Total CO2 (mol/kg)	= 4.055e-03
Temperature (°C)	= 91.90
Electrical balance (eq)	= 2.747e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 19.68
Iterations	= 7
Total H	= 1.110161e+02
Total O	= 5.551854e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	9.410e-06	8.473e-06	-5.026	-5.072	-0.046	-5.22
H+	5.493e-08	5.012e-08	-7.260	-7.300	-0.040	0.00
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.69
C(4)	4.055e-03					
HCO3-	3.615e-03	3.271e-03	-2.442	-2.485	-0.043	25.20
CO2	3.987e-04	3.994e-04	-3.399	-3.399	0.001	38.25
NaCO3-	1.041e-05	9.387e-06	-4.982	-5.027	-0.045	-1.85
NaHCO3	9.093e-06	9.108e-06	-5.041	-5.041	0.001	1.80
CaHCO3+	7.604e-06	6.891e-06	-5.119	-5.162	-0.043	10.63
CO3-2	7.083e-06	4.749e-06	-5.150	-5.323	-0.174	-11.45
CaCO3	5.736e-06	5.746e-06	-5.241	-5.241	0.001	-14.45
MgHCO3+	1.792e-06	1.616e-06	-5.747	-5.792	-0.045	5.70
MgCO3	2.802e-07	2.806e-07	-6.553	-6.552	0.001	-17.07
(CO2)2	1.327e-08	1.329e-08	-7.877	-7.876	0.001	76.49
Ca	1.673e-04					
Ca+2	1.516e-04	1.015e-04	-3.819	-3.993	-0.174	-19.07
CaHCO3+	7.604e-06	6.891e-06	-5.119	-5.162	-0.043	10.63
CaCO3	5.736e-06	5.746e-06	-5.241	-5.241	0.001	-14.45
CaSO4	2.320e-06	2.324e-06	-5.634	-5.634	0.001	8.78
CaOH+	3.728e-10	3.361e-10	-9.429	-9.474	-0.045	(0)
CaHSO4+	3.265e-12	2.943e-12	-11.486	-11.531	-0.045	(0)
Cl	1.693e-03					
Cl-	1.693e-03	1.526e-03	-2.771	-2.817	-0.045	16.81
H(0)	2.061e-26					
H2	1.030e-26	1.032e-26	-25.987	-25.986	0.001	28.57
K	5.016e-04					
K+	5.008e-04	4.510e-04	-3.300	-3.346	-0.045	10.08
KSO4-	7.765e-07	7.026e-07	-6.110	-6.153	-0.043	33.59

```
Mg              3.704e-05
   Mg+2              3.291e-05   2.216e-05    -4.483    -4.654    -0.172    -24.49
   MgSO4             1.811e-06   1.814e-06    -5.742    -5.741     0.001      7.13
   MgHCO3+           1.792e-06   1.616e-06    -5.747    -5.792    -0.045      5.70
   MgCO3             2.802e-07   2.806e-07    -6.553    -6.552     0.001    -17.07
   MgOH+             2.458e-07   2.230e-07    -6.609    -6.652    -0.042      (0)
Na              7.495e-03
   Na+               7.471e-03   6.746e-03    -2.127    -2.171    -0.044      0.31
   NaCO3-            1.041e-05   9.387e-06    -4.982    -5.027    -0.045     -1.85
   NaHCO3            9.093e-06   9.108e-06    -5.041    -5.041     0.001      1.80
   NaSO4-            4.515e-06   4.086e-06    -5.345    -5.389    -0.043      7.72
   NaOH              5.706e-18   5.716e-18   -17.244   -17.243     0.001      (0)
O(0)            3.359e-23
   O2                1.680e-23   1.682e-23   -22.775   -22.774     0.001     33.61
S(6)            1.375e-04
   SO4-2             1.281e-04   8.546e-05    -3.893    -4.068    -0.176     14.18
   NaSO4-            4.515e-06   4.086e-06    -5.345    -5.389    -0.043      7.72
   CaSO4             2.320e-06   2.324e-06    -5.634    -5.634     0.001      8.78
   MgSO4             1.811e-06   1.814e-06    -5.742    -5.741     0.001      7.13
   KSO4-             7.765e-07   7.026e-07    -6.110    -6.153    -0.043     33.59
   HSO4-             2.675e-09   2.412e-09    -8.573    -8.618    -0.045     41.10
   CaHSO4+           3.265e-12   2.943e-12   -11.486   -11.531    -0.045     (0)

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

  Phase               SI** log IAP   log K(365 K,   1 atm)

  Anhydrite         -2.92     -8.06   -5.15  CaSO4
  Aragonite         -0.27     -9.32   -9.04  CaCO3
  Calcite            0.13     -9.32   -9.44  CaCO3
  CO2(g)            -1.45     -3.40   -1.95  CO2
  Dolomite          -0.16    -19.29  -19.13  CaMg(CO3)2
  Gypsum            -3.26     -8.06   -4.80  CaSO4:2H2O
  H2(g)            -22.87    -25.99   -3.11  H2
  H2O(g)            -0.13     -0.00    0.13  H2O
  Halite            -6.60     -4.99    1.61  NaCl
  O2(g)            -19.66    -22.77   -3.11  O2
  Sylvite           -7.34     -6.16    1.17  KCl

**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 8.
------------------------------------

      Solution 9  #LF9  Água Prata 3
      temp        17.9
      pH          5.2
      pe          4
      redox       pe
      units mg/l
      Alkalinity  120.5 as Ca.5CO3.5
      Cl          20.7
      S(6)        12.8
      Na          37.1
      Mg          4
      K           21.8
      Ca          9.5
      END
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------
```

Initial solution 9.

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

Elements	Molality	Moles
Alkalinity	1.369e-03	1.369e-03
Ca	2.371e-04	2.371e-04
Cl	5.840e-04	5.840e-04
K	5.576e-04	5.576e-04
Mg	1.646e-04	1.646e-04
Na	1.614e-03	1.614e-03
S(6)	1.333e-04	1.333e-04

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

pH	= 5.200
pe	= 4.000
Specific Conductance (µS/cm, 18°C)	= 237
Density (g/cm³)	= 0.99897
Volume (L)	= 1.00212
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 3.104e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 2.168e-02
Total CO2 (mol/kg)	= 2.168e-02
Temperature (°C)	= 17.90
Electrical balance (eq)	= 7.557e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 14.61
Iterations	= 10
Total H	= 1.110138e+02
Total O	= 5.555149e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	6.670e-06	6.310e-06	-5.176	-5.200	-0.024	0.00
OH-	9.720e-10	9.147e-10	-9.012	-9.039	-0.026	-4.42
H2O	5.551e+01	9.996e-01	1.744	-0.000	0.000	18.04
C(4)	2.168e-02					
CO2	2.030e-02	2.031e-02	-1.693	-1.692	0.000	34.08
HCO3-	1.370e-03	1.291e-03	-2.863	-2.889	-0.026	24.11
(CO2)2	5.927e-06	5.931e-06	-5.227	-5.227	0.000	68.16
CaHCO3+	2.811e-06	2.652e-06	-5.551	-5.576	-0.025	9.39
MgHCO3+	1.982e-06	1.866e-06	-5.703	-5.729	-0.026	5.27
NaHCO3	1.149e-06	1.149e-06	-5.940	-5.940	0.000	1.80
CO3-2	1.038e-08	8.204e-09	-7.984	-8.086	-0.102	-5.91
CaCO3	2.224e-09	2.225e-09	-8.653	-8.653	0.000	-14.62
MgCO3	8.893e-10	8.899e-10	-9.051	-9.051	0.000	-17.08
NaCO3-	1.708e-10	1.608e-10	-9.768	-9.794	-0.026	-1.77
Ca	2.371e-04					
Ca+2	2.312e-04	1.826e-04	-3.636	-3.738	-0.102	-18.17
CaSO4	3.068e-06	3.070e-06	-5.513	-5.513	0.000	7.20
CaHCO3+	2.811e-06	2.652e-06	-5.551	-5.576	-0.025	9.39
CaCO3	2.224e-09	2.225e-09	-8.653	-8.653	0.000	-14.62
CaHSO4+	1.229e-10	1.157e-10	-9.911	-9.937	-0.026	(0)
CaOH+	5.099e-12	4.802e-12	-11.292	-11.319	-0.026	(0)
Cl	5.840e-04					
Cl-	5.840e-04	5.497e-04	-3.234	-3.260	-0.026	17.84
H(0)	6.056e-22					
H2	3.028e-22	3.030e-22	-21.519	-21.519	0.000	28.61
K	5.576e-04					
K+	5.573e-04	5.245e-04	-3.254	-3.280	-0.026	8.78
KSO4-	3.437e-07	3.241e-07	-6.464	-6.489	-0.026	33.91
Mg	1.646e-04					
Mg+2	1.601e-04	1.268e-04	-3.796	-3.897	-0.101	-21.48

```
   MgSO4           2.458e-06   2.460e-06    -5.609    -5.609     0.000      5.54
   MgHCO3+         1.982e-06   1.866e-06    -5.703    -5.729    -0.026      5.27
   MgCO3           8.893e-10   8.899e-10    -9.051    -9.051     0.000    -17.08
   MgOH+           4.006e-11   3.781e-11   -10.397   -10.422    -0.025      (0)
Na             1.614e-03
   Na+             1.612e-03   1.519e-03    -2.793    -2.818    -0.026     -1.86
   NaHCO3          1.149e-06   1.149e-06    -5.940    -5.940     0.000      1.80
   NaSO4-          7.698e-07   7.258e-07    -6.114    -6.139    -0.026     14.10
   NaCO3-          1.708e-10   1.608e-10    -9.768    -9.794    -0.026     -1.77
   NaOH            1.388e-22   1.389e-22   -21.857   -21.857     0.000      (0)
O(0)           0.000e+00
   O2              0.000e+00   0.000e+00   -51.691   -51.691     0.000     29.79
S(6)           1.333e-04
   SO4-2           1.266e-04   9.984e-05    -3.898    -4.001    -0.103     13.53
   CaSO4           3.068e-06   3.070e-06    -5.513    -5.513     0.000      7.20
   MgSO4           2.458e-06   2.460e-06    -5.609    -5.609     0.000      5.54
   NaSO4-          7.698e-07   7.258e-07    -6.114    -6.139    -0.026     14.10
   KSO4-           3.437e-07   3.241e-07    -6.464    -6.489    -0.026     33.91
   HSO4-           5.597e-08   5.270e-08    -7.252    -7.278    -0.026     39.75
   CaHSO4+         1.229e-10   1.157e-10    -9.911    -9.937    -0.026      (0)

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

  Phase               SI** log IAP   log K(291 K,   1 atm)

  Anhydrite        -3.54     -7.74   -4.20  CaSO4
  Aragonite        -3.53    -11.82   -8.29  CaCO3
  Calcite          -3.39    -11.82   -8.44  CaCO3
  CO2(g)           -0.31     -1.69   -1.38  CO2
  Dolomite         -6.83    -23.81  -16.97  CaMg(CO3)2
  Gypsum           -3.15     -7.74   -4.59  CaSO4:2H2O
  H2(g)           -18.44    -21.52   -3.08  H2
  H2O(g)           -1.69     -0.00    1.69  H2O
  Halite           -7.64     -6.08    1.56  NaCl
  O2(g)           -48.85    -51.69   -2.84  O2
  Sylvite          -7.40     -6.54    0.86  KCl

**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 9.
------------------------------------

      Solution 10 #LF10 Azeda
      temp        16.4
      pH          5.2
      pe          5.38
      redox       pe
      units mg/l
      Alkalinity  130.9 as Ca.5CO3.5
      Cl          19.9
      S(6)        8.2
      Na          33.3
      Mg          4
      K           19.5
      Ca          8.7
      Si          98.82 as SiO2
      Al          0.8149
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------
```

Initial solution 10.

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

Elements	Molality	Moles
Al	3.021e-05	3.021e-05
Alkalinity	1.487e-03	1.487e-03
Ca	2.171e-04	2.171e-04
Cl	5.615e-04	5.615e-04
K	4.989e-04	4.989e-04
Mg	1.646e-04	1.646e-04
Na	1.449e-03	1.449e-03
S(6)	8.539e-05	8.539e-05
Si	1.645e-03	1.645e-03

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

pH	= 5.200
pe	= 5.380
Specific Conductance (µS/cm, 16°C)	= 215
Density (g/cm³)	= 0.99932
Volume (L)	= 1.00201
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 2.987e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 2.385e-02
Total CO2 (mol/kg)	= 2.385e-02
Temperature (°C)	= 16.40
Electrical balance (eq)	= 5.825e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 11.74
Iterations	= 10
Total H	= 1.110205e+02
Total O	= 5.556233e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	6.663e-06	6.310e-06	-5.176	-5.200	-0.024	0.00
OH-	8.577e-10	8.081e-10	-9.067	-9.093	-0.026	-4.51
H2O	5.551e+01	9.995e-01	1.744	-0.000	0.000	18.04
Al	3.021e-05					
Al+3	1.417e-05	8.676e-06	-4.849	-5.062	-0.213	-41.55
AlOH+2	9.726e-06	7.721e-06	-5.012	-5.112	-0.100	-27.37
Al(OH)2+	4.607e-06	4.348e-06	-5.337	-5.362	-0.025	(0)
AlSO4+	1.640e-06	1.547e-06	-5.785	-5.811	-0.025	(0)
Al(OH)3	5.184e-08	5.187e-08	-7.285	-7.285	0.000	(0)
Al(OH)4-	1.493e-08	1.408e-08	-7.826	-7.851	-0.025	(0)
Al(SO4)2-	3.148e-09	2.969e-09	-8.502	-8.527	-0.025	(0)
AlHSO4+2	1.026e-12	8.101e-13	-11.989	-12.091	-0.102	(0)
C(4)	2.385e-02					
CO2	2.236e-02	2.238e-02	-1.651	-1.650	0.000	34.00
HCO3-	1.469e-03	1.386e-03	-2.833	-2.858	-0.025	23.95
(CO2)2	6.815e-06	6.819e-06	-5.167	-5.166	0.000	68.01
CaHCO3+	2.699e-06	2.549e-06	-5.569	-5.594	-0.025	9.32
MgHCO3+	2.136e-06	2.014e-06	-5.670	-5.696	-0.026	5.21
NaHCO3	1.118e-06	1.119e-06	-5.951	-5.951	0.000	1.80
CO3-2	1.069e-08	8.489e-09	-7.971	-8.071	-0.100	-6.12
CaCO3	2.083e-09	2.084e-09	-8.681	-8.681	0.000	-14.63
MgCO3	9.079e-10	9.085e-10	-9.042	-9.042	0.000	-17.08
NaCO3-	1.465e-10	1.381e-10	-9.834	-9.860	-0.026	-1.97
Ca	2.171e-04					
Ca+2	2.127e-04	1.688e-04	-3.672	-3.773	-0.100	-18.20
CaHCO3+	2.699e-06	2.549e-06	-5.569	-5.594	-0.025	9.32
CaSO4	1.775e-06	1.776e-06	-5.751	-5.751	0.000	7.13
CaCO3	2.083e-09	2.084e-09	-8.681	-8.681	0.000	-14.63

```
   CaHSO4+         6.968e-11   6.569e-11   -10.157   -10.183    -0.026      (0)
   CaOH+           4.706e-12   4.437e-12   -11.327   -11.353    -0.026      (0)
Cl             5.615e-04
   Cl-             5.615e-04   5.292e-04    -3.251    -3.276    -0.026     17.77
H(0)           1.069e-24
   H2              5.346e-25   5.349e-25   -24.272   -24.272     0.000     28.62
K              4.989e-04
   K+              4.987e-04   4.699e-04    -3.302    -3.328    -0.026      8.71
   KSO4-           1.895e-07   1.789e-07    -6.722    -6.747    -0.025     33.85
Mg             1.646e-04
   Mg+2            1.609e-04   1.280e-04    -3.793    -3.893    -0.099    -21.43
   MgHCO3+         2.136e-06   2.014e-06    -5.670    -5.696    -0.026      5.21
   MgSO4           1.509e-06   1.510e-06    -5.821    -5.821     0.000      5.47
   MgCO3           9.079e-10   9.085e-10    -9.042    -9.042     0.000    -17.08
   MgOH+           3.502e-11   3.309e-11   -10.456   -10.480    -0.025      (0)
Na             1.449e-03
   Na+             1.447e-03   1.365e-03    -2.839    -2.865    -0.025     -1.96
   NaHCO3          1.118e-06   1.119e-06    -5.951    -5.951     0.000      1.80
   NaSO4-          4.334e-07   4.091e-07    -6.363    -6.388    -0.025     14.11
   NaCO3-          1.465e-10   1.381e-10    -9.834    -9.860    -0.026     -1.97
   NaOH            1.103e-22   1.103e-22   -21.958   -21.957     0.000      (0)
O(0)           0.000e+00
   O2              0.000e+00   0.000e+00   -46.695   -46.695     0.000     29.65
S(6)           8.539e-05
   SO4-2           7.980e-05   6.324e-05    -4.098    -4.199    -0.101     13.24
   CaSO4           1.775e-06   1.776e-06    -5.751    -5.751     0.000      7.13
   AlSO4+          1.640e-06   1.547e-06    -5.785    -5.811    -0.025      (0)
   MgSO4           1.509e-06   1.510e-06    -5.821    -5.821     0.000      5.47
   NaSO4-          4.334e-07   4.091e-07    -6.363    -6.388    -0.025     14.11
   KSO4-           1.895e-07   1.789e-07    -6.722    -6.747    -0.025     33.85
   HSO4-           3.434e-08   3.238e-08    -7.464    -7.490    -0.026     39.61
   Al(SO4)2-       3.148e-09   2.969e-09    -8.502    -8.527    -0.025      (0)
   CaHSO4+         6.968e-11   6.569e-11   -10.157   -10.183    -0.026      (0)
   AlHSO4+2        1.026e-12   8.101e-13   -11.989   -12.091    -0.102      (0)
Si             1.645e-03
   H4SiO4          1.645e-03   1.646e-03    -2.784    -2.783     0.000     52.90
   H3SiO4-         2.974e-08   2.803e-08    -7.527    -7.552    -0.026     27.72
   H2SiO4-2        2.111e-16   1.676e-16   -15.675   -15.776    -0.100      (0)

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

  Phase               SI** log IAP   log K(289 K,   1 atm)

  Al(OH)3(a)       -0.84     10.54    11.38  Al(OH)3
  Albite           -0.50    -19.06   -18.57  NaAlSi3O8
  Alunite           4.59      4.29    -0.31  KAl3(SO4)2(OH)6
  Anhydrite        -3.79     -7.97    -4.19  CaSO4
  Anorthite        -5.07    -25.04   -19.97  CaAl2Si2O8
  Aragonite        -3.56    -11.84    -8.29  CaCO3
  Ca-Montmorillonite   6.77    -39.53   -46.30  Ca0.165Al2.33Si3.67O10(OH)2
  Calcite          -3.42    -11.84    -8.43  CaCO3
  Chalcedony        0.87     -2.78    -3.65  SiO2
  Chlorite(14A)   -26.42     45.26    71.68  Mg5Al2Si3O10(OH)8
  Chrysotile      -19.34     13.95    33.30  Mg3Si2O5(OH)4
  CO2(g)           -0.29     -1.65    -1.36  CO2
  Dolomite         -6.85    -23.81   -16.95  CaMg(CO3)2
  Gibbsite          1.93     10.54     8.61  Al(OH)3
  Gypsum           -3.38     -7.97    -4.59  CaSO4:2H2O
  H2(g)           -21.19    -24.27    -3.08  H2
  H2O(g)           -1.73     -0.00     1.73  H2O
  Halite           -7.70     -6.14     1.56  NaCl
  Illite            4.45    -37.01   -41.46  K0.6Mg0.25Al2.3Si3.5O10(OH)2
  K-feldspar        1.72    -19.53   -21.24  KAlSi3O8
  K-mica           11.14     25.14    14.00  KAl3Si3O10(OH)2
  Kaolinite         7.31     15.51     8.20  Al2Si2O5(OH)4
  O2(g)           -43.87    -46.69    -2.82  O2
  Quartz            1.33     -2.78    -4.11  SiO2
  Sepiolite       -11.33      4.66    15.99  Mg2Si3O7.5OH:3H2O
```

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  Sepiolite(d)    -14.00      4.66   18.66  Mg2Si3O7.5OH:3H2O
  SiO2(a)           0.00     -2.78   -2.78  SiO2
  Sylvite          -7.46     -6.60    0.86  KCl
  Talc            -14.02      8.39   22.41  Mg3Si4O10(OH)2

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

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

------------------------------------
Reading input data for simulation 10.
------------------------------------

      Solution 11 #LF11 Tio José de Sousa 1
      temp        17
      pH          5.4
      pe          4
      redox       pe
      units mg/l
      Alkalinity  81.9 as Ca.5CO3.5
      Cl          22.9
      S(6)        11
      Na          44
      Mg          2.4
      K           23.4
      Ca          7.1
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 11.

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

      Elements           Molality       Moles

      Alkalinity        9.303e-04   9.303e-04
      Ca                1.772e-04   1.772e-04
      Cl                6.461e-04   6.461e-04
      K                 5.986e-04   5.986e-04
      Mg                9.874e-05   9.874e-05
      Na                1.914e-03   1.914e-03
      S(6)              1.145e-04   1.145e-04

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

                                       pH  =   5.400
                                       pe  =   4.000
      Specific Conductance (µS/cm,  17°C)  = 222
                           Density (g/cm³)  =   0.99900
                                Volume (L)  =   1.00156
                        Activity of water  =   1.000
                  Ionic strength (mol/kgw)  =   2.809e-03
                       Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)  =   9.802e-03
                     Total CO2 (mol/kg)  =   9.802e-03
                       Temperature (°C)  =  17.00
                   Electrical balance (eq)  =   1.259e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  25.93
                                 Iterations  =   8
                                    Total H  = 1.110134e+02
                                    Total O  = 5.552721e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	4.198e-06	3.981e-06	-5.377	-5.400	-0.023	0.00
OH-	1.427e-09	1.346e-09	-8.846	-8.871	-0.025	-4.48
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.04
C(4)	9.802e-03					
CO2	8.865e-03	8.871e-03	-2.052	-2.052	0.000	34.03
HCO3-	9.313e-04	8.805e-04	-3.031	-3.055	-0.024	24.01
CaHCO3+	1.425e-06	1.348e-06	-5.846	-5.870	-0.024	9.34
(CO2)2	1.095e-06	1.095e-06	-5.961	-5.960	0.000	68.07
NaHCO3	9.366e-07	9.373e-07	-6.028	-6.028	0.000	1.80
MgHCO3+	8.197e-07	7.739e-07	-6.086	-6.111	-0.025	5.23
CO3-2	1.086e-08	8.674e-09	-7.964	-8.062	-0.098	-6.04
CaCO3	1.763e-09	1.765e-09	-8.754	-8.753	0.000	-14.63
MgCO3	5.656e-10	5.659e-10	-9.248	-9.247	0.000	-17.08
NaCO3-	2.042e-10	1.928e-10	-9.690	-9.715	-0.025	-1.89
Ca	1.772e-04					
Ca+2	1.737e-04	1.387e-04	-3.760	-3.858	-0.098	-18.19
CaSO4	2.034e-06	2.036e-06	-5.692	-5.691	0.000	7.16
CaHCO3+	1.425e-06	1.348e-06	-5.846	-5.870	-0.024	9.34
CaCO3	1.763e-09	1.765e-09	-8.754	-8.753	0.000	-14.63
CaHSO4+	5.069e-11	4.786e-11	-10.295	-10.320	-0.025	(0)
CaOH+	6.123e-12	5.781e-12	-11.213	-11.238	-0.025	(0)
Cl	6.461e-04					
Cl-	6.461e-04	6.098e-04	-3.190	-3.215	-0.025	17.80
H(0)	2.434e-22					
H2	1.217e-22	1.218e-22	-21.915	-21.914	0.000	28.62
K	5.986e-04					
K+	5.982e-04	5.646e-04	-3.223	-3.248	-0.025	8.74
KSO4-	3.191e-07	3.017e-07	-6.496	-6.520	-0.024	33.87
Mg	9.874e-05					
Mg+2	9.663e-05	7.732e-05	-4.015	-4.112	-0.097	-21.45
MgSO4	1.286e-06	1.287e-06	-5.891	-5.890	0.000	5.50
MgHCO3+	8.197e-07	7.739e-07	-6.086	-6.111	-0.025	5.23
MgCO3	5.656e-10	5.659e-10	-9.248	-9.247	0.000	-17.08
MgOH+	3.546e-11	3.356e-11	-10.450	-10.474	-0.024	(0)
Na	1.914e-03					
Na+	1.913e-03	1.807e-03	-2.718	-2.743	-0.025	-1.92
NaHCO3	9.366e-07	9.373e-07	-6.028	-6.028	0.000	1.80
NaSO4-	7.980e-07	7.545e-07	-6.098	-6.122	-0.024	14.09
NaCO3-	2.042e-10	1.928e-10	-9.690	-9.715	-0.025	-1.89
NaOH	2.431e-22	2.433e-22	-21.614	-21.614	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-51.205	-51.204	0.000	29.71
S(6)	1.145e-04					
SO4-2	1.101e-04	8.777e-05	-3.958	-4.057	-0.098	13.35
CaSO4	2.034e-06	2.036e-06	-5.692	-5.691	0.000	7.16
MgSO4	1.286e-06	1.287e-06	-5.891	-5.890	0.000	5.50
NaSO4-	7.980e-07	7.545e-07	-6.098	-6.122	-0.024	14.09
KSO4-	3.191e-07	3.017e-07	-6.496	-6.520	-0.024	33.87
HSO4-	3.039e-08	2.870e-08	-7.517	-7.542	-0.025	39.67
CaHSO4+	5.069e-11	4.786e-11	-10.295	-10.320	-0.025	(0)

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

Phase	SI**	log IAP	log K(290 K, 1 atm)	
Anhydrite	-3.72	-7.91	-4.19	CaSO4
Aragonite	-3.63	-11.92	-8.29	CaCO3
Calcite	-3.49	-11.92	-8.43	CaCO3
CO2(g)	-0.68	-2.05	-1.37	CO2
Dolomite	-7.13	-24.09	-16.96	CaMg(CO3)2
Gypsum	-3.33	-7.91	-4.59	CaSO4:2H2O
H2(g)	-18.84	-21.91	-3.08	H2
H2O(g)	-1.71	-0.00	1.71	H2O
Halite	-7.52	-5.96	1.56	NaCl

```
  O2(g)           -48.37    -51.20   -2.83  O2
  Sylvite          -7.32     -6.46    0.86  KCl

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

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

------------------------------------
Reading input data for simulation 11.
------------------------------------

      Solution 12 #LF12 Tio José de Sousa 2
      temp        15.8
      pH          5.4
      pe          4
      redox       pe
      units mg/l
      Alkalinity  96.7 as Ca.5CO3.5
      Cl          22
      S(6)        10.1
      Na          36.8
      Mg          3.6
      K           20.4
      Ca          7.7
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 12.

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

      Elements           Molality       Moles

      Alkalinity        1.098e-03   1.098e-03
      Ca                1.922e-04   1.922e-04
      Cl                6.207e-04   6.207e-04
      K                 5.218e-04   5.218e-04
      Mg                1.481e-04   1.481e-04
      Na                1.601e-03   1.601e-03
      S(6)              1.052e-04   1.052e-04

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

                                       pH  =   5.400
                                       pe  =   4.000
      Specific Conductance (µS/cm,  16°C)  = 207
                           Density (g/cm³)  =   0.99922
                                Volume (L)  =   1.00142
                        Activity of water   =   1.000
                  Ionic strength (mol/kgw)  =   2.792e-03
                       Mass of water (kg)   =   1.000e+00
                  Total carbon (mol/kg)     =   1.179e-02
                     Total CO2 (mol/kg)     =   1.179e-02
                       Temperature (°C)     =  15.80
                   Electrical balance (eq)  =   8.739e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   =  18.53
                                 Iterations  =   9
                                    Total H  = 1.110135e+02
                                    Total O  = 5.553132e+01

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

                                                Log       Log       Log    mole V
```

Species	Molality	Activity	Molality	Activity	Gamma	cm³/mol
H+	4.197e-06	3.981e-06	-5.377	-5.400	-0.023	0.00
OH-	1.291e-09	1.218e-09	-8.889	-8.914	-0.025	-4.55
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.03
C(4)	1.179e-02					
CO2	1.068e-02	1.069e-02	-1.971	-1.971	0.000	33.97
HCO3-	1.098e-03	1.039e-03	-2.959	-2.983	-0.024	23.88
CaHCO3+	1.777e-06	1.681e-06	-5.750	-5.774	-0.024	9.28
(CO2)2	1.522e-06	1.523e-06	-5.818	-5.817	0.000	67.94
MgHCO3+	1.447e-06	1.367e-06	-5.839	-5.864	-0.025	5.19
NaHCO3	9.311e-07	9.317e-07	-6.031	-6.031	0.000	1.80
CO3-2	1.242e-08	9.931e-09	-7.906	-8.003	-0.097	-6.22
CaCO3	2.158e-09	2.159e-09	-8.666	-8.666	0.000	-14.63
MgCO3	9.546e-10	9.552e-10	-9.020	-9.020	0.000	-17.08
NaCO3-	1.833e-10	1.732e-10	-9.737	-9.762	-0.025	-2.06
Ca	1.922e-04					
Ca+2	1.884e-04	1.506e-04	-3.725	-3.822	-0.097	-18.22
CaSO4	2.001e-06	2.002e-06	-5.699	-5.699	0.000	7.10
CaHCO3+	1.777e-06	1.681e-06	-5.750	-5.774	-0.024	9.28
CaCO3	2.158e-09	2.159e-09	-8.666	-8.666	0.000	-14.63
CaHSO4+	4.911e-11	4.638e-11	-10.309	-10.334	-0.025	(0)
CaOH+	6.644e-12	6.275e-12	-11.178	-11.202	-0.025	(0)
Cl	6.207e-04					
Cl-	6.207e-04	5.860e-04	-3.207	-3.232	-0.025	17.74
H(0)	2.465e-22					
H2	1.232e-22	1.233e-22	-21.909	-21.909	0.000	28.62
K	5.218e-04					
K+	5.216e-04	4.924e-04	-3.283	-3.308	-0.025	8.69
KSO4-	2.489e-07	2.354e-07	-6.604	-6.628	-0.024	33.83
Mg	1.481e-04					
Mg+2	1.449e-04	1.161e-04	-3.839	-3.935	-0.096	-21.41
MgSO4	1.710e-06	1.711e-06	-5.767	-5.767	0.000	5.44
MgHCO3+	1.447e-06	1.367e-06	-5.839	-5.864	-0.025	5.19
MgCO3	9.546e-10	9.552e-10	-9.020	-9.020	0.000	-17.08
MgOH+	4.745e-11	4.492e-11	-10.324	-10.348	-0.024	(0)
Na	1.601e-03					
Na+	1.599e-03	1.512e-03	-2.796	-2.821	-0.025	-2.01
NaHCO3	9.311e-07	9.317e-07	-6.031	-6.031	0.000	1.80
NaSO4-	6.056e-07	5.727e-07	-6.218	-6.242	-0.024	14.10
NaCO3-	1.833e-10	1.732e-10	-9.737	-9.762	-0.025	-2.06
NaOH	1.841e-22	1.842e-22	-21.735	-21.735	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-51.626	-51.626	0.000	29.59
S(6)	1.052e-04					
SO4-2	1.006e-04	8.028e-05	-3.998	-4.095	-0.098	13.12
CaSO4	2.001e-06	2.002e-06	-5.699	-5.699	0.000	7.10
MgSO4	1.710e-06	1.711e-06	-5.767	-5.767	0.000	5.44
NaSO4-	6.056e-07	5.727e-07	-6.218	-6.242	-0.024	14.10
KSO4-	2.489e-07	2.354e-07	-6.604	-6.628	-0.024	33.83
HSO4-	2.713e-08	2.562e-08	-7.567	-7.591	-0.025	39.55
CaHSO4+	4.911e-11	4.638e-11	-10.309	-10.334	-0.025	(0)

Saturation indices

Phase	SI**	log IAP	log K(288 K, 1 atm)	
Anhydrite	-3.74	-7.92	-4.18	CaSO4
Aragonite	-3.54	-11.83	-8.28	CaCO3
Calcite	-3.40	-11.83	-8.43	CaCO3
CO2(g)	-0.62	-1.97	-1.35	CO2
Dolomite	-6.82	-23.76	-16.95	CaMg(CO3)2
Gypsum	-3.33	-7.92	-4.59	CaSO4:2H2O
H2(g)	-18.83	-21.91	-3.08	H2
H2O(g)	-1.75	-0.00	1.75	H2O
Halite	-7.62	-6.05	1.56	NaCl
O2(g)	-48.81	-51.63	-2.82	O2
Sylvite	-7.39	-6.54	0.85	KCl

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

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

-------------------------------------
Reading input data for simulation 12.
-------------------------------------

      Solution 13 #LF13 Tio José de Sousa 3
      temp        15.8
      pH          5.4
      pe          4
      redox       pe
      units mg/l
      Alkalinity  92.4 as Ca.5CO3.5
      Cl          21.2
      S(6)        10
      Na          36.2
      Mg          3.7
      K           20.3
      Ca          8.5
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 13.

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

      Elements           Molality       Moles

      Alkalinity        1.050e-03   1.050e-03
      Ca                2.121e-04   2.121e-04
      Cl                5.981e-04   5.981e-04
      K                 5.193e-04   5.193e-04
      Mg                1.522e-04   1.522e-04
      Na                1.575e-03   1.575e-03
      S(6)              1.041e-04   1.041e-04

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

                                       pH  =   5.400
                                       pe  =   4.000
      Specific Conductance (µS/cm,  16°C)  = 205
                           Density (g/cm³)  =   0.99921
                                Volume (L)  =   1.00140
                        Activity of water   =   1.000
                  Ionic strength (mol/kgw)  =   2.787e-03
                       Mass of water (kg)   =   1.000e+00
                  Total carbon (mol/kg)     =   1.127e-02
                     Total CO2 (mol/kg)     =   1.127e-02
                       Temperature (°C)     =  15.80
                   Electrical balance (eq)  =   9.669e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   =  20.74
                                 Iterations  =   9
                                    Total H  = 1.110135e+02
                                    Total O  = 5.553022e+01

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

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

H+	4.197e-06	3.981e-06	-5.377	-5.400	-0.023	0.00
OH-	1.291e-09	1.218e-09	-8.889	-8.914	-0.025	-4.55
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.03
C(4)	1.127e-02					
CO2	1.021e-02	1.022e-02	-1.991	-1.991	0.000	33.97
HCO3-	1.050e-03	9.926e-04	-2.979	-3.003	-0.024	23.88
CaHCO3+	1.876e-06	1.775e-06	-5.727	-5.751	-0.024	9.28
MgHCO3+	1.422e-06	1.343e-06	-5.847	-5.872	-0.025	5.19
(CO2)2	1.390e-06	1.391e-06	-5.857	-5.857	0.000	67.94
NaHCO3	8.753e-07	8.758e-07	-6.058	-6.058	0.000	1.80
CO3-2	1.186e-08	9.489e-09	-7.926	-8.023	-0.097	-6.22
CaCO3	2.278e-09	2.279e-09	-8.643	-8.642	0.000	-14.63
MgCO3	9.382e-10	9.388e-10	-9.028	-9.027	0.000	-17.08
NaCO3-	1.723e-10	1.628e-10	-9.764	-9.788	-0.025	-2.06
Ca	2.121e-04					
Ca+2	2.081e-04	1.663e-04	-3.682	-3.779	-0.097	-18.22
CaSO4	2.183e-06	2.185e-06	-5.661	-5.661	0.000	7.10
CaHCO3+	1.876e-06	1.775e-06	-5.727	-5.751	-0.024	9.28
CaCO3	2.278e-09	2.279e-09	-8.643	-8.642	0.000	-14.63
CaHSO4+	5.359e-11	5.062e-11	-10.271	-10.296	-0.025	(0)
CaOH+	7.339e-12	6.932e-12	-11.134	-11.159	-0.025	(0)
Cl	5.981e-04					
Cl-	5.981e-04	5.648e-04	-3.223	-3.248	-0.025	17.74
H(0)	2.465e-22					
H2	1.232e-22	1.233e-22	-21.909	-21.909	0.000	28.62
K	5.193e-04					
K+	5.190e-04	4.900e-04	-3.285	-3.310	-0.025	8.69
KSO4-	2.447e-07	2.314e-07	-6.611	-6.636	-0.024	33.83
Mg	1.522e-04					
Mg+2	1.491e-04	1.194e-04	-3.827	-3.923	-0.096	-21.41
MgSO4	1.737e-06	1.739e-06	-5.760	-5.760	0.000	5.44
MgHCO3+	1.422e-06	1.343e-06	-5.847	-5.872	-0.025	5.19
MgCO3	9.382e-10	9.388e-10	-9.028	-9.027	0.000	-17.08
MgOH+	4.881e-11	4.620e-11	-10.312	-10.335	-0.024	(0)
Na	1.575e-03					
Na+	1.573e-03	1.487e-03	-2.803	-2.828	-0.025	-2.01
NaHCO3	8.753e-07	8.758e-07	-6.058	-6.058	0.000	1.80
NaSO4-	5.885e-07	5.566e-07	-6.230	-6.254	-0.024	14.10
NaCO3-	1.723e-10	1.628e-10	-9.764	-9.788	-0.025	-2.06
NaOH	1.811e-22	1.812e-22	-21.742	-21.742	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-51.626	-51.626	0.000	29.59
S(6)	1.041e-04					
SO4-2	9.934e-05	7.931e-05	-4.003	-4.101	-0.098	13.12
CaSO4	2.183e-06	2.185e-06	-5.661	-5.661	0.000	7.10
MgSO4	1.737e-06	1.739e-06	-5.760	-5.760	0.000	5.44
NaSO4-	5.885e-07	5.566e-07	-6.230	-6.254	-0.024	14.10
KSO4-	2.447e-07	2.314e-07	-6.611	-6.636	-0.024	33.83
HSO4-	2.680e-08	2.531e-08	-7.572	-7.597	-0.025	39.55
CaHSO4+	5.359e-11	5.062e-11	-10.271	-10.296	-0.025	(0)

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

Phase	SI**	log IAP	log K(288 K, 1 atm)	
Anhydrite	-3.70	-7.88	-4.18	CaSO4
Aragonite	-3.52	-11.80	-8.28	CaCO3
Calcite	-3.38	-11.80	-8.43	CaCO3
CO2(g)	-0.64	-1.99	-1.35	CO2
Dolomite	-6.80	-23.75	-16.95	CaMg(CO3)2
Gypsum	-3.29	-7.88	-4.59	CaSO4:2H2O
H2(g)	-18.83	-21.91	-3.08	H2
H2O(g)	-1.75	-0.00	1.75	H2O
Halite	-7.64	-6.08	1.56	NaCl
O2(g)	-48.81	-51.63	-2.82	O2
Sylvite	-7.41	-6.56	0.85	KCl

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

For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 13.

```
      Solution 14 #LF14 Água do Rêgo
      temp        16.3
      pH          5.2
      pe          4
      redox       pe
      units mg/l
      Alkalinity  128.1 as Ca.5CO3.5
      Cl          21.4
      S(6)        8.9
      Na          38.9
      Mg          3.4
      K           21.3
      Ca          8.4
      END
```

Beginning of initial solution calculations.

Initial solution 14.

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

Elements	Molality	Moles
Alkalinity	1.455e-03	1.455e-03
Ca	2.096e-04	2.096e-04
Cl	6.038e-04	6.038e-04
K	5.449e-04	5.449e-04
Mg	1.399e-04	1.399e-04
Na	1.692e-03	1.692e-03
S(6)	9.267e-05	9.267e-05

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

pH	= 5.200
pe	= 4.000
Specific Conductance (µS/cm, 16°C)	= 226
Density (g/cm³)	= 0.99927
Volume (L)	= 1.00191
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 3.014e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 2.368e-02
Total CO2 (mol/kg)	= 2.368e-02
Temperature (°C)	= 16.30
Electrical balance (eq)	= 6.921e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 13.39
Iterations	= 10
Total H	= 1.110139e+02
Total O	= 5.555541e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	6.664e-06	6.310e-06	-5.176	-5.200	-0.024	0.00
OH-	8.508e-10	8.014e-10	-9.070	-9.096	-0.026	-4.52

H2O	5.551e+01	9.995e-01	1.744	-0.000	0.000	18.04
C(4)	2.368e-02					
CO2	2.220e-02	2.222e-02	-1.654	-1.653	0.000	34.00
HCO3-	1.456e-03	1.374e-03	-2.837	-2.862	-0.025	23.94
(CO2)2	6.695e-06	6.700e-06	-5.174	-5.174	0.000	68.00
CaHCO3+	2.573e-06	2.430e-06	-5.590	-5.614	-0.025	9.31
MgHCO3+	1.797e-06	1.693e-06	-5.745	-5.771	-0.026	5.21
NaHCO3	1.295e-06	1.296e-06	-5.888	-5.887	0.000	1.80
CO3-2	1.058e-08	8.394e-09	-7.975	-8.076	-0.101	-6.14
CaCO3	1.983e-09	1.984e-09	-8.703	-8.702	0.000	-14.63
MgCO3	7.605e-10	7.610e-10	-9.119	-9.119	0.000	-17.08
NaCO3-	1.683e-10	1.586e-10	-9.774	-9.800	-0.026	-1.98
Ca	2.096e-04					
Ca+2	2.052e-04	1.627e-04	-3.688	-3.789	-0.101	-18.20
CaHCO3+	2.573e-06	2.430e-06	-5.590	-5.614	-0.025	9.31
CaSO4	1.894e-06	1.896e-06	-5.723	-5.722	0.000	7.13
CaCO3	1.983e-09	1.984e-09	-8.703	-8.702	0.000	-14.63
CaHSO4+	7.431e-11	7.003e-11	-10.129	-10.155	-0.026	(0)
CaOH+	4.537e-12	4.276e-12	-11.343	-11.369	-0.026	(0)
Cl	6.038e-04					
Cl-	6.038e-04	5.689e-04	-3.219	-3.245	-0.026	17.76
H(0)	6.159e-22					
H2	3.079e-22	3.081e-22	-21.512	-21.511	0.000	28.62
K	5.449e-04					
K+	5.446e-04	5.131e-04	-3.264	-3.290	-0.026	8.71
KSO4-	2.290e-07	2.161e-07	-6.640	-6.665	-0.025	33.85
Mg	1.399e-04					
Mg+2	1.367e-04	1.086e-04	-3.864	-3.964	-0.100	-21.42
MgHCO3+	1.797e-06	1.693e-06	-5.745	-5.771	-0.026	5.21
MgSO4	1.415e-06	1.416e-06	-5.849	-5.849	0.000	5.46
MgCO3	7.605e-10	7.610e-10	-9.119	-9.119	0.000	-17.08
MgOH+	2.943e-11	2.781e-11	-10.531	-10.556	-0.025	(0)
Na	1.692e-03					
Na+	1.691e-03	1.594e-03	-2.772	-2.797	-0.025	-1.97
NaHCO3	1.295e-06	1.296e-06	-5.888	-5.887	0.000	1.80
NaSO4-	5.607e-07	5.291e-07	-6.251	-6.276	-0.025	14.12
NaCO3-	1.683e-10	1.586e-10	-9.774	-9.800	-0.026	-1.98
NaOH	1.277e-22	1.278e-22	-21.894	-21.894	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-52.250	-52.250	0.000	29.64
S(6)	9.267e-05					
SO4-2	8.853e-05	7.009e-05	-4.053	-4.154	-0.101	13.23
CaSO4	1.894e-06	1.896e-06	-5.723	-5.722	0.000	7.13
MgSO4	1.415e-06	1.416e-06	-5.849	-5.849	0.000	5.46
NaSO4-	5.607e-07	5.291e-07	-6.251	-6.276	-0.025	14.12
KSO4-	2.290e-07	2.161e-07	-6.640	-6.665	-0.025	33.85
HSO4-	3.800e-08	3.581e-08	-7.420	-7.446	-0.026	39.60
CaHSO4+	7.431e-11	7.003e-11	-10.129	-10.155	-0.026	(0)

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

Phase	SI**	log IAP	log K(289 K, 1 atm)	
Anhydrite	-3.76	-7.94	-4.18	CaSO4
Aragonite	-3.58	-11.86	-8.29	CaCO3
Calcite	-3.44	-11.86	-8.43	CaCO3
CO2(g)	-0.29	-1.65	-1.36	CO2
Dolomite	-6.95	-23.90	-16.95	CaMg(CO3)2
Gypsum	-3.36	-7.94	-4.59	CaSO4:2H2O
H2(g)	-18.43	-21.51	-3.08	H2
H2O(g)	-1.73	-0.00	1.73	H2O
Halite	-7.61	-6.04	1.56	NaCl
O2(g)	-49.43	-52.25	-2.82	O2
Sylvite	-7.39	-6.53	0.86	KCl

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

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

--------------------------------------
Reading input data for simulation 14.
--------------------------------------

      Solution 15 #LF15 Caldeira dos Inhames
      temp        61.8
      pH          5.6
      pe          4
      redox       pe
      units mg/l
      Alkalinity  85.8 as Ca.5CO3.5
      Cl          34.1
      S(6)        23.5
      Na          33.9
      Mg          4.9
      K           18.1
      Ca          11.3
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 15.

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

      Elements           Molality       Moles

      Alkalinity        9.746e-04   9.746e-04
      Ca                2.820e-04   2.820e-04
      Cl                9.620e-04   9.620e-04
      K                 4.630e-04   4.630e-04
      Mg                2.016e-04   2.016e-04
      Na                1.475e-03   1.475e-03
      S(6)              2.447e-04   2.447e-04

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

                                       pH  =   5.600
                                       pe  =   4.000
      Specific Conductance (µS/cm,  62°C)  = 544
                           Density (g/cm³)  =   0.98243
                                Volume (L)  =   1.01827
                        Activity of water  =   1.000
                  Ionic strength (mol/kgw)  =   3.294e-03
                       Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)  =   5.457e-03
                     Total CO2 (mol/kg)  =   5.457e-03
                       Temperature (°C)  =  61.80
                   Electrical balance (eq)  =   4.790e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   9.15
                                 Iterations  =   8
                                    Total H  = 1.110134e+02
                                    Total O  = 5.551909e+01

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

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

   H+              2.672e-06   2.512e-06    -5.573    -5.600    -0.027      0.00
   OH-             4.529e-08   4.232e-08    -7.344    -7.373    -0.029     -3.96
   H2O             5.551e+01   9.998e-01     1.744    -0.000     0.000     18.34
C(4)          5.457e-03
```

CO2	4.478e-03	4.482e-03	-2.349	-2.349	0.000	36.29
HCO3-	9.710e-04	9.094e-04	-3.013	-3.041	-0.028	25.81
CaHCO3+	3.448e-06	3.231e-06	-5.462	-5.491	-0.028	10.47
MgHCO3+	2.165e-06	2.024e-06	-5.665	-5.694	-0.029	5.91
(CO2)2	9.869e-07	9.876e-07	-6.006	-6.005	0.000	72.58
NaHCO3	5.849e-07	5.854e-07	-6.233	-6.233	0.000	1.80
CO3-2	3.410e-08	2.623e-08	-7.467	-7.581	-0.114	-6.24
CaCO3	2.581e-08	2.583e-08	-7.588	-7.588	0.000	-14.51
MgCO3	6.315e-09	6.320e-09	-8.200	-8.199	0.000	-17.09
NaCO3-	3.756e-09	3.512e-09	-8.425	-8.454	-0.029	-0.10
Ca	2.820e-04					
Ca+2	2.705e-04	2.079e-04	-3.568	-3.682	-0.114	-18.30
CaSO4	8.006e-06	8.012e-06	-5.097	-5.096	0.000	8.40
CaHCO3+	3.448e-06	3.231e-06	-5.462	-5.491	-0.028	10.47
CaCO3	2.581e-08	2.583e-08	-7.588	-7.588	0.000	-14.51
CaHSO4+	2.735e-10	2.557e-10	-9.563	-9.592	-0.029	(0)
CaOH+	1.469e-11	1.374e-11	-10.833	-10.862	-0.029	(0)
Cl	9.620e-04					
Cl-	9.620e-04	8.992e-04	-3.017	-3.046	-0.029	18.05
H(0)	6.442e-23					
H2	3.221e-23	3.224e-23	-22.492	-22.492	0.000	28.58
K	4.630e-04					
K+	4.620e-04	4.318e-04	-3.335	-3.365	-0.029	9.78
KSO4-	9.723e-07	9.105e-07	-6.012	-6.041	-0.028	34.27
Mg	2.016e-04					
Mg+2	1.862e-04	1.435e-04	-3.730	-3.843	-0.113	-23.15
MgSO4	1.324e-05	1.325e-05	-4.878	-4.878	0.000	6.75
MgHCO3+	2.165e-06	2.024e-06	-5.665	-5.694	-0.029	5.91
MgCO3	6.315e-09	6.320e-09	-8.200	-8.199	0.000	-17.09
MgOH+	4.259e-09	3.993e-09	-8.371	-8.399	-0.028	(0)
Na	1.475e-03					
Na+	1.473e-03	1.378e-03	-2.832	-2.861	-0.029	-0.20
NaSO4-	1.538e-06	1.441e-06	-5.813	-5.841	-0.028	11.46
NaHCO3	5.849e-07	5.854e-07	-6.233	-6.233	0.000	1.80
NaCO3-	3.756e-09	3.512e-09	-8.425	-8.454	-0.029	-0.10
NaOH	5.827e-21	5.831e-21	-20.235	-20.234	0.000	(0)
O(0)	2.988e-37					
O2	1.494e-37	1.495e-37	-36.826	-36.825	0.000	32.46
S(6)	2.447e-04					
SO4-2	2.208e-04	1.695e-04	-3.656	-3.771	-0.115	16.09
MgSO4	1.324e-05	1.325e-05	-4.878	-4.878	0.000	6.75
CaSO4	8.006e-06	8.012e-06	-5.097	-5.096	0.000	8.40
NaSO4-	1.538e-06	1.441e-06	-5.813	-5.841	-0.028	11.46
KSO4-	9.723e-07	9.105e-07	-6.012	-6.041	-0.028	34.27
HSO4-	1.094e-07	1.023e-07	-6.961	-6.990	-0.029	41.42
CaHSO4+	2.735e-10	2.557e-10	-9.563	-9.592	-0.029	(0)

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

Phase	SI**	log IAP	log K(334 K, 1 atm)	
Anhydrite	-2.72	-7.45	-4.73	CaSO4
Aragonite	-2.61	-11.26	-8.66	CaCO3
Calcite	-2.36	-11.26	-8.90	CaCO3
CO2(g)	-0.55	-2.35	-1.80	CO2
Dolomite	-4.67	-22.69	-18.02	CaMg(CO3)2
Gypsum	-2.80	-7.45	-4.66	CaSO4:2H2O
H2(g)	-19.35	-22.49	-3.14	H2
H2O(g)	-0.67	-0.00	0.67	H2O
Halite	-7.50	-5.91	1.60	NaCl
O2(g)	-33.76	-36.83	-3.07	O2
Sylvite	-7.47	-6.41	1.06	KCl

**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 15.
------------------------------------

      Solution 16 #LF16 Caldeira dos Vimes
      temp        20.2
      pH          5.4
      pe          4
      redox       pe
      units mg/l
      Alkalinity  110.9 as Ca.5CO3.5
      Cl          28.9
      S(6)        11.9
      Na          35.2
      Mg          3.8
      K           19
      Ca          9.4
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 16.

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

      Elements           Molality       Moles

      Alkalinity        1.260e-03   1.260e-03
      Ca                2.346e-04   2.346e-04
      Cl                8.153e-04   8.153e-04
      K                 4.860e-04   4.860e-04
      Mg                1.563e-04   1.563e-04
      Na                1.531e-03   1.531e-03
      S(6)              1.239e-04   1.239e-04

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

                                     pH  =   5.400
                                     pe  =   4.000
      Specific Conductance (µS/cm,  20°C)  = 250
                          Density (g/cm³)  =   0.99842
                               Volume (L)  =   1.00227
                      Activity of water    =   1.000
                 Ionic strength (mol/kgw)  =   3.048e-03
                       Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)    =   1.261e-02
                     Total CO2 (mol/kg)    =   1.261e-02
                       Temperature (°C)    =  20.20
                  Electrical balance (eq)  =   4.764e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   9.35
                                Iterations  =   9
                                   Total H  = 1.110137e+02
                                   Total O  = 5.553320e+01

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

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

   H+              4.207e-06   3.981e-06    -5.376    -5.400    -0.024       0.00
   OH-             1.856e-09   1.747e-09    -8.731    -8.758    -0.026      -4.30
   H2O             5.551e+01   9.997e-01     1.744    -0.000     0.000      18.05
C(4)          1.261e-02
   CO2             1.134e-02   1.135e-02    -1.945    -1.945     0.000      34.20
   HCO3-           1.259e-03   1.187e-03    -2.900    -2.926    -0.025      24.32
```

CaHCO3+	2.680e-06	2.529e-06	-5.572	-5.597	-0.025	9.50
(CO2)2	2.009e-06	2.010e-06	-5.697	-5.697	0.000	68.39
MgHCO3+	1.746e-06	1.645e-06	-5.758	-5.784	-0.026	5.35
NaHCO3	9.885e-07	9.892e-07	-6.005	-6.005	0.000	1.80
CO3-2	1.594e-08	1.261e-08	-7.797	-7.899	-0.102	-5.63
CaCO3	3.513e-09	3.515e-09	-8.454	-8.454	0.000	-14.61
MgCO3	1.348e-09	1.349e-09	-8.870	-8.870	0.000	-17.08
NaCO3-	2.811e-10	2.648e-10	-9.551	-9.577	-0.026	-1.49
Ca	2.346e-04					
Ca+2	2.290e-04	1.811e-04	-3.640	-3.742	-0.102	-18.13
CaSO4	2.883e-06	2.885e-06	-5.540	-5.540	0.000	7.31
CaHCO3+	2.680e-06	2.529e-06	-5.572	-5.597	-0.025	9.50
CaCO3	3.513e-09	3.515e-09	-8.454	-8.454	0.000	-14.61
CaHSO4+	7.504e-11	7.068e-11	-10.125	-10.151	-0.026	(0)
CaOH+	8.013e-12	7.547e-12	-11.096	-11.122	-0.026	(0)
Cl	8.153e-04					
Cl-	8.153e-04	7.677e-04	-3.089	-3.115	-0.026	17.94
H(0)	2.354e-22					
H2	1.177e-22	1.178e-22	-21.929	-21.929	0.000	28.61
K	4.860e-04					
K+	4.857e-04	4.573e-04	-3.314	-3.340	-0.026	8.86
KSO4-	2.908e-07	2.742e-07	-6.536	-6.562	-0.025	33.99
Mg	1.563e-04					
Mg+2	1.523e-04	1.207e-04	-3.817	-3.918	-0.101	-21.57
MgSO4	2.317e-06	2.319e-06	-5.635	-5.635	0.000	5.64
MgHCO3+	1.746e-06	1.645e-06	-5.758	-5.784	-0.026	5.35
MgCO3	1.348e-09	1.349e-09	-8.870	-8.870	0.000	-17.08
MgOH+	7.502e-11	7.082e-11	-10.125	-10.150	-0.025	(0)
Na	1.531e-03					
Na+	1.530e-03	1.442e-03	-2.815	-2.841	-0.026	-1.71
NaHCO3	9.885e-07	9.892e-07	-6.005	-6.005	0.000	1.80
NaSO4-	6.903e-07	6.510e-07	-6.161	-6.186	-0.025	14.06
NaCO3-	2.811e-10	2.648e-10	-9.551	-9.577	-0.026	-1.49
NaOH	2.517e-22	2.518e-22	-21.599	-21.599	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-50.097	-50.097	0.000	30.00
S(6)	1.239e-04					
SO4-2	1.177e-04	9.293e-05	-3.929	-4.032	-0.103	13.91
CaSO4	2.883e-06	2.885e-06	-5.540	-5.540	0.000	7.31
MgSO4	2.317e-06	2.319e-06	-5.635	-5.635	0.000	5.64
NaSO4-	6.903e-07	6.510e-07	-6.161	-6.186	-0.025	14.06
KSO4-	2.908e-07	2.742e-07	-6.536	-6.562	-0.025	33.99
HSO4-	3.446e-08	3.246e-08	-7.463	-7.489	-0.026	39.95
CaHSO4+	7.504e-11	7.068e-11	-10.125	-10.151	-0.026	(0)

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

Phase	SI**	log IAP	log K(293 K, 1 atm)	
Anhydrite	-3.55	-7.77	-4.23	CaSO4
Aragonite	-3.33	-11.64	-8.31	CaCO3
Calcite	-3.19	-11.64	-8.45	CaCO3
CO2(g)	-0.54	-1.94	-1.41	CO2
Dolomite	-6.45	-23.46	-17.01	CaMg(CO3)2
Gypsum	-3.19	-7.77	-4.58	CaSO4:2H2O
H2(g)	-18.84	-21.93	-3.09	H2
H2O(g)	-1.63	-0.00	1.63	H2O
Halite	-7.52	-5.96	1.57	NaCl
O2(g)	-47.24	-50.10	-2.86	O2
Sylvite	-7.33	-6.45	0.88	KCl

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

End of simulation.

```
------------------------------------
Reading input data for simulation 16.
------------------------------------

      Solution 17 #LF17 Caldeira do Esguicho
      temp        95.4
      pH          7.6
      pe          4
      redox       pe
      units mg/l
      Alkalinity  570.9 as Ca.5CO3.5
      Cl          127.7
      S(6)        21.3
      Na          371.5
      Mg          1.6
      K           28.8
      Ca          3
      END
----------------------------------------
Beginning of initial solution calculations.
----------------------------------------

Initial solution 17.

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

      Elements           Molality       Moles

      Alkalinity        6.491e-03   6.491e-03
      Ca                7.493e-05   7.493e-05
      Cl                3.606e-03   3.606e-03
      K                 7.374e-04   7.374e-04
      Mg                6.589e-05   6.589e-05
      Na                1.618e-02   1.618e-02
      S(6)              2.220e-04   2.220e-04

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

                                     pH  =   7.600
                                     pe  =   4.000
      Specific Conductance (µS/cm,  95°C)  = 3703
                           Density (g/cm³)  =   0.96230
                                Volume (L)  =   1.04017
                        Activity of water  =   1.000
                  Ionic strength (mol/kgw)  =   1.405e-02
                         Mass of water (kg)  =   1.000e+00
                     Total carbon (mol/kg)  =   6.695e-03
                        Total CO2 (mol/kg)  =   6.695e-03
                          Temperature (°C)  =  95.40
                   Electrical balance (eq)  =   6.656e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  24.29
                                Iterations  =   7
                                   Total H  = 1.110187e+02
                                   Total O  = 5.552687e+01

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

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

   OH-             2.231e-05   1.936e-05    -4.651    -4.713    -0.062     -5.38
   H+              2.828e-08   2.512e-08    -7.548    -7.600    -0.052      0.00
   H2O             5.551e+01   9.995e-01     1.744    -0.000     0.000     18.74
C(4)          6.695e-03
   HCO3-           6.193e-03   5.423e-03    -2.208    -2.266    -0.058     25.13
   CO2             3.438e-04   3.449e-04    -3.464    -3.462     0.001     38.52
   NaCO3-          8.199e-05   7.135e-05    -4.086    -4.147    -0.060     -2.09
   NaHCO3          3.084e-05   3.094e-05    -4.511    -4.509     0.001      1.80
```

CO3-2	2.632e-05	1.547e-05	-4.580	-4.810	-0.231	-12.10
CaCO3	7.314e-06	7.338e-06	-5.136	-5.134	0.001	-14.44
CaHCO3+	4.807e-06	4.220e-06	-5.318	-5.375	-0.057	10.67
MgHCO3+	4.744e-06	4.127e-06	-5.324	-5.384	-0.061	5.70
MgCO3	1.413e-06	1.417e-06	-5.850	-5.849	0.001	-17.07
(CO2)2	1.037e-08	1.040e-08	-7.984	-7.983	0.001	77.04
Ca	7.493e-05					
Ca+2	6.166e-05	3.618e-05	-4.210	-4.442	-0.232	-19.03
CaCO3	7.314e-06	7.338e-06	-5.136	-5.134	0.001	-14.44
CaHCO3+	4.807e-06	4.220e-06	-5.318	-5.375	-0.057	10.67
CaSO4	1.156e-06	1.160e-06	-5.937	-5.936	0.001	8.82
CaOH+	2.745e-10	2.389e-10	-9.561	-9.622	-0.060	(0)
CaHSO4+	9.221e-13	8.025e-13	-12.035	-12.096	-0.060	(0)
Cl	3.606e-03					
Cl-	3.606e-03	3.133e-03	-2.443	-2.504	-0.061	16.65
H(0)	5.051e-27					
H2	2.525e-27	2.533e-27	-26.598	-26.596	0.001	28.57
K	7.374e-04					
K+	7.357e-04	6.388e-04	-3.133	-3.195	-0.061	10.16
KSO4-	1.629e-06	1.426e-06	-5.788	-5.846	-0.058	33.52
Mg	6.589e-05					
Mg+2	5.493e-05	3.256e-05	-4.260	-4.487	-0.227	-24.51
MgHCO3+	4.744e-06	4.127e-06	-5.324	-5.384	-0.061	5.70
MgSO4	3.879e-06	3.892e-06	-5.411	-5.410	0.001	7.16
MgCO3	1.413e-06	1.417e-06	-5.850	-5.849	0.001	-17.07
MgOH+	9.154e-07	8.053e-07	-6.038	-6.094	-0.056	(0)
Na	1.618e-02					
Na+	1.605e-02	1.401e-02	-1.794	-1.854	-0.059	0.40
NaCO3-	8.199e-05	7.135e-05	-4.086	-4.147	-0.060	-2.09
NaHCO3	3.084e-05	3.094e-05	-4.511	-4.509	0.001	1.80
NaSO4-	1.353e-05	1.185e-05	-4.869	-4.926	-0.058	7.50
NaOH	2.703e-17	2.712e-17	-16.568	-16.567	0.001	(0)
O(0)	3.102e-21					
O2	1.551e-21	1.556e-21	-20.809	-20.808	0.001	33.73
S(6)	2.220e-04					
SO4-2	2.018e-04	1.176e-04	-3.695	-3.930	-0.234	14.02
NaSO4-	1.353e-05	1.185e-05	-4.869	-4.926	-0.058	7.50
MgSO4	3.879e-06	3.892e-06	-5.411	-5.410	0.001	7.16
KSO4-	1.629e-06	1.426e-06	-5.788	-5.846	-0.058	33.52
CaSO4	1.156e-06	1.160e-06	-5.937	-5.936	0.001	8.82
HSO4-	2.120e-09	1.845e-09	-8.674	-8.734	-0.060	41.06
CaHSO4+	9.221e-13	8.025e-13	-12.035	-12.096	-0.060	(0)

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

Phase	SI**	log IAP	log K(368 K, 1 atm)	
Anhydrite	-3.18	-8.37	-5.20	CaSO4
Aragonite	-0.16	-9.25	-9.10	CaCO3
Calcite	0.26	-9.25	-9.52	CaCO3
CO2(g)	-1.50	-3.46	-1.96	CO2
Dolomite	0.73	-18.55	-19.28	CaMg(CO3)2
Gypsum	-3.55	-8.37	-4.82	CaSO4:2H2O
H2(g)	-23.49	-26.60	-3.11	H2
H2O(g)	-0.08	-0.00	0.08	H2O
Halite	-5.97	-4.36	1.62	NaCl
O2(g)	-17.69	-20.81	-3.11	O2
Sylvite	-6.88	-5.70	1.18	KCl

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

End of simulation.

Reading input data for simulation 17.

```
------------------------------------

      Solution 18 #LF18 Caldeira Asmodeu
      temp        90.8
      pH          7.2
      pe          4
      redox       pe
      units mg/l
      Alkalinity  522.3 as Ca.5CO3.5
      Cl          270.4
      S(6)        65.6
      Na          514.3
      Mg          0.4
      K           23.2
      Ca          6
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 18.

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

      Elements           Molality       Moles

      Alkalinity        5.940e-03   5.940e-03
      Ca                1.499e-04   1.499e-04
      Cl                7.638e-03   7.638e-03
      K                 5.942e-04   5.942e-04
      Mg                1.648e-05   1.648e-05
      Na                2.240e-02   2.240e-02
      S(6)              6.838e-04   6.838e-04

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

                                       pH  =   7.200
                                       pe  =   4.000
      Specific Conductance (µS/cm,  91°C)  = 5011
                           Density (g/cm³)  =   0.96569
                                Volume (L)  =   1.03685
                        Activity of water  =   0.999
                  Ionic strength (mol/kgw)  =   1.974e-02
                       Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)  =   6.633e-03
                     Total CO2 (mol/kg)  =   6.633e-03
                       Temperature (°C)  =  90.80
                   Electrical balance (eq)  =   8.384e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  22.10
                                 Iterations  =   8
                                    Total H  = 1.110183e+02
                                    Total O  = 5.552811e+01

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

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

   OH-             7.576e-06   6.439e-06    -5.121    -5.191    -0.071     -5.04
   H+              7.204e-08   6.310e-08    -7.142    -7.200    -0.058      0.00
   H2O             5.551e+01   9.994e-01     1.744    -0.000     0.000     18.67
C(4)          6.633e-03
   HCO3-           5.781e-03   4.972e-03    -2.238    -2.303    -0.065     25.37
   CO2             7.524e-04   7.558e-04    -3.124    -3.122     0.002     38.16
   NaHCO3          3.913e-05   3.931e-05    -4.407    -4.406     0.002      1.80
   NaCO3-          3.633e-05   3.101e-05    -4.440    -4.509    -0.069     -1.58
   CO3-2           1.052e-05   5.758e-06    -4.978    -5.240    -0.262    -10.81
   CaHCO3+         8.428e-06   7.273e-06    -5.074    -5.138    -0.064     10.70
```

CaCO3	4.719e-06	4.741e-06	-5.326	-5.324	0.002	-14.45
MgHCO3+	9.283e-07	7.917e-07	-6.032	-6.101	-0.069	5.80
MgCO3	1.090e-07	1.094e-07	-6.963	-6.961	0.002	-17.08
(CO2)2	4.665e-08	4.687e-08	-7.331	-7.329	0.002	76.33
Ca	1.499e-04					
Ca+2	1.304e-04	7.124e-05	-3.885	-4.147	-0.263	-18.74
CaHCO3+	8.428e-06	7.273e-06	-5.074	-5.138	-0.064	10.70
CaSO4	6.331e-06	6.360e-06	-5.199	-5.197	0.002	8.77
CaCO3	4.719e-06	4.741e-06	-5.326	-5.324	0.002	-14.45
CaOH+	2.194e-10	1.873e-10	-9.659	-9.728	-0.069	(0)
CaHSO4+	1.156e-11	9.870e-12	-10.937	-11.006	-0.069	(0)
Cl	7.638e-03					
Cl-	7.638e-03	6.503e-03	-2.117	-2.187	-0.070	16.97
H(0)	3.281e-26					
H2	1.640e-26	1.648e-26	-25.785	-25.783	0.002	28.57
K	5.942e-04					
K+	5.906e-04	5.024e-04	-3.229	-3.299	-0.070	10.16
KSO4-	3.523e-06	3.030e-06	-5.453	-5.519	-0.065	33.72
Mg	1.648e-05					
Mg+2	1.310e-05	7.251e-06	-4.883	-5.140	-0.257	-24.15
MgSO4	2.273e-06	2.283e-06	-5.643	-5.641	0.002	7.12
MgHCO3+	9.283e-07	7.917e-07	-6.032	-6.101	-0.069	5.80
MgCO3	1.090e-07	1.094e-07	-6.963	-6.961	0.002	-17.08
MgOH+	6.265e-08	5.421e-08	-7.203	-7.266	-0.063	(0)
Na	2.240e-02					
Na+	2.227e-02	1.908e-02	-1.652	-1.720	-0.067	0.38
NaSO4-	5.242e-05	4.509e-05	-4.280	-4.346	-0.065	8.53
NaHCO3	3.913e-05	3.931e-05	-4.407	-4.406	0.002	1.80
NaCO3-	3.633e-05	3.101e-05	-4.440	-4.509	-0.069	-1.58
NaOH	1.223e-17	1.228e-17	-16.913	-16.911	0.002	(0)
O(0)	7.599e-24					
O2	3.799e-24	3.817e-24	-23.420	-23.418	0.002	33.57
S(6)	6.838e-04					
SO4-2	6.193e-04	3.351e-04	-3.208	-3.475	-0.267	14.70
NaSO4-	5.242e-05	4.509e-05	-4.280	-4.346	-0.065	8.53
CaSO4	6.331e-06	6.360e-06	-5.199	-5.197	0.002	8.77
KSO4-	3.523e-06	3.030e-06	-5.453	-5.519	-0.065	33.72
MgSO4	2.273e-06	2.283e-06	-5.643	-5.641	0.002	7.12
HSO4-	1.350e-08	1.152e-08	-7.870	-7.938	-0.069	41.22
CaHSO4+	1.156e-11	9.870e-12	-10.937	-11.006	-0.069	(0)

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

Phase	SI**	log IAP	log K(363 K, 1 atm)	
Anhydrite	-2.49	-7.62	-5.13	CaSO4
Aragonite	-0.36	-9.39	-9.03	CaCO3
Calcite	0.03	-9.39	-9.42	CaCO3
CO2(g)	-1.18	-3.12	-1.95	CO2
Dolomite	-0.68	-19.77	-19.09	CaMg(CO3)2
Gypsum	-2.83	-7.62	-4.80	CaSO4:2H2O
H2(g)	-22.67	-25.78	-3.12	H2
H2O(g)	-0.15	-0.00	0.15	H2O
Halite	-5.52	-3.91	1.61	NaCl
O2(g)	-20.30	-23.42	-3.11	O2
Sylvite	-6.66	-5.49	1.17	KCl

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

End of simulation.

Reading input data for simulation 18.

```
      Solution 19 #LF19 Caldeira Grande
      temp        89.5
      pH          7.9
      pe          -2.432
      redox       pe
      units mg/l
      Alkalinity  610.8 as Ca.5CO3.5
      Cl          253.8
      S(6)        32.5
      Na          458.6
      Mg          0.3
      K           20.2
      Ca          3.5
      Si          306.88 as SiO2
      Al          0.2304
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 19.

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

      Elements           Molality       Moles

      Al                8.554e-06   8.554e-06
      Alkalinity        6.949e-03   6.949e-03
      Ca                8.747e-05   8.747e-05
      Cl                7.171e-03   7.171e-03
      K                 5.175e-04   5.175e-04
      Mg                1.236e-05   1.236e-05
      Na                1.998e-02   1.998e-02
      S(6)              3.389e-04   3.389e-04
      Si                5.116e-03   5.116e-03

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

                                       pH  =   7.900
                                       pe  =  -2.432
      Specific Conductance (µS/cm,  90°C)  = 4521
                           Density (g/cm³)  =   0.96674
                                Volume (L)  =   1.03612
                        Activity of water  =   0.999
                  Ionic strength (mol/kgw)  =   1.791e-02
                         Mass of water (kg)  =   1.000e+00
                     Total carbon (mol/kg)  =   6.498e-03
                        Total CO2 (mol/kg)  =   6.498e-03
                          Temperature (°C)  =  89.50
                   Electrical balance (eq)  =   5.927e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  16.96
                                 Iterations  =   7
                                    Total H  = 1.110388e+02
                                    Total O  = 5.554744e+01

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

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

   OH-             3.578e-05   3.063e-05    -4.446    -4.514    -0.067     -4.98
   H+              1.431e-08   1.259e-08    -7.845    -7.900    -0.055      0.00
   H2O             5.551e+01   9.993e-01     1.744    -0.000     0.000     18.66
Al            8.554e-06
   Al(OH)4-        8.545e-06   7.359e-06    -5.068    -5.133    -0.065       (0)
   Al(OH)3         8.271e-09   8.305e-09    -8.082    -8.081     0.002       (0)
   Al(OH)2+        3.837e-11   3.320e-11   -10.416   -10.479    -0.063       (0)
   AlOH+2          1.962e-15   1.101e-15   -14.707   -14.958    -0.251    -30.48
```

Al+3	1.082e-19	3.426e-20	-18.966	-19.465	-0.499	-46.99
AlSO4+	4.317e-20	3.718e-20	-19.365	-19.430	-0.065	(0)
Al(SO4)2-	3.014e-22	2.595e-22	-21.521	-21.586	-0.065	(0)
AlHSO4+2	2.065e-28	1.126e-28	-27.685	-27.948	-0.263	(0)
C(4)	6.498e-03					
HCO3-	6.067e-03	5.250e-03	-2.217	-2.280	-0.063	25.40
NaCO3-	1.639e-04	1.408e-04	-3.785	-3.851	-0.066	-1.48
CO2	1.565e-04	1.571e-04	-3.805	-3.804	0.002	38.07
CO3-2	5.458e-05	3.061e-05	-4.263	-4.514	-0.251	-10.55
NaHCO3	3.709e-05	3.724e-05	-4.431	-4.429	0.002	1.80
CaCO3	1.295e-05	1.300e-05	-4.888	-4.886	0.002	-14.46
CaHCO3+	4.679e-06	4.062e-06	-5.330	-5.391	-0.061	10.69
MgHCO3+	7.507e-07	6.446e-07	-6.125	-6.191	-0.066	5.80
MgCO3	4.457e-07	4.475e-07	-6.351	-6.349	0.002	-17.08
(CO2)2	1.980e-09	1.988e-09	-8.703	-8.702	0.002	76.13
Ca	8.747e-05					
Ca+2	6.811e-05	3.813e-05	-4.167	-4.419	-0.252	-18.73
CaCO3	1.295e-05	1.300e-05	-4.888	-4.886	0.002	-14.46
CaHCO3+	4.679e-06	4.062e-06	-5.330	-5.391	-0.061	10.69
CaSO4	1.735e-06	1.742e-06	-5.761	-5.759	0.002	8.76
CaOH+	5.846e-10	5.023e-10	-9.233	-9.299	-0.066	(0)
CaHSO4+	6.081e-13	5.225e-13	-12.216	-12.282	-0.066	(0)
Cl	7.171e-03					
Cl-	7.171e-03	6.148e-03	-2.144	-2.211	-0.067	17.03
H(0)	9.637e-15					
H2	4.818e-15	4.838e-15	-14.317	-14.315	0.002	28.57
K	5.175e-04					
K+	5.159e-04	4.419e-04	-3.287	-3.355	-0.067	10.14
KSO4-	1.562e-06	1.352e-06	-5.806	-5.869	-0.063	33.76
Mg	1.236e-05					
Mg+2	1.004e-05	5.689e-06	-4.998	-5.245	-0.247	-24.11
MgSO4	8.983e-07	9.020e-07	-6.047	-6.045	0.002	7.10
MgHCO3+	7.507e-07	6.446e-07	-6.125	-6.191	-0.066	5.80
MgCO3	4.457e-07	4.475e-07	-6.351	-6.349	0.002	-17.08
MgOH+	2.263e-07	1.970e-07	-6.645	-6.706	-0.060	(0)
Na	1.998e-02					
Na+	1.976e-02	1.703e-02	-1.704	-1.769	-0.065	0.36
NaCO3-	1.639e-04	1.408e-04	-3.785	-3.851	-0.066	-1.48
NaHCO3	3.709e-05	3.724e-05	-4.431	-4.429	0.002	1.80
NaSO4-	2.382e-05	2.062e-05	-4.623	-4.686	-0.063	8.66
NaOH	5.195e-17	5.216e-17	-16.284	-16.283	0.002	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-46.638	-46.636	0.002	33.52
S(6)	3.389e-04					
SO4-2	3.109e-04	1.726e-04	-3.507	-3.763	-0.256	14.78
NaSO4-	2.382e-05	2.062e-05	-4.623	-4.686	-0.063	8.66
CaSO4	1.735e-06	1.742e-06	-5.761	-5.759	0.002	8.76
KSO4-	1.562e-06	1.352e-06	-5.806	-5.869	-0.063	33.76
MgSO4	8.983e-07	9.020e-07	-6.047	-6.045	0.002	7.10
HSO4-	1.326e-09	1.140e-09	-8.877	-8.943	-0.066	41.24
CaHSO4+	6.081e-13	5.225e-13	-12.216	-12.282	-0.066	(0)
AlSO4+	4.317e-20	3.718e-20	-19.365	-19.430	-0.065	(0)
Al(SO4)2-	3.014e-22	2.595e-22	-21.521	-21.586	-0.065	(0)
AlHSO4+2	2.065e-28	1.126e-28	-27.685	-27.948	-0.263	(0)
Si	5.116e-03					
H4SiO4	4.811e-03	4.831e-03	-2.318	-2.316	0.002	49.10
H3SiO4-	3.053e-04	2.621e-04	-3.515	-3.581	-0.066	27.11
H2SiO4-2	4.468e-08	2.506e-08	-7.350	-7.601	-0.251	(0)

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

Phase	SI**	log IAP	log K(362 K, 1 atm)	
Al(OH)3(a)	-3.11	4.23	7.35	Al(OH)3
Albite	0.78	-13.85	-14.63	NaAlSi3O8
Alunite	-13.93	-21.88	-7.95	KAl3(SO4)2(OH)6
Anhydrite	-3.07	-8.18	-5.11	CaSO4
Anorthite	-1.11	-19.31	-18.20	CaAl2Si2O8

Aragonite	0.08	-8.93	-9.01	CaCO3
Ca-Montmorillonite	0.43	-36.99	-37.42	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	0.46	-8.93	-9.40	CaCO3
Chalcedony	0.62	-2.32	-2.94	SiO2
Chlorite(14A)	5.66	54.30	48.63	Mg5Al2Si3O10(OH)8
Chrysotile	1.45	27.03	25.58	Mg3Si2O5(OH)4
CO2(g)	-1.86	-3.80	-1.94	CO2
Dolomite	0.34	-18.69	-19.04	CaMg(CO3)2
Gibbsite	-0.90	4.23	5.14	Al(OH)3
Gypsum	-3.39	-8.18	-4.79	CaSO4:2H2O
H2(g)	-11.20	-14.32	-3.12	H2
H2O(g)	-0.17	-0.00	0.17	H2O
Halite	-5.59	-3.98	1.61	NaCl
Illite	0.42	-32.71	-33.14	K0.6Mg0.25Al2.3Si3.5O10(OH)2
K-feldspar	1.12	-15.43	-16.56	KAlSi3O8
K-mica	5.34	10.30	4.96	KAl3Si3O10(OH)2
Kaolinite	1.00	3.84	2.83	Al2Si2O5(OH)4
O2(g)	-43.52	-46.64	-3.11	O2
Quartz	0.88	-2.32	-3.20	SiO2
Sepiolite	-0.20	14.16	14.37	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-4.50	14.16	18.66	Mg2Si3O7.5OH:3H2O
SiO2(a)	-0.04	-2.32	-2.28	SiO2
Sylvite	-6.73	-5.57	1.16	KCl
Talc	7.05	22.40	15.36	Mg3Si4O10(OH)2

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

End of simulation.

Reading input data for simulation 19.

```
      Solution 20 #LF20 Água Padre José
      temp        62.3
      pH          6.1
      pe          4
      redox       pe
      units mg/l
      Alkalinity  311.1 as Ca.5CO3.5
      Cl          39.2
      S(6)        20.3
      Na          121.6
      Mg          5.5
      K           40.2
      Ca          14.7
      END
```

Beginning of initial solution calculations.

Initial solution 20.

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

Elements	Molality	Moles
Alkalinity	3.535e-03	3.535e-03
Ca	3.670e-04	3.670e-04
Cl	1.106e-03	1.106e-03
K	1.029e-03	1.029e-03
Mg	2.264e-04	2.264e-04
Na	5.292e-03	5.292e-03
S(6)	2.114e-04	2.114e-04

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

pH	= 6.100
pe	= 4.000
Specific Conductance (µS/cm, 62°C)	= 1174
Density (g/cm³)	= 0.98237
Volume (L)	= 1.01863
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 6.957e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 8.522e-03
Total CO2 (mol/kg)	= 8.522e-03
Temperature (°C)	= 62.30
Electrical balance (eq)	= 2.443e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 19.65
Iterations	= 8
Total H	= 1.110160e+02
Total O	= 5.552764e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	8.641e-07	7.943e-07	-6.063	-6.100	-0.037	0.00
OH-	1.512e-07	1.374e-07	-6.820	-6.862	-0.042	-3.93
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.35
C(4)	8.522e-03					
CO2	4.985e-03	4.993e-03	-2.302	-2.302	0.001	36.32
HCO3-	3.504e-03	3.198e-03	-2.455	-2.495	-0.040	25.85
CaHCO3+	1.433e-05	1.310e-05	-4.844	-4.883	-0.039	10.51
MgHCO3+	7.939e-06	7.221e-06	-5.100	-5.141	-0.041	5.94
NaHCO3	7.159e-06	7.170e-06	-5.145	-5.144	0.001	1.80
(CO2)2	1.237e-06	1.239e-06	-5.908	-5.907	0.001	72.64
CO3-2	4.217e-07	2.924e-07	-6.375	-6.534	-0.159	-6.16
CaCO3	3.359e-07	3.364e-07	-6.474	-6.473	0.001	-14.51
NaCO3-	1.532e-07	1.394e-07	-6.815	-6.856	-0.041	-0.06
MgCO3	7.152e-08	7.164e-08	-7.146	-7.145	0.001	-17.09
Ca	3.670e-04					
Ca+2	3.452e-04	2.391e-04	-3.462	-3.621	-0.159	-18.19
CaHCO3+	1.433e-05	1.310e-05	-4.844	-4.883	-0.039	10.51
CaSO4	7.070e-06	7.082e-06	-5.151	-5.150	0.001	8.41
CaCO3	3.359e-07	3.364e-07	-6.474	-6.473	0.001	-14.51
CaHSO4+	7.939e-11	7.222e-11	-10.100	-10.141	-0.041	(0)
CaOH+	5.490e-11	4.995e-11	-10.260	-10.301	-0.041	(0)
Cl	1.106e-03					
Cl-	1.106e-03	1.006e-03	-2.956	-2.998	-0.041	18.07
H(0)	6.412e-24					
H2	3.206e-24	3.211e-24	-23.494	-23.493	0.001	28.58
K	1.029e-03					
K+	1.027e-03	9.332e-04	-2.988	-3.030	-0.042	9.81
KSO4-	1.664e-06	1.519e-06	-5.779	-5.819	-0.040	34.29
Mg	2.264e-04					
Mg+2	2.080e-04	1.448e-04	-3.682	-3.839	-0.157	-23.06
MgSO4	1.034e-05	1.035e-05	-4.986	-4.985	0.001	6.75
MgHCO3+	7.939e-06	7.221e-06	-5.100	-5.141	-0.041	5.94
MgCO3	7.152e-08	7.164e-08	-7.146	-7.145	0.001	-17.09
MgOH+	1.444e-08	1.321e-08	-7.840	-7.879	-0.039	(0)
Na	5.292e-03					
Na+	5.281e-03	4.810e-03	-2.277	-2.318	-0.041	-0.16
NaHCO3	7.159e-06	7.170e-06	-5.145	-5.144	0.001	1.80
NaSO4-	4.234e-06	3.863e-06	-5.373	-5.413	-0.040	11.67
NaCO3-	1.532e-07	1.394e-07	-6.815	-6.856	-0.041	-0.06
NaOH	6.599e-20	6.609e-20	-19.181	-19.180	0.001	(0)
O(0)	4.036e-35					
O2	2.018e-35	2.021e-35	-34.695	-34.694	0.001	32.48
S(6)	2.114e-04					
SO4-2	1.881e-04	1.299e-04	-3.726	-3.887	-0.161	16.21

MgSO4	1.034e-05	1.035e-05	-4.986	-4.985	0.001	6.75
CaSO4	7.070e-06	7.082e-06	-5.151	-5.150	0.001	8.41
NaSO4-	4.234e-06	3.863e-06	-5.373	-5.413	-0.040	11.67
KSO4-	1.664e-06	1.519e-06	-5.779	-5.819	-0.040	34.29
HSO4-	2.761e-08	2.512e-08	-7.559	-7.600	-0.041	41.46
CaHSO4+	7.939e-11	7.222e-11	-10.100	-10.141	-0.041	(0)

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

Phase	SI**	log IAP	log K(335 K, 1 atm)	
Anhydrite	-2.77	-7.51	-4.74	CaSO4
Aragonite	-1.49	-10.16	-8.66	CaCO3
Calcite	-1.24	-10.16	-8.91	CaCO3
CO2(g)	-0.50	-2.30	-1.80	CO2
Dolomite	-2.50	-20.53	-18.03	CaMg(CO3)2
Gypsum	-2.85	-7.51	-4.66	CaSO4:2H2O
H2(g)	-20.35	-23.49	-3.14	H2
H2O(g)	-0.66	-0.00	0.66	H2O
Halite	-6.91	-5.32	1.60	NaCl
O2(g)	-31.62	-34.69	-3.07	O2
Sylvite	-7.09	-6.03	1.07	KCl

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

End of simulation.

Reading input data for simulation 20.

End of Run after 0.326 Seconds.

```
   Input file: F:\Doutoramento\artigos originais\Furnas springs - modelling\Phreeqc
\Especiação\Speciation3_L.pqi
  Output file: F:\Doutoramento\artigos originais\Furnas springs - modelling\Phreeqc
\Especiação\Speciation3_L.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
      Solution 21 #LF21 Poça da Dona Beija
      temp  38.9
      pH    5.8
      pe    4
      redox pe
      units mg/l
      Alkalinity  169 as Ca.5CO3.5
      Cl    67.5
      S(6)  11.8
      Na    75
      Mg    6.2
      K     16.8
      Ca    11.7
      END
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 21.

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

      Elements           Molality       Moles

      Alkalinity        1.920e-03   1.920e-03
      Ca                2.920e-04   2.920e-04
      Cl                1.905e-03   1.905e-03
      K                 4.298e-04   4.298e-04
      Mg                2.551e-04   2.551e-04
      Na                3.263e-03   3.263e-03
      S(6)              1.229e-04   1.229e-04

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

                                       pH  =   5.800
                                       pe  =   4.000
      Specific Conductance (µS/cm,  39°C)  = 616
                           Density (g/cm³)  =   0.99291
                                Volume (L)  =   1.00770
                        Activity of water  =   1.000
                  Ionic strength (mol/kgw)  =   5.040e-03
                       Mass of water (kg)  =   1.000e+00
```

```
                  Total carbon (mol/kg)  =   7.509e-03
                     Total CO2 (mol/kg)  =   7.509e-03
                       Temperature (°C)  =  38.90
                 Electrical balance (eq) =   7.171e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|) =   8.15
                               Iterations =   7
                                  Total H  = 1.110144e+02
                                  Total O  = 5.552365e+01
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.701e-06	1.585e-06	-5.769	-5.800	-0.031	0.00
OH-	1.859e-08	1.718e-08	-7.731	-7.765	-0.034	-3.75
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.15
C(4)	7.509e-03					
CO2	5.586e-03	5.592e-03	-2.253	-2.252	0.001	35.11
HCO3-	1.908e-03	1.769e-03	-2.719	-2.752	-0.033	25.47
CaHCO3+	5.946e-06	5.517e-06	-5.226	-5.258	-0.033	10.12
MgHCO3+	4.413e-06	4.081e-06	-5.355	-5.389	-0.034	5.79
NaHCO3	2.781e-06	2.784e-06	-5.556	-5.555	0.001	1.80
(CO2)2	8.758e-07	8.769e-07	-6.058	-6.057	0.001	70.21
CO3-2	8.943e-08	6.602e-08	-7.049	-7.180	-0.132	-4.70
CaCO3	3.234e-08	3.238e-08	-7.490	-7.490	0.001	-14.56
MgCO3	1.417e-08	1.419e-08	-7.849	-7.848	0.001	-17.10
NaCO3-	7.837e-09	7.248e-09	-8.106	-8.140	-0.034	-0.13
Ca	2.920e-04					
Ca+2	2.826e-04	2.085e-04	-3.549	-3.681	-0.132	-17.97
CaHCO3+	5.946e-06	5.517e-06	-5.226	-5.258	-0.033	10.12
CaSO4	3.394e-06	3.398e-06	-5.469	-5.469	0.001	7.93
CaCO3	3.234e-08	3.238e-08	-7.490	-7.490	0.001	-14.56
CaHSO4+	4.768e-11	4.410e-11	-10.322	-10.356	-0.034	(0)
CaOH+	2.360e-11	2.183e-11	-10.627	-10.661	-0.034	(0)
Cl	1.905e-03					
Cl-	1.905e-03	1.761e-03	-2.720	-2.754	-0.034	18.32
H(0)	3.112e-23					
H2	1.556e-23	1.558e-23	-22.808	-22.807	0.001	28.59
K	4.298e-04					
K+	4.295e-04	3.969e-04	-3.367	-3.401	-0.034	9.41
KSO4-	3.147e-07	2.917e-07	-6.502	-6.535	-0.033	34.36
Mg	2.551e-04					
Mg+2	2.457e-04	1.819e-04	-3.610	-3.740	-0.131	-22.20
MgSO4	4.975e-06	4.980e-06	-5.303	-5.303	0.001	6.27
MgHCO3+	4.413e-06	4.081e-06	-5.355	-5.389	-0.034	5.79
MgCO3	1.417e-08	1.419e-08	-7.849	-7.848	0.001	-17.10
MgOH+	1.489e-09	1.382e-09	-8.827	-8.859	-0.032	(0)
Na	3.263e-03					
Na+	3.259e-03	3.017e-03	-2.487	-2.520	-0.033	-0.82
NaHCO3	2.781e-06	2.784e-06	-5.556	-5.555	0.001	1.80
NaSO4-	1.472e-06	1.365e-06	-5.832	-5.865	-0.033	13.44
NaCO3-	7.837e-09	7.248e-09	-8.106	-8.140	-0.034	-0.13
NaOH	5.177e-21	5.183e-21	-20.286	-20.285	0.001	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-42.480	-42.479	0.001	31.34
S(6)	1.229e-04					
SO4-2	1.127e-04	8.295e-05	-3.948	-4.081	-0.133	15.89
MgSO4	4.975e-06	4.980e-06	-5.303	-5.303	0.001	6.27
CaSO4	3.394e-06	3.398e-06	-5.469	-5.469	0.001	7.93
NaSO4-	1.472e-06	1.365e-06	-5.832	-5.865	-0.033	13.44
KSO4-	3.147e-07	2.917e-07	-6.502	-6.535	-0.033	34.36
HSO4-	1.902e-08	1.759e-08	-7.721	-7.755	-0.034	41.01
CaHSO4+	4.768e-11	4.410e-11	-10.322	-10.356	-0.034	(0)

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

Phase	SI**	log IAP	log K(312 K, 1 atm)

```
  Anhydrite        -3.32     -7.76   -4.44  CaSO4
  Aragonite        -2.42    -10.86   -8.44  CaCO3
  Calcite          -2.26    -10.86   -8.60  CaCO3
  CO2(g)           -0.64     -2.25   -1.61  CO2
  Dolomite         -4.41    -21.78  -17.37  CaMg(CO3)2
  Gypsum           -3.17     -7.76   -4.59  CaSO4:2H2O
  H2(g)           -19.68    -22.81   -3.13  H2
  H2O(g)           -1.16     -0.00    1.16  H2O
  Halite           -6.86     -5.27    1.58  NaCl
  O2(g)           -39.50    -42.48   -2.98  O2
  Sylvite          -7.12     -6.16    0.97  KCl

**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.
-----------------------------------

      Solution 22 #LF22 Dr. Bruno
      temp  19.8
      pH    6.1
      pe    4
      redox pe
      units mg/l
      Alkalinity  214.1 as Ca.5CO3.5
      Cl    27.6
      S(6)  5.7
      Na    63.8
      Mg    8.4
      K     19
      Ca    19.4
      END
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 22.

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

      Elements           Molality       Moles

      Alkalinity        2.432e-03   2.432e-03
      Ca                4.842e-04   4.842e-04
      Cl                7.788e-04   7.788e-04
      K                 4.861e-04   4.861e-04
      Mg                3.456e-04   3.456e-04
      Na                2.776e-03   2.776e-03
      S(6)              5.936e-05   5.936e-05

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

                                       pH  =   6.100
                                       pe  =   4.000
      Specific Conductance (µS/cm,  20°C)  = 366
                           Density (g/cm³)  =   0.99852
                                Volume (L)  =   1.00196
                        Activity of water  =   1.000
                  Ionic strength (mol/kgw)  =   4.959e-03
                       Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)  =   6.735e-03
                     Total CO2 (mol/kg)  =   6.735e-03
```

Temperature (°C) = 19.80
Electrical balance (eq) = 1.592e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 19.43
Iterations = 8
Total H = 1.110149e+02
Total O = 5.552236e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	8.501e-07	7.943e-07	-6.071	-6.100	-0.029	0.00
OH-	9.147e-09	8.479e-09	-8.039	-8.072	-0.033	-4.30
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.05
C(4)	6.735e-03					
CO2	4.301e-03	4.306e-03	-2.366	-2.366	0.000	34.18
HCO3-	2.413e-03	2.243e-03	-2.618	-2.649	-0.032	24.30
CaHCO3+	9.914e-06	9.225e-06	-5.004	-5.035	-0.031	9.49
MgHCO3+	6.990e-06	6.484e-06	-5.156	-5.188	-0.033	5.35
NaHCO3	3.342e-06	3.346e-06	-5.476	-5.475	0.000	1.80
(CO2)2	2.849e-07	2.852e-07	-6.545	-6.545	0.000	68.35
CO3-2	1.584e-07	1.184e-07	-6.800	-6.927	-0.127	-5.62
CaCO3	6.368e-08	6.375e-08	-7.196	-7.196	0.000	-14.62
MgCO3	2.626e-08	2.629e-08	-7.581	-7.580	0.000	-17.08
NaCO3-	4.683e-09	4.345e-09	-8.329	-8.362	-0.033	-1.51
Ca	4.842e-04					
Ca+2	4.718e-04	3.523e-04	-3.326	-3.453	-0.127	-18.09
CaHCO3+	9.914e-06	9.225e-06	-5.004	-5.035	-0.031	9.49
CaSO4	2.427e-06	2.430e-06	-5.615	-5.614	0.000	7.29
CaCO3	6.368e-08	6.375e-08	-7.196	-7.196	0.000	-14.62
CaOH+	7.931e-11	7.359e-11	-10.101	-10.133	-0.033	(0)
CaHSO4+	1.273e-11	1.181e-11	-10.895	-10.928	-0.033	(0)
Cl	7.788e-04					
Cl-	7.788e-04	7.222e-04	-3.109	-3.141	-0.033	17.93
H(0)	9.406e-24					
H2	4.703e-24	4.709e-24	-23.328	-23.327	0.000	28.61
K	4.861e-04					
K+	4.860e-04	4.505e-04	-3.313	-3.346	-0.033	8.86
KSO4-	1.253e-07	1.165e-07	-6.902	-6.934	-0.032	33.99
Mg	3.456e-04					
Mg+2	3.365e-04	2.521e-04	-3.473	-3.598	-0.125	-21.51
MgHCO3+	6.990e-06	6.484e-06	-5.156	-5.188	-0.033	5.35
MgSO4	2.079e-06	2.082e-06	-5.682	-5.682	0.000	5.62
MgCO3	2.626e-08	2.629e-08	-7.581	-7.580	0.000	-17.08
MgOH+	7.673e-10	7.145e-10	-9.115	-9.146	-0.031	(0)
Na	2.776e-03					
Na+	2.772e-03	2.575e-03	-2.557	-2.589	-0.032	-1.72
NaHCO3	3.342e-06	3.346e-06	-5.476	-5.475	0.000	1.80
NaSO4-	5.417e-07	5.036e-07	-6.266	-6.298	-0.032	14.20
NaCO3-	4.683e-09	4.345e-09	-8.329	-8.362	-0.033	-1.51
NaOH	2.180e-21	2.183e-21	-20.661	-20.661	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-47.434	-47.434	0.000	29.97
S(6)	5.936e-05					
SO4-2	5.418e-05	4.036e-05	-4.266	-4.394	-0.128	13.90
CaSO4	2.427e-06	2.430e-06	-5.615	-5.614	0.000	7.29
MgSO4	2.079e-06	2.082e-06	-5.682	-5.682	0.000	5.62
NaSO4-	5.417e-07	5.036e-07	-6.266	-6.298	-0.032	14.20
KSO4-	1.253e-07	1.165e-07	-6.902	-6.934	-0.032	33.99
HSO4-	3.006e-09	2.789e-09	-8.522	-8.554	-0.033	39.93
CaHSO4+	1.273e-11	1.181e-11	-10.895	-10.928	-0.033	(0)

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

Phase	SI**	log IAP	log K(292 K, 1 atm)	
Anhydrite	-3.63	-7.85	-4.22	CaSO4

Aragonite	-2.08	-10.38	-8.30	CaCO3
Calcite	-1.93	-10.38	-8.45	CaCO3
CO2(g)	-0.96	-2.37	-1.40	CO2
Dolomite	-3.90	-20.90	-17.00	CaMg(CO3)2
Gypsum	-3.26	-7.85	-4.58	CaSO4:2H2O
H2(g)	-20.24	-23.33	-3.09	H2
H2O(g)	-1.64	-0.00	1.64	H2O
Halite	-7.30	-5.73	1.57	NaCl
O2(g)	-44.58	-47.43	-2.85	O2
Sylvite	-7.36	-6.49	0.87	KCl

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

End of simulation.

Reading input data for simulation 3.

```
Solution 23 #LF23 Banhos Férreos I
temp  37.5
pH    6.2
pe    4
redox pe
units mg/l
Alkalinity  880.9 as Ca.5CO3.5
Cl    56.7
S(6)  21.1
Na    275.9
Mg    36.2
K     46.8
Ca    53
END
```

Beginning of initial solution calculations.

Initial solution 23.

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

Elements	Molality	Moles
Alkalinity	1.002e-02	1.002e-02
Ca	1.324e-03	1.324e-03
Cl	1.601e-03	1.601e-03
K	1.199e-03	1.199e-03
Mg	1.491e-03	1.491e-03
Na	1.202e-02	1.202e-02
S(6)	2.199e-04	2.199e-04

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

pH	=	6.200
pe	=	4.000
Specific Conductance (µS/cm, 38°C)	=	1777
Density (g/cm³)	=	0.99411
Volume (L)	=	1.00752
Activity of water	=	0.999
Ionic strength (mol/kgw)	=	1.785e-02
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	2.086e-02
Total CO2 (mol/kg)	=	2.086e-02
Temperature (°C)	=	37.50
Electrical balance (eq)	=	6.787e-03

Percent error, 100*(Cat-|An|)/(Cat+|An|) = 22.46
Iterations = 9
Total H = 1.110224e+02
Total O = 5.555882e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	7.077e-07	6.310e-07	-6.150	-6.200	-0.050	0.00
OH-	4.513e-08	3.927e-08	-7.346	-7.406	-0.060	-3.68
H2O	5.551e+01	9.993e-01	1.744	-0.000	0.000	18.14
C(4)	2.086e-02					
CO2	1.084e-02	1.088e-02	-1.965	-1.963	0.002	35.04
HCO3-	9.760e-03	8.574e-03	-2.011	-2.067	-0.056	25.51
CaHCO3+	1.032e-04	9.091e-05	-3.986	-4.041	-0.055	10.13
MgHCO3+	1.012e-04	8.827e-05	-3.995	-4.054	-0.059	5.82
NaHCO3	4.701e-05	4.720e-05	-4.328	-4.326	0.002	1.80
(CO2)2	3.177e-06	3.190e-06	-5.498	-5.496	0.002	70.08
CO3-2	1.324e-06	7.885e-07	-5.878	-6.103	-0.225	-4.43
CaCO3	1.275e-06	1.281e-06	-5.894	-5.893	0.002	-14.56
MgCO3	7.442e-07	7.473e-07	-6.128	-6.126	0.002	-17.09
NaCO3-	3.225e-07	2.818e-07	-6.491	-6.550	-0.059	-0.05
Ca	1.324e-03					
Ca+2	1.206e-03	7.175e-04	-2.919	-3.144	-0.225	-17.76
CaHCO3+	1.032e-04	9.091e-05	-3.986	-4.041	-0.055	10.13
CaSO4	1.410e-05	1.415e-05	-4.851	-4.849	0.002	7.90
CaCO3	1.275e-06	1.281e-06	-5.894	-5.893	0.002	-14.56
CaOH+	2.159e-10	1.886e-10	-9.666	-9.724	-0.059	(0)
CaHSO4+	8.174e-11	7.141e-11	-10.088	-10.146	-0.059	(0)
Cl	1.601e-03					
Cl-	1.601e-03	1.396e-03	-2.795	-2.855	-0.060	18.38
H(0)	4.982e-24					
H2	2.491e-24	2.501e-24	-23.604	-23.602	0.002	28.60
K	1.199e-03					
K+	1.197e-03	1.043e-03	-2.922	-2.982	-0.060	9.44
KSO4-	1.043e-06	9.159e-07	-5.982	-6.038	-0.056	34.41
Mg	1.491e-03					
Mg+2	1.363e-03	8.197e-04	-2.866	-3.086	-0.221	-21.95
MgHCO3+	1.012e-04	8.827e-05	-3.995	-4.054	-0.059	5.82
MgSO4	2.643e-05	2.654e-05	-4.578	-4.576	0.002	6.24
MgCO3	7.442e-07	7.473e-07	-6.128	-6.126	0.002	-17.09
MgOH+	1.578e-08	1.393e-08	-7.802	-7.856	-0.054	(0)
Na	1.202e-02					
Na+	1.196e-02	1.048e-02	-1.922	-1.980	-0.058	-0.78
NaHCO3	4.701e-05	4.720e-05	-4.328	-4.326	0.002	1.80
NaSO4-	6.540e-06	5.746e-06	-5.184	-5.241	-0.056	14.10
NaCO3-	3.225e-07	2.818e-07	-6.491	-6.550	-0.059	-0.05
NaOH	4.098e-20	4.115e-20	-19.387	-19.386	0.002	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-41.307	-41.305	0.002	31.25
S(6)	2.199e-04					
SO4-2	1.718e-04	1.014e-04	-3.765	-3.994	-0.229	16.07
MgSO4	2.643e-05	2.654e-05	-4.578	-4.576	0.002	6.24
CaSO4	1.410e-05	1.415e-05	-4.851	-4.849	0.002	7.90
NaSO4-	6.540e-06	5.746e-06	-5.184	-5.241	-0.056	14.10
KSO4-	1.043e-06	9.159e-07	-5.982	-6.038	-0.056	34.41
HSO4-	9.476e-09	8.278e-09	-8.023	-8.082	-0.059	41.02
CaHSO4+	8.174e-11	7.141e-11	-10.088	-10.146	-0.059	(0)

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

Phase	SI**	log IAP	log K(310 K, 1 atm)	
Anhydrite	-2.72	-7.14	-4.42	CaSO4
Aragonite	-0.82	-9.25	-8.43	CaCO3
Calcite	-0.66	-9.25	-8.59	CaCO3

```
  CO2(g)           -0.36     -1.96   -1.60  CO2
  Dolomite         -1.10    -18.44  -17.34  CaMg(CO3)2
  Gypsum           -2.55     -7.14   -4.59  CaSO4:2H2O
  H2(g)           -20.48    -23.60   -3.12  H2
  H2O(g)           -1.20     -0.00    1.20  H2O
  Halite           -6.41     -4.83    1.58  NaCl
  O2(g)           -38.33    -41.31   -2.97  O2
  Sylvite          -6.80     -5.84    0.96  KCl

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

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

-----------------------------------
Reading input data for simulation 4.
-----------------------------------

      Solution 24 #LF24 Banhos Férreos II
      temp  32.6
      pH    6.5
      pe    4
      redox pe
      units mg/l
      Alkalinity  829   as Ca.5CO3.5
      Cl    81.7
      S(6)  46.1
      Na    264.7
      Mg    35.3
      K     48.5
      Ca    56.2
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 24.

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

      Elements           Molality       Moles

      Alkalinity        9.428e-03   9.428e-03
      Ca                1.404e-03   1.404e-03
      Cl                2.308e-03   2.308e-03
      K                 1.242e-03   1.242e-03
      Mg                1.454e-03   1.454e-03
      Na                1.153e-02   1.153e-02
      S(6)              4.805e-04   4.805e-04

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

                                       pH  =   6.500
                                       pe  =   4.000
      Specific Conductance (µS/cm,  33°C)  = 1664
                           Density (g/cm³)  =   0.99575
                                Volume (L)  =   1.00561
                        Activity of water  =   0.999
                  Ionic strength (mol/kgw)  =   1.814e-02
                       Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)  =   1.471e-02
                     Total CO2 (mol/kg)  =   1.471e-02
                       Temperature (°C)  =  32.60
                   Electrical balance (eq)  =   5.791e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  19.08
                                 Iterations  =   8
```

Total H = 1.110219e+02
Total O = 5.554699e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	3.546e-07	3.162e-07	-6.450	-6.500	-0.050	0.00
OH-	6.421e-08	5.589e-08	-7.192	-7.253	-0.060	-3.76
H2O	5.551e+01	9.994e-01	1.744	-0.000	0.000	18.11
C(4)	1.471e-02					
HCO3-	9.186e-03	8.072e-03	-2.037	-2.093	-0.056	25.29
CO2	5.290e-03	5.313e-03	-2.277	-2.275	0.002	34.80
CaHCO3+	9.778e-05	8.615e-05	-4.010	-4.065	-0.055	10.00
MgHCO3+	8.904e-05	7.771e-05	-4.050	-4.110	-0.059	5.73
NaHCO3	4.356e-05	4.374e-05	-4.361	-4.359	0.002	1.80
CO3-2	2.306e-06	1.375e-06	-5.637	-5.862	-0.225	-4.49
CaCO3	2.069e-06	2.077e-06	-5.684	-5.682	0.002	-14.58
MgCO3	1.161e-06	1.166e-06	-5.935	-5.933	0.002	-17.09
(CO2)2	6.559e-07	6.587e-07	-6.183	-6.181	0.002	69.60
NaCO3-	4.279e-07	3.739e-07	-6.369	-6.427	-0.059	-0.29
Ca	1.404e-03					
Ca+2	1.272e-03	7.580e-04	-2.895	-3.120	-0.225	-17.77
CaHCO3+	9.778e-05	8.615e-05	-4.010	-4.065	-0.055	10.00
CaSO4	3.204e-05	3.217e-05	-4.494	-4.492	0.002	7.76
CaCO3	2.069e-06	2.077e-06	-5.684	-5.682	0.002	-14.58
CaOH+	4.549e-10	3.976e-10	-9.342	-9.401	-0.059	(0)
CaHSO4+	8.587e-11	7.504e-11	-10.066	-10.125	-0.059	(0)
Cl	2.308e-03					
Cl-	2.308e-03	2.011e-03	-2.637	-2.696	-0.060	18.33
H(0)	1.310e-24					
H2	6.548e-25	6.576e-25	-24.184	-24.182	0.002	28.60
K	1.242e-03					
K+	1.240e-03	1.080e-03	-2.907	-2.967	-0.060	9.32
KSO4-	2.219e-06	1.950e-06	-5.654	-5.710	-0.056	34.35
Mg	1.454e-03					
Mg+2	1.313e-03	7.909e-04	-2.882	-3.102	-0.220	-21.78
MgHCO3+	8.904e-05	7.771e-05	-4.050	-4.110	-0.059	5.73
MgSO4	5.046e-05	5.067e-05	-4.297	-4.295	0.002	6.09
MgCO3	1.161e-06	1.166e-06	-5.935	-5.933	0.002	-17.09
MgOH+	2.007e-08	1.772e-08	-7.697	-7.751	-0.054	(0)
Na	1.153e-02					
Na+	1.147e-02	1.005e-02	-1.940	-1.998	-0.057	-0.97
NaHCO3	4.356e-05	4.374e-05	-4.361	-4.359	0.002	1.80
NaSO4-	1.357e-05	1.192e-05	-4.868	-4.924	-0.056	14.35
NaCO3-	4.279e-07	3.739e-07	-6.369	-6.427	-0.059	-0.29
NaOH	5.594e-20	5.617e-20	-19.252	-19.250	0.002	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-41.626	-41.625	0.002	30.95
S(6)	4.805e-04					
SO4-2	3.823e-04	2.258e-04	-3.418	-3.646	-0.229	15.71
MgSO4	5.046e-05	5.067e-05	-4.297	-4.295	0.002	6.09
CaSO4	3.204e-05	3.217e-05	-4.494	-4.492	0.002	7.76
NaSO4-	1.357e-05	1.192e-05	-4.868	-4.924	-0.056	14.35
KSO4-	2.219e-06	1.950e-06	-5.654	-5.710	-0.056	34.35
HSO4-	9.423e-09	8.235e-09	-8.026	-8.084	-0.059	40.81
CaHSO4+	8.587e-11	7.504e-11	-10.066	-10.125	-0.059	(0)

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

Phase	SI**	log IAP	log K(305 K, 1 atm)	
Anhydrite	-2.40	-6.77	-4.36	CaSO4
Aragonite	-0.59	-8.98	-8.39	CaCO3
Calcite	-0.44	-8.98	-8.54	CaCO3
CO2(g)	-0.72	-2.27	-1.55	CO2
Dolomite	-0.72	-17.95	-17.23	CaMg(CO3)2

```
  Gypsum           -2.18     -6.77   -4.59  CaSO4:2H2O
  H2(g)           -21.07    -24.18   -3.12  H2
  H2O(g)           -1.31     -0.00    1.31  H2O
  Halite           -6.27     -4.69    1.58  NaCl
  O2(g)           -38.68    -41.62   -2.94  O2
  Sylvite          -6.60     -5.66    0.94  KCl

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

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

------------------------------------
Reading input data for simulation 5.
------------------------------------

      Solution 25 #LF25 Banhos Férreos III
      temp  33.6
      pH    6.4
      pe    4
      redox pe
      units mg/l
      Alkalinity  775.3 as Ca.5CO3.5
      Cl    54.2
      S(6)  7.8
      Na    260.6
      Mg    31.8
      K     43.3
      Ca    50.1
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 25.

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

      Elements           Molality       Moles

      Alkalinity        8.816e-03   8.816e-03
      Ca                1.252e-03   1.252e-03
      Cl                1.531e-03   1.531e-03
      K                 1.109e-03   1.109e-03
      Mg                1.310e-03   1.310e-03
      Na                1.135e-02   1.135e-02
      S(6)              8.130e-05   8.130e-05

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

                                       pH  =   6.400
                                       pe  =   4.000
      Specific Conductance (µS/cm,  34°C)  = 1517
                           Density (g/cm³)  =   0.99534
                                Volume (L)  =   1.00595
                        Activity of water  =   0.999
                  Ionic strength (mol/kgw)  =   1.625e-02
                       Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)  =   1.504e-02
                     Total CO2 (mol/kg)  =   1.504e-02
                       Temperature (°C)  =  33.60
                   Electrical balance (eq)  =   7.071e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  25.61
                                 Iterations  =   7
                                    Total H  = 1.110212e+02
                                    Total O  = 5.554543e+01
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	4.445e-07	3.981e-07	-6.352	-6.400	-0.048	0.00
OH-	5.438e-08	4.763e-08	-7.265	-7.322	-0.058	-3.75
H2O	5.551e+01	9.995e-01	1.744	-0.000	0.000	18.12
C(4)	1.504e-02					
HCO3-	8.601e-03	7.599e-03	-2.065	-2.119	-0.054	25.33
CO2	6.223e-03	6.247e-03	-2.206	-2.204	0.002	34.85
CaHCO3+	8.615e-05	7.630e-05	-4.065	-4.117	-0.053	10.02
MgHCO3+	7.955e-05	6.985e-05	-4.099	-4.156	-0.057	5.75
NaHCO3	4.045e-05	4.060e-05	-4.393	-4.391	0.002	1.80
CO3-2	1.715e-06	1.045e-06	-5.766	-5.981	-0.215	-4.49
CaCO3	1.501e-06	1.507e-06	-5.824	-5.822	0.002	-14.57
(CO2)2	9.349e-07	9.384e-07	-6.029	-6.028	0.002	69.70
MgCO3	8.508e-07	8.540e-07	-6.070	-6.069	0.002	-17.09
NaCO3-	3.361e-07	2.954e-07	-6.474	-6.530	-0.056	-0.25
Ca	1.252e-03					
Ca+2	1.159e-03	7.054e-04	-2.936	-3.152	-0.216	-17.79
CaHCO3+	8.615e-05	7.630e-05	-4.065	-4.117	-0.053	10.02
CaSO4	5.215e-06	5.235e-06	-5.283	-5.281	0.002	7.79
CaCO3	1.501e-06	1.507e-06	-5.824	-5.822	0.002	-14.57
CaOH+	3.344e-10	2.939e-10	-9.476	-9.532	-0.056	(0)
CaHSO4+	1.777e-11	1.562e-11	-10.750	-10.806	-0.056	(0)
Cl	1.531e-03					
Cl-	1.531e-03	1.342e-03	-2.815	-2.872	-0.057	18.34
H(0)	2.057e-24					
H2	1.029e-24	1.032e-24	-23.988	-23.986	0.002	28.60
K	1.109e-03					
K+	1.108e-03	9.714e-04	-2.955	-3.013	-0.057	9.34
KSO4-	3.503e-07	3.095e-07	-6.456	-6.509	-0.054	34.36
Mg	1.310e-03					
Mg+2	1.221e-03	7.506e-04	-2.913	-3.125	-0.211	-21.84
MgHCO3+	7.955e-05	6.985e-05	-4.099	-4.156	-0.057	5.75
MgSO4	8.521e-06	8.553e-06	-5.070	-5.068	0.002	6.13
MgCO3	8.508e-07	8.540e-07	-6.070	-6.069	0.002	-17.09
MgOH+	1.640e-08	1.455e-08	-7.785	-7.837	-0.052	(0)
Na	1.135e-02					
Na+	1.131e-02	9.961e-03	-1.947	-2.002	-0.055	-0.94
NaHCO3	4.045e-05	4.060e-05	-4.393	-4.391	0.002	1.80
NaSO4-	2.335e-06	2.063e-06	-5.632	-5.685	-0.054	14.24
NaCO3-	3.361e-07	2.954e-07	-6.474	-6.530	-0.056	-0.25
NaOH	4.727e-20	4.745e-20	-19.325	-19.324	0.002	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-41.712	-41.711	0.002	31.01
S(6)	8.130e-05					
SO4-2	6.487e-05	3.919e-05	-4.188	-4.407	-0.219	15.77
MgSO4	8.521e-06	8.553e-06	-5.070	-5.068	0.002	6.13
CaSO4	5.215e-06	5.235e-06	-5.283	-5.281	0.002	7.79
NaSO4-	2.335e-06	2.063e-06	-5.632	-5.685	-0.054	14.24
KSO4-	3.503e-07	3.095e-07	-6.456	-6.509	-0.054	34.36
HSO4-	2.095e-09	1.842e-09	-8.679	-8.735	-0.056	40.85
CaHSO4+	1.777e-11	1.562e-11	-10.750	-10.806	-0.056	(0)

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

Phase	SI**	log IAP	log K(306 K, 1 atm)	
Anhydrite	-3.18	-7.56	-4.38	CaSO4
Aragonite	-0.74	-9.13	-8.40	CaCO3
Calcite	-0.58	-9.13	-8.55	CaCO3
CO2(g)	-0.64	-2.20	-1.56	CO2
Dolomite	-0.99	-18.24	-17.25	CaMg(CO3)2
Gypsum	-2.97	-7.56	-4.59	CaSO4:2H2O
H2(g)	-20.87	-23.99	-3.12	H2

```
  H2O(g)           -1.29     -0.00    1.29  H2O
  Halite           -6.45     -4.87    1.58  NaCl
  O2(g)           -38.76    -41.71   -2.95  O2
  Sylvite          -6.83     -5.88    0.94  KCl

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

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

------------------------------------
Reading input data for simulation 6.
------------------------------------

      Solution 26 #LF26 Camarça
      temp  15.5
      pH    6
      pe    4
      redox pe
      units mg/l
      Alkalinity  79    as Ca.5CO3.5
      Cl    42.2
      S(6)  4
      Na    77.6
      Mg    7.6
      K     15.5
      Ca    12.3
      END
----------------------------------------
Beginning of initial solution calculations.
----------------------------------------

Initial solution 26.

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

      Elements           Molality       Moles

      Alkalinity        8.974e-04   8.974e-04
      Ca                3.070e-04   3.070e-04
      Cl                1.191e-03   1.191e-03
      K                 3.965e-04   3.965e-04
      Mg                3.127e-04   3.127e-04
      Na                3.376e-03   3.376e-03
      S(6)              4.165e-05   4.165e-05

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

                                       pH  =   6.000
                                       pe  =   4.000
      Specific Conductance (µS/cm,  16°C)  = 305
                           Density (g/cm³)  =   0.99923
                                Volume (L)  =   1.00108
                        Activity of water  =   1.000
                  Ionic strength (mol/kgw)  =   4.233e-03
                       Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)  =   3.064e-03
                     Total CO2 (mol/kg)  =   3.064e-03
                       Temperature (°C)  =  15.50
                   Electrical balance (eq)  =   2.841e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  39.66
                                 Iterations  =   8
                                    Total H  = 1.110133e+02
                                    Total O  = 5.551341e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.065e-06	1.000e-06	-5.973	-6.000	-0.027	0.00
OH-	5.074e-09	4.731e-09	-8.295	-8.325	-0.030	-4.56
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.03
C(4)	3.064e-03					
CO2	2.166e-03	2.168e-03	-2.664	-2.664	0.000	33.96
HCO3-	8.922e-04	8.340e-04	-3.050	-3.079	-0.029	23.87
MgHCO3+	2.394e-06	2.234e-06	-5.621	-5.651	-0.030	5.18
CaHCO3+	2.206e-06	2.063e-06	-5.656	-5.685	-0.029	9.28
NaHCO3	1.561e-06	1.562e-06	-5.807	-5.806	0.000	1.80
(CO2)2	6.186e-08	6.192e-08	-7.209	-7.208	0.000	67.91
CO3-2	4.126e-08	3.150e-08	-7.384	-7.502	-0.117	-6.22
CaCO3	1.049e-08	1.050e-08	-7.979	-7.979	0.000	-14.63
MgCO3	6.138e-09	6.144e-09	-8.212	-8.212	0.000	-17.08
NaCO3-	1.207e-09	1.127e-09	-8.918	-8.948	-0.030	-2.08
Ca	3.070e-04					
Ca+2	3.036e-04	2.317e-04	-3.518	-3.635	-0.117	-18.19
CaHCO3+	2.206e-06	2.063e-06	-5.656	-5.685	-0.029	9.28
CaSO4	1.128e-06	1.129e-06	-5.948	-5.947	0.000	7.09
CaCO3	1.049e-08	1.050e-08	-7.979	-7.979	0.000	-14.63
CaOH+	4.120e-11	3.845e-11	-10.385	-10.415	-0.030	(0)
CaHSO4+	7.013e-12	6.545e-12	-11.154	-11.184	-0.030	(0)
Cl	1.191e-03					
Cl-	1.191e-03	1.110e-03	-2.924	-2.954	-0.030	17.73
H(0)	1.560e-23					
H2	7.798e-24	7.806e-24	-23.108	-23.108	0.000	28.62
K	3.965e-04					
K+	3.964e-04	3.697e-04	-3.402	-3.432	-0.030	8.68
KSO4-	6.904e-08	6.453e-08	-7.161	-7.190	-0.029	33.82
Mg	3.127e-04					
Mg+2	3.090e-04	2.365e-04	-3.510	-3.626	-0.116	-21.36
MgHCO3+	2.394e-06	2.234e-06	-5.621	-5.651	-0.030	5.18
MgSO4	1.268e-06	1.270e-06	-5.897	-5.896	0.000	5.42
MgCO3	6.138e-09	6.144e-09	-8.212	-8.212	0.000	-17.08
MgOH+	3.781e-10	3.540e-10	-9.422	-9.451	-0.029	(0)
Na	3.376e-03					
Na+	3.374e-03	3.151e-03	-2.472	-2.502	-0.030	-2.01
NaHCO3	1.561e-06	1.562e-06	-5.807	-5.806	0.000	1.80
NaSO4-	4.681e-07	4.376e-07	-6.330	-6.359	-0.029	14.21
NaCO3-	1.207e-09	1.127e-09	-8.918	-8.948	-0.030	-2.08
NaOH	1.489e-21	1.491e-21	-20.827	-20.827	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-49.332	-49.332	0.000	29.56
S(6)	4.165e-05					
SO4-2	3.871e-05	2.948e-05	-4.412	-4.530	-0.118	13.10
MgSO4	1.268e-06	1.270e-06	-5.897	-5.896	0.000	5.42
CaSO4	1.128e-06	1.129e-06	-5.948	-5.947	0.000	7.09
NaSO4-	4.681e-07	4.376e-07	-6.330	-6.359	-0.029	14.21
KSO4-	6.904e-08	6.453e-08	-7.161	-7.190	-0.029	33.82
HSO4-	2.518e-09	2.349e-09	-8.599	-8.629	-0.030	39.53
CaHSO4+	7.013e-12	6.545e-12	-11.154	-11.184	-0.030	(0)

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

Phase	SI**	log IAP	log K(288 K, 1 atm)	
Anhydrite	-3.99	-8.17	-4.18	CaSO4
Aragonite	-2.86	-11.14	-8.28	CaCO3
Calcite	-2.71	-11.14	-8.42	CaCO3
CO2(g)	-1.32	-2.66	-1.35	CO2
Dolomite	-5.32	-22.26	-16.94	CaMg(CO3)2
Gypsum	-3.58	-8.17	-4.59	CaSO4:2H2O
H2(g)	-20.03	-23.11	-3.07	H2
H2O(g)	-1.76	-0.00	1.76	H2O
Halite	-7.02	-5.46	1.56	NaCl

```
  O2(g)           -46.52    -49.33   -2.82  O2
  Sylvite          -7.24     -6.39    0.85  KCl

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

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

------------------------------------
Reading input data for simulation 7.
------------------------------------

      Solution 27 #LF27 Poça da Tia Silvina
      temp  44.8
      pH    6.3
      pe    4
      redox pe
      units mg/l
      Alkalinity  713.6 as Ca.5CO3.5
      Cl    85.2
      S(6)  13.2
      Na    284.7
      Mg    17.9
      K     41.5
      Ca    38.1
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 27.

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

      Elements           Molality       Moles

      Alkalinity        8.114e-03   8.114e-03
      Ca                9.517e-04   9.517e-04
      Cl                2.406e-03   2.406e-03
      K                 1.063e-03   1.063e-03
      Mg                7.371e-04   7.371e-04
      Na                1.240e-02   1.240e-02
      S(6)              1.376e-04   1.376e-04

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

                                       pH  =   6.300
                                       pe  =   4.000
      Specific Conductance (µS/cm,  45°C)  = 1872
                           Density (g/cm³)  =   0.99110
                                Volume (L)  =   1.01027
                        Activity of water   =   0.999
                  Ionic strength (mol/kgw)  =   1.529e-02
                       Mass of water (kg)   =   1.000e+00
                  Total carbon (mol/kg)     =   1.496e-02
                     Total CO2 (mol/kg)     =   1.496e-02
                       Temperature (°C)     =  44.80
                   Electrical balance (eq)  =   6.044e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)   =  22.18
                                 Iterations  =   7
                                    Total H  = 1.110205e+02
                                    Total O  = 5.554480e+01

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

                                                 Log       Log       Log    mole V
```

Species	Molality	Activity	Molality	Activity	Gamma	cm³/mol
H+	5.595e-07	5.012e-07	-6.252	-6.300	-0.048	0.00
OH-	9.063e-08	7.945e-08	-7.043	-7.100	-0.057	-3.65
H2O	5.551e+01	9.994e-01	1.744	-0.000	0.000	18.19
C(4)	1.496e-02					
HCO3-	7.957e-03	7.034e-03	-2.099	-2.153	-0.054	25.73
CO2	6.848e-03	6.872e-03	-2.164	-2.163	0.002	35.40
CaHCO3+	6.633e-05	5.877e-05	-4.178	-4.231	-0.053	10.29
MgHCO3+	4.454e-05	3.913e-05	-4.351	-4.407	-0.056	5.90
NaHCO3	3.864e-05	3.878e-05	-4.413	-4.411	0.002	1.80
(CO2)2	1.548e-06	1.554e-06	-5.810	-5.809	0.002	70.79
CO3-2	1.461e-06	8.921e-07	-5.835	-6.050	-0.214	-4.61
CaCO3	1.324e-06	1.329e-06	-5.878	-5.877	0.002	-14.55
NaCO3-	5.248e-07	4.615e-07	-6.280	-6.336	-0.056	0.13
MgCO3	4.825e-07	4.842e-07	-6.317	-6.315	0.002	-17.10
Ca	9.517e-04					
Ca+2	8.766e-04	5.348e-04	-3.057	-3.272	-0.215	-17.82
CaHCO3+	6.633e-05	5.877e-05	-4.178	-4.231	-0.053	10.29
CaSO4	7.500e-06	7.527e-06	-5.125	-5.123	0.002	8.08
CaCO3	1.324e-06	1.329e-06	-5.878	-5.877	0.002	-14.55
CaOH+	2.012e-10	1.770e-10	-9.696	-9.752	-0.056	(0)
CaHSO4+	3.900e-11	3.430e-11	-10.409	-10.465	-0.056	(0)
Cl	2.406e-03					
Cl-	2.406e-03	2.112e-03	-2.619	-2.675	-0.057	18.38
H(0)	2.946e-24					
H2	1.473e-24	1.478e-24	-23.832	-23.830	0.002	28.59
K	1.063e-03					
K+	1.062e-03	9.313e-04	-2.974	-3.031	-0.057	9.58
KSO4-	7.048e-07	6.230e-07	-6.152	-6.206	-0.054	34.44
Mg	7.371e-04					
Mg+2	6.812e-04	4.196e-04	-3.167	-3.377	-0.210	-22.24
MgHCO3+	4.454e-05	3.913e-05	-4.351	-4.407	-0.056	5.90
MgSO4	1.089e-05	1.093e-05	-4.963	-4.962	0.002	6.42
MgCO3	4.825e-07	4.842e-07	-6.317	-6.315	0.002	-17.10
MgOH+	1.830e-08	1.625e-08	-7.738	-7.789	-0.052	(0)
Na	1.240e-02					
Na+	1.235e-02	1.089e-02	-1.908	-1.963	-0.055	-0.55
NaHCO3	3.864e-05	3.878e-05	-4.413	-4.411	0.002	1.80
NaSO4-	4.783e-06	4.228e-06	-5.320	-5.374	-0.054	13.56
NaCO3-	5.248e-07	4.615e-07	-6.280	-6.336	-0.056	0.13
NaOH	8.621e-20	8.652e-20	-19.064	-19.063	0.002	(0)
O(0)	3.729e-39					
O2	1.865e-39	1.871e-39	-38.729	-38.728	0.002	31.66
S(6)	1.376e-04					
SO4-2	1.137e-04	6.886e-05	-3.944	-4.162	-0.218	16.38
MgSO4	1.089e-05	1.093e-05	-4.963	-4.962	0.002	6.42
CaSO4	7.500e-06	7.527e-06	-5.125	-5.123	0.002	8.08
NaSO4-	4.783e-06	4.228e-06	-5.320	-5.374	-0.054	13.56
KSO4-	7.048e-07	6.230e-07	-6.152	-6.206	-0.054	34.44
HSO4-	6.067e-09	5.335e-09	-8.217	-8.273	-0.056	41.25
CaHSO4+	3.900e-11	3.430e-11	-10.409	-10.465	-0.056	(0)

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

Phase	SI**	log IAP	log K(317 K, 1 atm)	
Anhydrite	-2.92	-7.43	-4.51	CaSO4
Aragonite	-0.83	-9.32	-8.49	CaCO3
Calcite	-0.65	-9.32	-8.67	CaCO3
CO2(g)	-0.49	-2.16	-1.67	CO2
Dolomite	-1.23	-18.75	-17.52	CaMg(CO3)2
Gypsum	-2.83	-7.43	-4.61	CaSO4:2H2O
H2(g)	-20.70	-23.83	-3.13	H2
H2O(g)	-1.03	-0.00	1.03	H2O
Halite	-6.22	-4.64	1.58	NaCl
O2(g)	-35.72	-38.73	-3.01	O2
Sylvite	-6.70	-5.71	0.99	KCl

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

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

-----------------------------------
Reading input data for simulation 8.
-----------------------------------

      Solution 28 #LF28 Morangueira
      temp  32.2
      pH    6.4
      pe    4
      redox pe
      units mg/l
      Alkalinity  641.9 as Ca.5CO3.5
      Cl    99.7
      S(6)  12.6
      Na    323.4
      Mg    20.1
      K     46.2
      Ca    43.4
      END
----------------------------------------
Beginning of initial solution calculations.
----------------------------------------

Initial solution 28.

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

      Elements           Molality       Moles

      Alkalinity        7.299e-03   7.299e-03
      Ca                1.084e-03   1.084e-03
      Cl                2.816e-03   2.816e-03
      K                 1.183e-03   1.183e-03
      Mg                8.277e-04   8.277e-04
      Na                1.408e-02   1.408e-02
      S(6)              1.313e-04   1.313e-04

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

                                     pH  =   6.400
                                     pe  =   4.000
      Specific Conductance (µS/cm,  32°C)  = 1607
                           Density (g/cm³)  =   0.99580
                                Volume (L)  =   1.00545
                        Activity of water  =   0.999
                  Ionic strength (mol/kgw)  =   1.645e-02
                       Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)  =   1.253e-02
                     Total CO2 (mol/kg)  =   1.253e-02
                       Temperature (°C)  =  32.20
                   Electrical balance (eq)  =   8.714e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  29.95
                                 Iterations  =   8
                                    Total H  = 1.110197e+02
                                    Total O  = 5.553909e+01

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

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

H+	4.446e-07	3.981e-07	-6.352	-6.400	-0.048	0.00
OH-	4.929e-08	4.316e-08	-7.307	-7.365	-0.058	-3.78
H2O	5.551e+01	9.994e-01	1.744	-0.000	0.000	18.11
C(4)	1.253e-02					
HCO3-	7.147e-03	6.313e-03	-2.146	-2.200	-0.054	25.26
CO2	5.228e-03	5.248e-03	-2.282	-2.280	0.002	34.78
CaHCO3+	6.162e-05	5.456e-05	-4.210	-4.263	-0.053	9.98
NaHCO3	4.201e-05	4.217e-05	-4.377	-4.375	0.002	1.80
MgHCO3+	4.167e-05	3.658e-05	-4.380	-4.437	-0.057	5.72
CO3-2	1.394e-06	8.485e-07	-5.856	-6.071	-0.216	-4.52
CaCO3	1.029e-06	1.033e-06	-5.988	-5.986	0.002	-14.58
(CO2)2	6.327e-07	6.351e-07	-6.199	-6.197	0.002	69.56
MgCO3	4.298e-07	4.315e-07	-6.367	-6.365	0.002	-17.09
NaCO3-	3.169e-07	2.785e-07	-6.499	-6.555	-0.056	-0.33
Ca	1.084e-03					
Ca+2	1.014e-03	6.165e-04	-2.994	-3.210	-0.216	-17.79
CaHCO3+	6.162e-05	5.456e-05	-4.210	-4.263	-0.053	9.98
CaSO4	7.602e-06	7.631e-06	-5.119	-5.117	0.002	7.75
CaCO3	1.029e-06	1.033e-06	-5.988	-5.986	0.002	-14.58
CaOH+	2.923e-10	2.569e-10	-9.534	-9.590	-0.056	(0)
CaHSO4+	2.534e-11	2.227e-11	-10.596	-10.652	-0.056	(0)
Cl	2.816e-03					
Cl-	2.816e-03	2.468e-03	-2.550	-2.608	-0.057	18.32
H(0)	2.084e-24					
H2	1.042e-24	1.046e-24	-23.982	-23.980	0.002	28.60
K	1.183e-03					
K+	1.182e-03	1.036e-03	-2.927	-2.985	-0.057	9.30
KSO4-	6.151e-07	5.433e-07	-6.211	-6.265	-0.054	34.34
Mg	8.277e-04					
Mg+2	7.768e-04	4.771e-04	-3.110	-3.321	-0.212	-21.79
MgHCO3+	4.167e-05	3.658e-05	-4.380	-4.437	-0.057	5.72
MgSO4	8.818e-06	8.851e-06	-5.055	-5.053	0.002	6.08
MgCO3	4.298e-07	4.315e-07	-6.367	-6.365	0.002	-17.09
MgOH+	9.248e-09	8.205e-09	-8.034	-8.086	-0.052	(0)
Na	1.408e-02					
Na+	1.404e-02	1.236e-02	-1.853	-1.908	-0.055	-1.00
NaHCO3	4.201e-05	4.217e-05	-4.377	-4.375	0.002	1.80
NaSO4-	4.843e-06	4.278e-06	-5.315	-5.369	-0.054	14.31
NaCO3-	3.169e-07	2.785e-07	-6.499	-6.555	-0.056	-0.33
NaOH	5.315e-20	5.335e-20	-19.274	-19.273	0.002	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-42.152	-42.151	0.002	30.92
S(6)	1.313e-04					
SO4-2	1.094e-04	6.603e-05	-3.961	-4.180	-0.219	15.65
MgSO4	8.818e-06	8.851e-06	-5.055	-5.053	0.002	6.08
CaSO4	7.602e-06	7.631e-06	-5.119	-5.117	0.002	7.75
NaSO4-	4.843e-06	4.278e-06	-5.315	-5.369	-0.054	14.31
KSO4-	6.151e-07	5.433e-07	-6.211	-6.265	-0.054	34.34
HSO4-	3.419e-09	3.004e-09	-8.466	-8.522	-0.056	40.78
CaHSO4+	2.534e-11	2.227e-11	-10.596	-10.652	-0.056	(0)

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

Phase	SI**	log IAP	log K(305 K, 1 atm)	
Anhydrite	-3.03	-7.39	-4.36	CaSO4
Aragonite	-0.90	-9.28	-8.39	CaCO3
Calcite	-0.74	-9.28	-8.54	CaCO3
CO2(g)	-0.73	-2.28	-1.55	CO2
Dolomite	-1.45	-18.67	-17.22	CaMg(CO3)2
Gypsum	-2.80	-7.39	-4.59	CaSO4:2H2O
H2(g)	-20.86	-23.98	-3.12	H2
H2O(g)	-1.32	-0.00	1.32	H2O
Halite	-6.09	-4.52	1.58	NaCl
O2(g)	-39.21	-42.15	-2.94	O2
Sylvite	-6.53	-5.59	0.94	KCl

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

For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 9.

```
      Solution 29 #LF29 Quenturas I
      temp  16.3
      pH    6.2
      pe    4
      redox pe
      units mg/l
      Alkalinity  136.6 as Ca.5CO3.5
      Cl    21.8
      S(6)  6.3
      Na    25.2
      Mg    5
      K     11.6
      Ca    7.2
      END
```

Beginning of initial solution calculations.

Initial solution 29.

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

Elements	Molality	Moles
Alkalinity	1.552e-03	1.552e-03
Ca	1.797e-04	1.797e-04
Cl	6.150e-04	6.150e-04
K	2.967e-04	2.967e-04
Mg	2.057e-04	2.057e-04
Na	1.096e-03	1.096e-03
S(6)	6.560e-05	6.560e-05

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

pH	= 6.200
pe	= 4.000
Specific Conductance (µS/cm, 16°C)	= 190
Density (g/cm³)	= 0.99905
Volume (L)	= 1.00123
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 2.660e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 3.917e-03
Total CO2 (mol/kg)	= 3.917e-03
Temperature (°C)	= 16.30
Electrical balance (eq)	= -1.341e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -3.02
Iterations	= 8
Total H	= 1.110140e+02
Total O	= 5.551586e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	6.645e-07	6.310e-07	-6.177	-6.200	-0.023	0.00
OH-	8.482e-09	8.017e-09	-8.072	-8.096	-0.024	-4.52

H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.04
C(4)	3.917e-03					
CO2	2.364e-03	2.366e-03	-2.626	-2.626	0.000	34.00
HCO3-	1.546e-03	1.464e-03	-2.811	-2.835	-0.024	23.94
MgHCO3+	2.846e-06	2.691e-06	-5.546	-5.570	-0.024	5.21
CaHCO3+	2.376e-06	2.250e-06	-5.624	-5.648	-0.024	9.31
NaHCO3	8.967e-07	8.973e-07	-6.047	-6.047	0.000	1.80
CO3-2	1.113e-07	8.941e-08	-6.954	-7.049	-0.095	-6.15
(CO2)2	7.591e-08	7.595e-08	-7.120	-7.119	0.000	68.00
CaCO3	1.836e-08	1.837e-08	-7.736	-7.736	0.000	-14.63
MgCO3	1.209e-08	1.209e-08	-7.918	-7.917	0.000	-17.08
NaCO3-	1.161e-09	1.098e-09	-8.935	-8.959	-0.024	-1.99
Ca	1.797e-04					
Ca+2	1.761e-04	1.414e-04	-3.754	-3.849	-0.095	-18.21
CaHCO3+	2.376e-06	2.250e-06	-5.624	-5.648	-0.024	9.31
CaSO4	1.179e-06	1.180e-06	-5.928	-5.928	0.000	7.13
CaCO3	1.836e-08	1.837e-08	-7.736	-7.736	0.000	-14.63
CaOH+	3.933e-11	3.720e-11	-10.405	-10.429	-0.024	(0)
CaHSO4+	4.610e-12	4.359e-12	-11.336	-11.361	-0.024	(0)
Cl	6.150e-04					
Cl-	6.150e-04	5.814e-04	-3.211	-3.235	-0.024	17.76
H(0)	6.159e-24					
H2	3.080e-24	3.081e-24	-23.512	-23.511	0.000	28.62
K	2.967e-04					
K+	2.966e-04	2.804e-04	-3.528	-3.552	-0.024	8.71
KSO4-	8.930e-08	8.455e-08	-7.049	-7.073	-0.024	33.85
Mg	2.057e-04					
Mg+2	2.013e-04	1.620e-04	-3.696	-3.790	-0.094	-21.43
MgHCO3+	2.846e-06	2.691e-06	-5.546	-5.570	-0.024	5.21
MgSO4	1.512e-06	1.513e-06	-5.820	-5.820	0.000	5.46
MgCO3	1.209e-08	1.209e-08	-7.918	-7.917	0.000	-17.08
MgOH+	4.379e-10	4.150e-10	-9.359	-9.382	-0.023	(0)
Na	1.096e-03					
Na+	1.095e-03	1.036e-03	-2.961	-2.985	-0.024	-1.97
NaHCO3	8.967e-07	8.973e-07	-6.047	-6.047	0.000	1.80
NaSO4-	2.600e-07	2.462e-07	-6.585	-6.609	-0.024	14.09
NaCO3-	1.161e-09	1.098e-09	-8.935	-8.959	-0.024	-1.99
NaOH	8.302e-22	8.308e-22	-21.081	-21.081	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-48.250	-48.250	0.000	29.64
S(6)	6.560e-05					
SO4-2	6.255e-05	5.018e-05	-4.204	-4.300	-0.096	13.21
MgSO4	1.512e-06	1.513e-06	-5.820	-5.820	0.000	5.46
CaSO4	1.179e-06	1.180e-06	-5.928	-5.928	0.000	7.13
NaSO4-	2.600e-07	2.462e-07	-6.585	-6.609	-0.024	14.09
KSO4-	8.930e-08	8.455e-08	-7.049	-7.073	-0.024	33.85
HSO4-	2.711e-09	2.564e-09	-8.567	-8.591	-0.024	39.60
CaHSO4+	4.610e-12	4.359e-12	-11.336	-11.361	-0.024	(0)

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

Phase	SI**	log IAP	log K(289 K, 1 atm)	
Anhydrite	-3.96	-8.15	-4.18	CaSO4
Aragonite	-2.61	-10.90	-8.29	CaCO3
Calcite	-2.47	-10.90	-8.43	CaCO3
CO2(g)	-1.27	-2.63	-1.36	CO2
Dolomite	-4.79	-21.74	-16.95	CaMg(CO3)2
Gypsum	-3.56	-8.15	-4.59	CaSO4:2H2O
H2(g)	-20.43	-23.51	-3.08	H2
H2O(g)	-1.73	-0.00	1.73	H2O
Halite	-7.78	-6.22	1.56	NaCl
O2(g)	-45.43	-48.25	-2.82	O2
Sylvite	-7.64	-6.79	0.86	KCl

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

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

--------------------------------------
Reading input data for simulation 10.
--------------------------------------

      Solution 30 #LF30 Quenturas II
      temp  57.2
      pH    6.4
      pe    4
      redox pe
      units mg/l
      Alkalinity  603.7 as Ca.5CO3.5
      Cl    74.4
      S(6)  31.7
      Na    223.5
      Mg    13.5
      K     44.1
      Ca    28.9
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 30.

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

      Elements           Molality       Moles

      Alkalinity        6.863e-03   6.863e-03
      Ca                7.218e-04   7.218e-04
      Cl                2.101e-03   2.101e-03
      K                 1.129e-03   1.129e-03
      Mg                5.558e-04   5.558e-04
      Na                9.732e-03   9.732e-03
      S(6)              3.303e-04   3.303e-04

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

                                       pH  =   6.400
                                       pe  =   4.000
      Specific Conductance (µS/cm,  57°C)  = 1922
                           Density (g/cm³)  =   0.98527
                                Volume (L)  =   1.01601
                        Activity of water  =   1.000
                  Ionic strength (mol/kgw)  =   1.275e-02
                       Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)  =   1.148e-02
                     Total CO2 (mol/kg)  =   1.148e-02
                       Temperature (°C)  =  57.20
                   Electrical balance (eq)  =   3.791e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  16.75
                                 Iterations  =   8
                                    Total H  = 1.110193e+02
                                    Total O  = 5.553736e+01

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

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

   H+              4.423e-07   3.981e-07    -6.354    -6.400    -0.046      0.00
   OH-             2.355e-07   2.079e-07    -6.628    -6.682    -0.054     -3.78
   H2O             5.551e+01   9.996e-01     1.744    -0.000     0.000     18.30
C(4)          1.148e-02
```

HCO3-	6.751e-03	6.005e-03	-2.171	-2.222	-0.051	25.90
CO2	4.624e-03	4.637e-03	-2.335	-2.334	0.001	36.04
CaHCO3+	4.634e-05	4.130e-05	-4.334	-4.384	-0.050	10.48
MgHCO3+	3.151e-05	2.787e-05	-4.502	-4.555	-0.053	5.97
NaHCO3	2.456e-05	2.464e-05	-4.610	-4.608	0.001	1.80
CaCO3	1.787e-06	1.792e-06	-5.748	-5.747	0.001	-14.52
CO3-2	1.703e-06	1.066e-06	-5.769	-5.972	-0.204	-5.48
(CO2)2	9.534e-07	9.562e-07	-6.021	-6.019	0.001	72.08
NaCO3-	8.352e-07	7.393e-07	-6.078	-6.131	-0.053	0.12
MgCO3	5.211e-07	5.227e-07	-6.283	-6.282	0.001	-17.10
Ca	7.218e-04					
Ca+2	6.581e-04	4.113e-04	-3.182	-3.386	-0.204	-17.99
CaHCO3+	4.634e-05	4.130e-05	-4.334	-4.384	-0.050	10.48
CaSO4	1.555e-05	1.560e-05	-4.808	-4.807	0.001	8.33
CaCO3	1.787e-06	1.792e-06	-5.748	-5.747	0.001	-14.52
CaOH+	1.936e-10	1.714e-10	-9.713	-9.766	-0.053	(0)
CaHSO4+	8.105e-11	7.174e-11	-10.091	-10.144	-0.053	(0)
Cl	2.101e-03					
Cl-	2.101e-03	1.856e-03	-2.678	-2.731	-0.054	18.22
H(0)	1.675e-24					
H2	8.376e-25	8.401e-25	-24.077	-24.076	0.001	28.58
K	1.129e-03					
K+	1.127e-03	9.951e-04	-2.948	-3.002	-0.054	9.78
KSO4-	2.238e-06	1.991e-06	-5.650	-5.701	-0.051	34.39
Mg	5.558e-04					
Mg+2	4.972e-04	3.134e-04	-3.303	-3.504	-0.200	-22.74
MgHCO3+	3.151e-05	2.787e-05	-4.502	-4.555	-0.053	5.97
MgSO4	2.655e-05	2.663e-05	-4.576	-4.575	0.001	6.67
MgCO3	5.211e-07	5.227e-07	-6.283	-6.282	0.001	-17.10
MgOH+	4.414e-08	3.941e-08	-7.355	-7.404	-0.049	(0)
Na	9.732e-03					
Na+	9.696e-03	8.601e-03	-2.013	-2.065	-0.052	-0.23
NaHCO3	2.456e-05	2.464e-05	-4.610	-4.608	0.001	1.80
NaSO4-	9.991e-06	8.886e-06	-5.000	-5.051	-0.051	12.46
NaCO3-	8.352e-07	7.393e-07	-6.078	-6.131	-0.053	0.12
NaOH	1.783e-19	1.788e-19	-18.749	-18.748	0.001	(0)
O(0)	2.815e-35					
O2	1.408e-35	1.412e-35	-34.851	-34.850	0.001	32.26
S(6)	3.303e-04					
SO4-2	2.760e-04	1.715e-04	-3.559	-3.766	-0.207	16.46
MgSO4	2.655e-05	2.663e-05	-4.576	-4.575	0.001	6.67
CaSO4	1.555e-05	1.560e-05	-4.808	-4.807	0.001	8.33
NaSO4-	9.991e-06	8.886e-06	-5.000	-5.051	-0.051	12.46
KSO4-	2.238e-06	1.991e-06	-5.650	-5.701	-0.051	34.39
HSO4-	1.639e-08	1.451e-08	-7.785	-7.838	-0.053	41.46
CaHSO4+	8.105e-11	7.174e-11	-10.091	-10.144	-0.053	(0)

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

Phase	SI**	log IAP	log K(330 K, 1 atm)	
Anhydrite	-2.48	-7.15	-4.67	CaSO4
Aragonite	-0.75	-9.36	-8.61	CaCO3
Calcite	-0.52	-9.36	-8.84	CaCO3
CO2(g)	-0.57	-2.33	-1.76	CO2
Dolomite	-0.96	-18.83	-17.87	CaMg(CO3)2
Gypsum	-2.51	-7.15	-4.64	CaSO4:2H2O
H2(g)	-20.94	-24.08	-3.14	H2
H2O(g)	-0.77	-0.00	0.77	H2O
Halite	-6.39	-4.80	1.59	NaCl
O2(g)	-31.79	-34.85	-3.06	O2
Sylvite	-6.78	-5.73	1.05	KCl

**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 11.
------------------------------------

      Solution 31 #LF31 Quenturas III
      temp  57.5
      pH    6.4
      pe    4
      redox pe
      units mg/l
      Alkalinity  643.5 as Ca.5CO3.5
      Cl    75.9
      S(6)  15
      Na    224.8
      Mg    13.6
      K     44.1
      Ca    28.3
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 31.

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

      Elements           Molality       Moles

      Alkalinity        7.316e-03   7.316e-03
      Ca                7.068e-04   7.068e-04
      Cl                2.143e-03   2.143e-03
      K                 1.129e-03   1.129e-03
      Mg                5.600e-04   5.600e-04
      Na                9.788e-03   9.788e-03
      S(6)              1.563e-04   1.563e-04

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

                                       pH  =   6.400
                                       pe  =   4.000
      Specific Conductance (µS/cm,  58°C)  = 1938
                           Density (g/cm³)  =   0.98513
                                Volume (L)  =   1.01618
                        Activity of water  =   1.000
                  Ionic strength (mol/kgw)  =   1.274e-02
                       Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)  =   1.224e-02
                     Total CO2 (mol/kg)  =   1.224e-02
                       Temperature (°C)  =  57.50
                   Electrical balance (eq)  =   3.679e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  16.07
                                 Iterations  =   8
                                    Total H  = 1.110197e+02
                                    Total O  = 5.553864e+01

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

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

   H+              4.423e-07   3.981e-07    -6.354    -6.400    -0.046      0.00
   OH-             2.395e-07   2.114e-07    -6.621    -6.675    -0.054     -3.78
   H2O             5.551e+01   9.995e-01     1.744    -0.000     0.000     18.30
C(4)          1.224e-02
   HCO3-           7.196e-03   6.400e-03    -2.143    -2.194    -0.051     25.90
   CO2             4.931e-03   4.945e-03    -2.307    -2.306     0.001     36.06
```

CaHCO3+	4.876e-05	4.346e-05	-4.312	-4.362	-0.050	10.48
MgHCO3+	3.466e-05	3.066e-05	-4.460	-4.513	-0.053	5.97
NaHCO3	2.631e-05	2.638e-05	-4.580	-4.579	0.001	1.80
CaCO3	1.899e-06	1.904e-06	-5.722	-5.720	0.001	-14.52
CO3-2	1.819e-06	1.138e-06	-5.740	-5.944	-0.204	-5.51
(CO2)2	1.092e-06	1.095e-06	-5.962	-5.961	0.001	72.11
NaCO3-	9.085e-07	8.041e-07	-6.042	-6.095	-0.053	0.11
MgCO3	5.752e-07	5.769e-07	-6.240	-6.239	0.001	-17.10
Ca	7.068e-04					
Ca+2	6.489e-04	4.055e-04	-3.188	-3.392	-0.204	-17.99
CaHCO3+	4.876e-05	4.346e-05	-4.312	-4.362	-0.050	10.48
CaSO4	7.248e-06	7.269e-06	-5.140	-5.139	0.001	8.33
CaCO3	1.899e-06	1.904e-06	-5.722	-5.720	0.001	-14.52
CaOH+	1.909e-10	1.690e-10	-9.719	-9.772	-0.053	(0)
CaHSO4+	3.801e-11	3.364e-11	-10.420	-10.473	-0.053	(0)
Cl	2.143e-03					
Cl-	2.143e-03	1.894e-03	-2.669	-2.723	-0.054	18.21
H(0)	1.671e-24					
H2	8.356e-25	8.381e-25	-24.078	-24.077	0.001	28.58
K	1.129e-03					
K+	1.128e-03	9.962e-04	-2.948	-3.002	-0.054	9.78
KSO4-	1.062e-06	9.444e-07	-5.974	-6.025	-0.051	34.39
Mg	5.600e-04					
Mg+2	5.117e-04	3.225e-04	-3.291	-3.491	-0.201	-22.75
MgHCO3+	3.466e-05	3.066e-05	-4.460	-4.513	-0.053	5.97
MgSO4	1.297e-05	1.301e-05	-4.887	-4.886	0.001	6.67
MgCO3	5.752e-07	5.769e-07	-6.240	-6.239	0.001	-17.10
MgOH+	4.643e-08	4.146e-08	-7.333	-7.382	-0.049	(0)
Na	9.788e-03					
Na+	9.757e-03	8.654e-03	-2.011	-2.063	-0.052	-0.22
NaHCO3	2.631e-05	2.638e-05	-4.580	-4.579	0.001	1.80
NaSO4-	4.752e-06	4.226e-06	-5.323	-5.374	-0.051	12.43
NaCO3-	9.085e-07	8.041e-07	-6.042	-6.095	-0.053	0.11
NaOH	1.824e-19	1.830e-19	-18.739	-18.738	0.001	(0)
O(0)	3.392e-35					
O2	1.696e-35	1.701e-35	-34.771	-34.769	0.001	32.27
S(6)	1.563e-04					
SO4-2	1.303e-04	8.092e-05	-3.885	-4.092	-0.207	16.46
MgSO4	1.297e-05	1.301e-05	-4.887	-4.886	0.001	6.67
CaSO4	7.248e-06	7.269e-06	-5.140	-5.139	0.001	8.33
NaSO4-	4.752e-06	4.226e-06	-5.323	-5.374	-0.051	12.43
KSO4-	1.062e-06	9.444e-07	-5.974	-6.025	-0.051	34.39
HSO4-	7.796e-09	6.900e-09	-8.108	-8.161	-0.053	41.46
CaHSO4+	3.801e-11	3.364e-11	-10.420	-10.473	-0.053	(0)

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

Phase	SI**	log IAP	log K(330 K, 1 atm)	
Anhydrite	-2.81	-7.48	-4.67	CaSO4
Aragonite	-0.72	-9.34	-8.61	CaCO3
Calcite	-0.50	-9.34	-8.84	CaCO3
CO2(g)	-0.54	-2.31	-1.77	CO2
Dolomite	-0.89	-18.77	-17.88	CaMg(CO3)2
Gypsum	-2.84	-7.48	-4.64	CaSO4:2H2O
H2(g)	-20.94	-24.08	-3.14	H2
H2O(g)	-0.76	-0.00	0.76	H2O
Halite	-6.38	-4.79	1.59	NaCl
O2(g)	-31.71	-34.77	-3.06	O2
Sylvite	-6.77	-5.72	1.05	KCl

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

End of simulation.

```
------------------------------------
Reading input data for simulation 12.
------------------------------------

      Solution 32 #LF32 Grutinha I
      temp  41
      pH    6.2
      pe    2.89
      redox pe
      units mg/l
      Alkalinity  683   as Ca.5CO3.5
      Cl    88.2
      S(6)  11.8
      Na    301
      Mg    15.8
      K     37.3
      Ca    34.9
      END
----------------------------------------
Beginning of initial solution calculations.
----------------------------------------

Initial solution 32.

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

      Elements           Molality       Moles

      Alkalinity        7.766e-03   7.766e-03
      Ca                8.718e-04   8.718e-04
      Cl                2.491e-03   2.491e-03
      K                 9.550e-04   9.550e-04
      Mg                6.506e-04   6.506e-04
      Na                1.311e-02   1.311e-02
      S(6)              1.230e-04   1.230e-04

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

                                       pH  =   6.200
                                       pe  =   2.890
      Specific Conductance (µS/cm,  41°C)  = 1760
                           Density (g/cm³)  =   0.99264
                                Volume (L)  =   1.00875
                        Activity of water  =   0.999
                  Ionic strength (mol/kgw)  =   1.515e-02
                         Mass of water (kg)  =   1.000e+00
                     Total carbon (mol/kg)  =   1.615e-02
                        Total CO2 (mol/kg)  =   1.615e-02
                          Temperature (°C)  =  41.00
                   Electrical balance (eq)  =   6.605e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  24.22
                                 Iterations  =   8
                                    Total H  = 1.110202e+02
                                    Total O  = 5.554678e+01

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

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

   H+              7.035e-07   6.310e-07    -6.153    -6.200    -0.047      0.00
   OH-             5.640e-08   4.951e-08    -7.249    -7.305    -0.057     -3.67
   H2O             5.551e+01   9.994e-01     1.744    -0.000     0.000     18.16
C(4)          1.615e-02
   CO2             8.386e-03   8.415e-03    -2.076    -2.075     0.002     35.21
   HCO3-           7.627e-03   6.751e-03    -2.118    -2.171    -0.053     25.62
   CaHCO3+         5.732e-05   5.085e-05    -4.242    -4.294    -0.052     10.21
   NaHCO3          4.003e-05   4.017e-05    -4.398    -4.396     0.002      1.80
```

MgHCO3+	3.702e-05	3.257e-05	-4.432	-4.487	-0.056	5.86
(CO2)2	2.097e-06	2.105e-06	-5.678	-5.677	0.002	70.42
CO3-2	1.060e-06	6.505e-07	-5.975	-6.187	-0.212	-4.51
CaCO3	8.008e-07	8.036e-07	-6.096	-6.095	0.002	-14.56
NaCO3-	3.411e-07	3.004e-07	-6.467	-6.522	-0.055	0.04
MgCO3	2.963e-07	2.974e-07	-6.528	-6.527	0.002	-17.10
Ca	8.718e-04					
Ca+2	8.075e-04	4.953e-04	-3.093	-3.305	-0.212	-17.80
CaHCO3+	5.732e-05	5.085e-05	-4.242	-4.294	-0.052	10.21
CaSO4	6.201e-06	6.223e-06	-5.208	-5.206	0.002	7.99
CaCO3	8.008e-07	8.036e-07	-6.096	-6.095	0.002	-14.56
CaOH+	1.478e-10	1.302e-10	-9.830	-9.885	-0.055	(0)
CaHSO4+	3.786e-11	3.335e-11	-10.422	-10.477	-0.055	(0)
Cl	2.491e-03					
Cl-	2.491e-03	2.189e-03	-2.604	-2.660	-0.056	18.39
H(0)	8.014e-22					
H2	4.007e-22	4.021e-22	-21.397	-21.396	0.002	28.59
K	9.550e-04					
K+	9.545e-04	8.384e-04	-3.020	-3.077	-0.056	9.51
KSO4-	5.469e-07	4.841e-07	-6.262	-6.315	-0.053	34.43
Mg	6.506e-04					
Mg+2	6.052e-04	3.747e-04	-3.218	-3.426	-0.208	-22.11
MgHCO3+	3.702e-05	3.257e-05	-4.432	-4.487	-0.056	5.86
MgSO4	8.160e-06	8.189e-06	-5.088	-5.087	0.002	6.33
MgCO3	2.963e-07	2.974e-07	-6.528	-6.527	0.002	-17.10
MgOH+	9.551e-09	8.491e-09	-8.020	-8.071	-0.051	(0)
Na	1.311e-02					
Na+	1.306e-02	1.153e-02	-1.884	-1.938	-0.054	-0.67
NaHCO3	4.003e-05	4.017e-05	-4.398	-4.396	0.002	1.80
NaSO4-	4.533e-06	4.012e-06	-5.344	-5.397	-0.053	13.80
NaCO3-	3.411e-07	3.004e-07	-6.467	-6.522	-0.055	0.04
NaOH	5.689e-20	5.709e-20	-19.245	-19.243	0.002	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-44.690	-44.689	0.002	31.46
S(6)	1.230e-04					
SO4-2	1.035e-04	6.305e-05	-3.985	-4.200	-0.215	16.22
MgSO4	8.160e-06	8.189e-06	-5.088	-5.087	0.002	6.33
CaSO4	6.201e-06	6.223e-06	-5.208	-5.206	0.002	7.99
NaSO4-	4.533e-06	4.012e-06	-5.344	-5.397	-0.053	13.80
KSO4-	5.469e-07	4.841e-07	-6.262	-6.315	-0.053	34.43
HSO4-	6.359e-09	5.601e-09	-8.197	-8.252	-0.055	41.14
CaHSO4+	3.786e-11	3.335e-11	-10.422	-10.477	-0.055	(0)

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

Phase	SI**	log IAP	log K(314 K, 1 atm)	
Anhydrite	-3.04	-7.51	-4.46	CaSO4
Aragonite	-1.04	-9.49	-8.45	CaCO3
Calcite	-0.86	-9.49	-8.63	CaCO3
CO2(g)	-0.44	-2.07	-1.63	CO2
Dolomite	-1.68	-19.11	-17.42	CaMg(CO3)2
Gypsum	-2.91	-7.51	-4.60	CaSO4:2H2O
H2(g)	-18.27	-21.40	-3.13	H2
H2O(g)	-1.12	-0.00	1.12	H2O
Halite	-6.18	-4.60	1.58	NaCl
O2(g)	-41.70	-44.69	-2.99	O2
Sylvite	-6.71	-5.74	0.98	KCl

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

End of simulation.

Reading input data for simulation 13.

```
------------------------------------

      Solution 33 #LF33 Grutinha II
      temp  41.7
      pH    6.1
      pe    2.846
      redox pe
      units mg/l
      Alkalinity  639.1 as Ca.5CO3.5
      Cl    84.5
      S(6)  13.3
      Na    261.2
      Mg    13.8
      K     35.9
      Ca    28.8
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 33.

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

      Elements           Molality       Moles

      Alkalinity        7.266e-03   7.266e-03
      Ca                7.193e-04   7.193e-04
      Cl                2.386e-03   2.386e-03
      K                 9.191e-04   9.191e-04
      Mg                5.682e-04   5.682e-04
      Na                1.137e-02   1.137e-02
      S(6)              1.386e-04   1.386e-04

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

                                       pH  =   6.100
                                       pe  =   2.846
      Specific Conductance (µS/cm,  42°C)  = 1614
                           Density (g/cm³)  =   0.99231
                                Volume (L)  =   1.00908
                        Activity of water  =   0.999
                  Ionic strength (mol/kgw)  =   1.357e-02
                        Mass of water (kg)  =   1.000e+00
                   Total carbon (mol/kg)  =   1.720e-02
                      Total CO2 (mol/kg)  =   1.720e-02
                        Temperature (°C)  =  41.70
                   Electrical balance (eq)  =   4.939e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  20.15
                                 Iterations  =   8
                                    Total H  = 1.110197e+02
                                    Total O  = 5.554844e+01

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

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

   H+              8.820e-07   7.943e-07    -6.055    -6.100    -0.045      0.00
   OH-             4.660e-08   4.115e-08    -7.332    -7.386    -0.054     -3.67
   H2O             5.551e+01   9.994e-01     1.744    -0.000     0.000     18.17
C(4)          1.720e-02
   CO2             9.929e-03   9.960e-03    -2.003    -2.002     0.001     35.24
   HCO3-           7.154e-03   6.366e-03    -2.145    -2.196    -0.051     25.63
   CaHCO3+         4.561e-05   4.067e-05    -4.341    -4.391    -0.050     10.22
   NaHCO3          3.283e-05   3.293e-05    -4.484    -4.482     0.001      1.80
   MgHCO3+         3.108e-05   2.750e-05    -4.508    -4.561    -0.053      5.86
   (CO2)2          2.996e-06   3.005e-06    -5.523    -5.522     0.001     70.49
```

CO3-2	7.838e-07	4.914e-07	-6.106	-6.309	-0.203	-4.55
CaCO3	5.209e-07	5.226e-07	-6.283	-6.282	0.001	-14.55
NaCO3-	2.308e-07	2.044e-07	-6.637	-6.689	-0.053	0.05
MgCO3	2.017e-07	2.023e-07	-6.695	-6.694	0.001	-17.10
Ca	7.193e-04					
Ca+2	6.671e-04	4.179e-04	-3.176	-3.379	-0.203	-17.82
CaHCO3+	4.561e-05	4.067e-05	-4.341	-4.391	-0.050	10.22
CaSO4	6.154e-06	6.173e-06	-5.211	-5.210	0.001	8.01
CaCO3	5.209e-07	5.226e-07	-6.283	-6.282	0.001	-14.55
CaOH+	9.851e-11	8.725e-11	-10.007	-10.059	-0.053	(0)
CaHSO4+	4.761e-11	4.216e-11	-10.322	-10.375	-0.053	(0)
Cl	2.386e-03					
Cl-	2.386e-03	2.109e-03	-2.622	-2.676	-0.053	18.38
H(0)	1.546e-21					
H2	7.731e-22	7.756e-22	-21.112	-21.110	0.001	28.59
K	9.191e-04					
K+	9.185e-04	8.115e-04	-3.037	-3.091	-0.054	9.52
KSO4-	6.230e-07	5.544e-07	-6.205	-6.256	-0.051	34.42
Mg	5.682e-04					
Mg+2	5.283e-04	3.338e-04	-3.277	-3.477	-0.199	-22.15
MgHCO3+	3.108e-05	2.750e-05	-4.508	-4.561	-0.053	5.86
MgSO4	8.649e-06	8.676e-06	-5.063	-5.062	0.001	6.35
MgCO3	2.017e-07	2.023e-07	-6.695	-6.694	0.001	-17.10
MgOH+	7.119e-09	6.360e-09	-8.148	-8.197	-0.049	(0)
Na	1.137e-02					
Na+	1.134e-02	1.006e-02	-1.946	-1.997	-0.052	-0.66
NaHCO3	3.283e-05	3.293e-05	-4.484	-4.482	0.001	1.80
NaSO4-	4.622e-06	4.113e-06	-5.335	-5.386	-0.051	13.69
NaCO3-	2.308e-07	2.044e-07	-6.637	-6.689	-0.053	0.05
NaOH	4.128e-20	4.141e-20	-19.384	-19.383	0.001	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-45.057	-45.056	0.001	31.49
S(6)	1.386e-04					
SO4-2	1.185e-04	7.378e-05	-3.926	-4.132	-0.206	16.23
MgSO4	8.649e-06	8.676e-06	-5.063	-5.062	0.001	6.35
CaSO4	6.154e-06	6.173e-06	-5.211	-5.210	0.001	8.01
NaSO4-	4.622e-06	4.113e-06	-5.335	-5.386	-0.051	13.69
KSO4-	6.230e-07	5.544e-07	-6.205	-6.256	-0.051	34.42
HSO4-	9.476e-09	8.393e-09	-8.023	-8.076	-0.053	41.15
CaHSO4+	4.761e-11	4.216e-11	-10.322	-10.375	-0.053	(0)

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

Phase	SI**	log IAP	log K(314 K, 1 atm)	
Anhydrite	-3.04	-7.51	-4.47	CaSO4
Aragonite	-1.23	-9.69	-8.46	CaCO3
Calcite	-1.05	-9.69	-8.64	CaCO3
CO2(g)	-0.36	-2.00	-1.64	CO2
Dolomite	-2.03	-19.47	-17.44	CaMg(CO3)2
Gypsum	-2.91	-7.51	-4.60	CaSO4:2H2O
H2(g)	-17.98	-21.11	-3.13	H2
H2O(g)	-1.10	-0.00	1.10	H2O
Halite	-6.26	-4.67	1.58	NaCl
O2(g)	-42.06	-45.06	-2.99	O2
Sylvite	-6.75	-5.77	0.98	KCl

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

End of simulation.

Reading input data for simulation 14.

```
      Solution 34 #LF34 Torno
      temp  39.4
      pH    6.2
      pe    2.294
      redox pe
      units mg/l
      Alkalinity  610.1 as Ca.5CO3.5
      Cl    90.8
      S(6)  12.8
      Na    284
      Mg    14.5
      K     31.9
      Ca    28.7
      Si    142.10 as SiO2
      Al    0.167
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 34.

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

      Elements           Molality       Moles

      Al                 6.197e-06   6.197e-06
      Alkalinity         6.937e-03   6.937e-03
      Ca                 7.169e-04   7.169e-04
      Cl                 2.564e-03   2.564e-03
      K                  8.168e-04   8.168e-04
      Mg                 5.971e-04   5.971e-04
      Na                 1.237e-02   1.237e-02
      S(6)               1.334e-04   1.334e-04
      Si                 2.368e-03   2.368e-03

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

                                       pH  =   6.200
                                       pe  =   2.294
      Specific Conductance (µS/cm,  39°C)  = 1601
                           Density (g/cm³)  =   0.99330
                                Volume (L)  =   1.00820
                        Activity of water  =   0.999
                  Ionic strength (mol/kgw)  =   1.398e-02
                       Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)  =   1.449e-02
                     Total CO2 (mol/kg)  =   1.449e-02
                       Temperature (°C)  =  39.40
                   Electrical balance (eq)  =   6.063e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  23.98
                                 Iterations  =   7
                                    Total H  = 1.110288e+02
                                    Total O  = 5.555214e+01

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

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

   H+             7.011e-07   6.310e-07    -6.154    -6.200    -0.046      0.00
   OH-            5.054e-08   4.458e-08    -7.296    -7.351    -0.054     -3.68
   H2O            5.551e+01   9.994e-01     1.744    -0.000     0.000     18.15
Al             6.197e-06
   Al(OH)4-       3.705e-06   3.282e-06    -5.431    -5.484    -0.053      (0)
   Al(OH)2+       1.580e-06   1.404e-06    -5.801    -5.853    -0.051      (0)
   Al(OH)3        8.523e-07   8.550e-07    -6.069    -6.068     0.001      (0)
   AlOH+2         5.716e-08   3.570e-08    -7.243    -7.447    -0.204    -28.03
```

Al+3	2.360e-09	9.140e-10	-8.627	-9.039	-0.412	-42.74
AlSO4+	2.757e-10	2.442e-10	-9.560	-9.612	-0.053	(0)
Al(SO4)2-	6.571e-13	5.821e-13	-12.182	-12.235	-0.053	(0)
AlHSO4+2	2.599e-17	1.593e-17	-16.585	-16.798	-0.213	(0)
C(4)	1.449e-02					
CO2	7.573e-03	7.597e-03	-2.121	-2.119	0.001	35.13
HCO3-	6.805e-03	6.050e-03	-2.167	-2.218	-0.051	25.56
CaHCO3+	4.251e-05	3.788e-05	-4.371	-4.422	-0.050	10.17
NaHCO3	3.430e-05	3.441e-05	-4.465	-4.463	0.001	1.80
MgHCO3+	3.059e-05	2.705e-05	-4.514	-4.568	-0.054	5.84
(CO2)2	1.636e-06	1.641e-06	-5.786	-5.785	0.001	70.26
CO3-2	9.142e-07	5.710e-07	-6.039	-6.243	-0.204	-4.50
CaCO3	5.658e-07	5.677e-07	-6.247	-6.246	0.001	-14.56
NaCO3-	2.626e-07	2.324e-07	-6.581	-6.634	-0.053	-0.02
MgCO3	2.380e-07	2.388e-07	-6.623	-6.622	0.001	-17.10
Ca	7.169e-04					
Ca+2	6.681e-04	4.169e-04	-3.175	-3.380	-0.205	-17.81
CaHCO3+	4.251e-05	3.788e-05	-4.371	-4.422	-0.050	10.17
CaSO4	5.793e-06	5.811e-06	-5.237	-5.236	0.001	7.95
CaCO3	5.658e-07	5.677e-07	-6.247	-6.246	0.001	-14.56
CaOH+	1.239e-10	1.096e-10	-9.907	-9.960	-0.053	(0)
CaHSO4+	3.423e-11	3.029e-11	-10.466	-10.519	-0.053	(0)
Cl	2.564e-03					
Cl-	2.564e-03	2.265e-03	-2.591	-2.645	-0.054	18.38
H(0)	1.265e-20					
H2	6.327e-21	6.347e-21	-20.199	-20.197	0.001	28.59
K	8.168e-04					
K+	8.163e-04	7.205e-04	-3.088	-3.142	-0.054	9.47
KSO4-	5.117e-07	4.549e-07	-6.291	-6.342	-0.051	34.41
Mg	5.971e-04					
Mg+2	5.580e-04	3.513e-04	-3.253	-3.454	-0.201	-22.06
MgHCO3+	3.059e-05	2.705e-05	-4.514	-4.568	-0.054	5.84
MgSO4	8.269e-06	8.296e-06	-5.083	-5.081	0.001	6.29
MgCO3	2.380e-07	2.388e-07	-6.623	-6.622	0.001	-17.10
MgOH+	7.825e-09	6.985e-09	-8.107	-8.156	-0.049	(0)
Na	1.237e-02					
Na+	1.233e-02	1.093e-02	-1.909	-1.961	-0.052	-0.73
NaHCO3	3.430e-05	3.441e-05	-4.465	-4.463	0.001	1.80
NaSO4-	4.755e-06	4.227e-06	-5.323	-5.374	-0.051	13.85
NaCO3-	2.626e-07	2.324e-07	-6.581	-6.634	-0.053	-0.02
NaOH	4.858e-20	4.874e-20	-19.314	-19.312	0.001	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-47.554	-47.553	0.001	31.36
S(6)	1.334e-04					
SO4-2	1.141e-04	7.072e-05	-3.943	-4.150	-0.208	16.12
MgSO4	8.269e-06	8.296e-06	-5.083	-5.081	0.001	6.29
CaSO4	5.793e-06	5.811e-06	-5.237	-5.236	0.001	7.95
NaSO4-	4.755e-06	4.227e-06	-5.323	-5.374	-0.051	13.85
KSO4-	5.117e-07	4.549e-07	-6.291	-6.342	-0.051	34.41
HSO4-	6.829e-09	6.042e-09	-8.166	-8.219	-0.053	41.08
AlSO4+	2.757e-10	2.442e-10	-9.560	-9.612	-0.053	(0)
CaHSO4+	3.423e-11	3.029e-11	-10.466	-10.519	-0.053	(0)
Al(SO4)2-	6.571e-13	5.821e-13	-12.182	-12.235	-0.053	(0)
AlHSO4+2	2.599e-17	1.593e-17	-16.585	-16.798	-0.213	(0)
Si	2.368e-03					
H4SiO4	2.367e-03	2.375e-03	-2.626	-2.624	0.001	51.07
H3SiO4-	9.915e-07	8.766e-07	-6.004	-6.057	-0.054	28.24
H2SiO4-2	3.579e-13	2.235e-13	-12.446	-12.651	-0.204	(0)

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

Phase	SI**	log IAP	log K(312 K, 1 atm)	
Al(OH)3(a)	-0.34	9.56	9.91	Al(OH)3
Albite	1.81	-15.32	-17.13	NaAlSi3O8
Alunite	1.73	-1.36	-3.10	KAl3(SO4)2(OH)6
Anhydrite	-3.09	-7.53	-4.44	CaSO4
Anorthite	-0.27	-19.59	-19.32	CaAl2Si2O8

```
  Aragonite          -1.18     -9.62   -8.44  CaCO3
  Ca-Montmorillonite   7.69    -35.36  -43.06  Ca0.165Al2.33Si3.67O10(OH)2
  Calcite            -1.01     -9.62   -8.61  CaCO3
  Chalcedony          0.77     -2.62   -3.39  SiO2
  Chlorite(14A)      -7.29     55.98   63.26  Mg5Al2Si3O10(OH)8
  Chrysotile         -8.91     21.59   30.50  Mg3Si2O5(OH)4
  CO2(g)             -0.50     -2.12   -1.62  CO2
  Dolomite           -1.94    -19.32  -17.38  CaMg(CO3)2
  Gibbsite            2.22      9.56    7.34  Al(OH)3
  Gypsum             -2.94     -7.53   -4.60  CaSO4:2H2O
  H2(g)             -17.07    -20.20   -3.13  H2
  H2O(g)             -1.15     -0.00    1.15  H2O
  Halite             -6.19     -4.61    1.58  NaCl
  Illite              6.44    -31.98  -38.42  K0.6Mg0.25Al2.3Si3.5O10(OH)2
  K-feldspar          3.03    -16.50  -19.53  KAlSi3O8
  K-mica             13.17     23.87   10.70  KAl3Si3O10(OH)2
  Kaolinite           7.63     13.87    6.24  Al2Si2O5(OH)4
  O2(g)             -44.57    -47.55   -2.98  O2
  Quartz              1.15     -2.62   -3.78  SiO2
  Sepiolite          -5.38     10.02   15.40  Mg2Si3O7.5OH:3H2O
  Sepiolite(d)       -8.64     10.02   18.66  Mg2Si3O7.5OH:3H2O
  SiO2(a)            -0.03     -2.62   -2.60  SiO2
  Sylvite            -6.76     -5.79    0.97  KCl
  Talc               -3.49     16.34   19.83  Mg3Si4O10(OH)2

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

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

------------------------------------
Reading input data for simulation 15.
------------------------------------

      Solution 35 #LF35 Nostra
      temp  18
      pH    6.5
      pe    4
      redox pe
      units mg/l
      Alkalinity  103.6 as Ca.5CO3.5
      Cl    22.7
      S(6)  7.5
      Na    45.2
      Mg    2.9
      K     13.6
      Ca    6.6
      END
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 35.

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

      Elements           Molality       Moles

      Alkalinity        1.177e-03   1.177e-03
      Ca                1.647e-04   1.647e-04
      Cl                6.404e-04   6.404e-04
      K                 3.479e-04   3.479e-04
      Mg                1.193e-04   1.193e-04
      Na                1.966e-03   1.966e-03
      S(6)              7.809e-05   7.809e-05
```

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

pH	= 6.500
pe	= 4.000
Specific Conductance (µS/cm, 18°C)	= 218
Density (g/cm³)	= 0.99874
Volume (L)	= 1.00147
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 2.772e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 2.049e-03
Total CO2 (mol/kg)	= 2.049e-03
Temperature (°C)	= 18.00
Electrical balance (eq)	= 9.090e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 18.79
Iterations	= 8
Total H	= 1.110136e+02
Total O	= 5.551180e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	3.334e-07	3.162e-07	-6.477	-6.500	-0.023	0.00
OH-	1.950e-08	1.841e-08	-7.710	-7.735	-0.025	-4.42
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.04
C(4)	2.049e-03					
HCO3-	1.173e-03	1.109e-03	-2.931	-2.955	-0.024	24.11
CO2	8.717e-04	8.723e-04	-3.060	-3.059	0.000	34.09
CaHCO3+	1.706e-06	1.615e-06	-5.768	-5.792	-0.024	9.39
MgHCO3+	1.254e-06	1.184e-06	-5.902	-5.927	-0.025	5.27
NaHCO3	1.205e-06	1.206e-06	-5.919	-5.919	0.000	1.80
CO3-2	1.762e-07	1.409e-07	-6.754	-6.851	-0.097	-5.91
CaCO3	2.706e-08	2.708e-08	-7.568	-7.567	0.000	-14.62
MgCO3	1.130e-08	1.131e-08	-7.947	-7.947	0.000	-17.08
(CO2)2	1.097e-08	1.098e-08	-7.960	-7.959	0.000	68.17
NaCO3-	3.593e-09	3.393e-09	-8.445	-8.469	-0.025	-1.76
Ca	1.647e-04					
Ca+2	1.617e-04	1.292e-04	-3.791	-3.889	-0.097	-18.17
CaHCO3+	1.706e-06	1.615e-06	-5.768	-5.792	-0.024	9.39
CaSO4	1.303e-06	1.304e-06	-5.885	-5.885	0.000	7.21
CaCO3	2.706e-08	2.708e-08	-7.568	-7.567	0.000	-14.62
CaOH+	7.179e-11	6.781e-11	-10.144	-10.169	-0.025	(0)
CaHSO4+	2.611e-12	2.466e-12	-11.583	-11.608	-0.025	(0)
Cl	6.404e-04					
Cl-	6.404e-04	6.047e-04	-3.194	-3.218	-0.025	17.84
H(0)	1.520e-24					
H2	7.598e-25	7.603e-25	-24.119	-24.119	0.000	28.61
K	3.479e-04					
K+	3.477e-04	3.283e-04	-3.459	-3.484	-0.025	8.78
KSO4-	1.289e-07	1.219e-07	-6.890	-6.914	-0.024	33.91
Mg	1.193e-04					
Mg+2	1.169e-04	9.366e-05	-3.932	-4.028	-0.096	-21.49
MgHCO3+	1.254e-06	1.184e-06	-5.902	-5.927	-0.025	5.27
MgSO4	1.092e-06	1.093e-06	-5.962	-5.961	0.000	5.54
MgCO3	1.130e-08	1.131e-08	-7.947	-7.947	0.000	-17.08
MgOH+	5.947e-10	5.629e-10	-9.226	-9.250	-0.024	(0)
Na	1.966e-03					
Na+	1.965e-03	1.857e-03	-2.707	-2.731	-0.025	-1.86
NaHCO3	1.205e-06	1.206e-06	-5.919	-5.919	0.000	1.80
NaSO4-	5.630e-07	5.323e-07	-6.250	-6.274	-0.024	14.08
NaCO3-	3.593e-09	3.393e-09	-8.445	-8.469	-0.025	-1.76
NaOH	3.415e-21	3.418e-21	-20.467	-20.466	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-46.456	-46.455	0.000	29.80
S(6)	7.809e-05					
SO4-2	7.500e-05	5.987e-05	-4.125	-4.223	-0.098	13.53

CaSO4	1.303e-06	1.304e-06	-5.885	-5.885	0.000	7.21
MgSO4	1.092e-06	1.093e-06	-5.962	-5.961	0.000	5.54
NaSO4-	5.630e-07	5.323e-07	-6.250	-6.274	-0.024	14.08
KSO4-	1.289e-07	1.219e-07	-6.890	-6.914	-0.024	33.91
HSO4-	1.680e-09	1.587e-09	-8.775	-8.799	-0.025	39.76
CaHSO4+	2.611e-12	2.466e-12	-11.583	-11.608	-0.025	(0)

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

Phase	SI**	log IAP	log K(291 K, 1 atm)	
Anhydrite	-3.91	-8.11	-4.20	CaSO4
Aragonite	-2.45	-10.74	-8.29	CaCO3
Calcite	-2.30	-10.74	-8.44	CaCO3
CO2(g)	-1.68	-3.06	-1.38	CO2
Dolomite	-4.64	-21.62	-16.97	CaMg(CO3)2
Gypsum	-3.53	-8.11	-4.59	CaSO4:2H2O
H2(g)	-21.04	-24.12	-3.08	H2
H2O(g)	-1.69	-0.00	1.69	H2O
Halite	-7.51	-5.95	1.56	NaCl
O2(g)	-43.62	-46.46	-2.84	O2
Sylvite	-7.57	-6.70	0.86	KCl

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

End of simulation.

Reading input data for simulation 16.

```
Solution 36 #LF36 Helena
temp  15.2
pH    5.3
pe    4
redox pe
units mg/l
Alkalinity  66.2  as Ca.5CO3.5
Cl    17.2
S(6)  4.6
Na    20.1
Mg    4.8
K     8.3
Ca    6.3
END
```

Beginning of initial solution calculations.

Initial solution 36.

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

Elements	Molality	Moles
Alkalinity	7.519e-04	7.519e-04
Ca	1.572e-04	1.572e-04
Cl	4.852e-04	4.852e-04
K	2.123e-04	2.123e-04
Mg	1.975e-04	1.975e-04
Na	8.744e-04	8.744e-04
S(6)	4.789e-05	4.789e-05

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

pH	= 5.300
pe	= 4.000
Specific Conductance (µS/cm, 15°C)	= 135
Density (g/cm³)	= 0.99925
Volume (L)	= 1.00127
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 1.959e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 1.018e-02
Total CO2 (mol/kg)	= 1.018e-02
Temperature (°C)	= 15.20
Electrical balance (eq)	= 4.631e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 14.82
Iterations	= 9
Total H	= 1.110132e+02
Total O	= 5.552753e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	5.244e-06	5.012e-06	-5.280	-5.300	-0.020	0.00
OH-	9.663e-10	9.203e-10	-9.015	-9.036	-0.021	-4.60
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.03
C(4)	1.018e-02					
CO2	9.421e-03	9.425e-03	-2.026	-2.026	0.000	33.94
HCO3-	7.544e-04	7.195e-04	-3.122	-3.143	-0.021	23.81
MgHCO3+	1.380e-06	1.315e-06	-5.860	-5.881	-0.021	5.15
(CO2)2	1.157e-06	1.158e-06	-5.937	-5.936	0.000	67.88
CaHCO3+	1.028e-06	9.803e-07	-5.988	-6.009	-0.020	9.25
NaHCO3	3.568e-07	3.569e-07	-6.448	-6.447	0.000	1.80
CO3-2	6.505e-09	5.380e-09	-8.187	-8.269	-0.082	-6.35
CaCO3	9.904e-10	9.909e-10	-9.004	-9.004	0.000	-14.63
MgCO3	7.128e-10	7.132e-10	-9.147	-9.147	0.000	-17.08
NaCO3-	5.254e-11	5.006e-11	-10.280	-10.300	-0.021	-2.15
Ca	1.572e-04					
Ca+2	1.554e-04	1.285e-04	-3.809	-3.891	-0.083	-18.26
CaHCO3+	1.028e-06	9.803e-07	-5.988	-6.009	-0.020	9.25
CaSO4	8.004e-07	8.007e-07	-6.097	-6.097	0.000	7.07
CaCO3	9.904e-10	9.909e-10	-9.004	-9.004	0.000	-14.63
CaHSO4+	2.434e-11	2.319e-11	-10.614	-10.635	-0.021	(0)
CaOH+	4.464e-12	4.254e-12	-11.350	-11.371	-0.021	(0)
Cl	4.852e-04					
Cl-	4.852e-04	4.622e-04	-3.314	-3.335	-0.021	17.70
H(0)	3.932e-22					
H2	1.966e-22	1.967e-22	-21.706	-21.706	0.000	28.62
K	2.123e-04					
K+	2.122e-04	2.022e-04	-3.673	-3.694	-0.021	8.65
KSO4-	4.720e-08	4.501e-08	-7.326	-7.347	-0.021	33.79
Mg	1.975e-04					
Mg+2	1.950e-04	1.615e-04	-3.710	-3.792	-0.082	-21.41
MgHCO3+	1.380e-06	1.315e-06	-5.860	-5.881	-0.021	5.15
MgSO4	1.102e-06	1.102e-06	-5.958	-5.958	0.000	5.41
MgCO3	7.128e-10	7.132e-10	-9.147	-9.147	0.000	-17.08
MgOH+	4.908e-11	4.684e-11	-10.309	-10.329	-0.020	(0)
Na	8.744e-04					
Na+	8.739e-04	8.330e-04	-3.059	-3.079	-0.021	-2.06
NaHCO3	3.568e-07	3.569e-07	-6.448	-6.447	0.000	1.80
NaSO4-	1.552e-07	1.480e-07	-6.809	-6.830	-0.021	14.04
NaCO3-	5.254e-11	5.006e-11	-10.280	-10.300	-0.021	-2.15
NaOH	7.663e-23	7.666e-23	-22.116	-22.115	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-52.238	-52.238	0.000	29.53
S(6)	4.789e-05					
SO4-2	4.577e-05	3.781e-05	-4.339	-4.422	-0.083	12.97
MgSO4	1.102e-06	1.102e-06	-5.958	-5.958	0.000	5.41
CaSO4	8.004e-07	8.007e-07	-6.097	-6.097	0.000	7.07

NaSO4-	1.552e-07	1.480e-07	-6.809	-6.830	-0.021	14.04
KSO4-	4.720e-08	4.501e-08	-7.326	-7.347	-0.021	33.79
HSO4-	1.575e-08	1.501e-08	-7.803	-7.824	-0.021	39.48
CaHSO4+	2.434e-11	2.319e-11	-10.614	-10.635	-0.021	(0)

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

Phase	SI**	log IAP	log K(288 K, 1 atm)	
Anhydrite	-4.14	-8.31	-4.17	CaSO4
Aragonite	-3.88	-12.16	-8.28	CaCO3
Calcite	-3.74	-12.16	-8.42	CaCO3
CO2(g)	-0.68	-2.03	-1.34	CO2
Dolomite	-7.28	-24.22	-16.94	CaMg(CO3)2
Gypsum	-3.72	-8.31	-4.59	CaSO4:2H2O
H2(g)	-18.63	-21.71	-3.07	H2
H2O(g)	-1.76	-0.00	1.76	H2O
Halite	-7.98	-6.41	1.56	NaCl
O2(g)	-49.42	-52.24	-2.81	O2
Sylvite	-7.88	-7.03	0.85	KCl

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

End of simulation.

Reading input data for simulation 17.

```
      Solution 37 #LF37  Glória Patri
      temp  14.5
      pH    6.8
      pe    6.661
      redox pe
      units mg/l
      Alkalinity  75.8  as Ca.5CO3.5
      Cl    18.5
      S(6)  4.8
      Na    24.1
      Mg    5
      K     11.7
      Ca    5.6
      END
```

Beginning of initial solution calculations.

Initial solution 37.

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

Elements	Molality	Moles
Alkalinity	8.610e-04	8.610e-04
Ca	1.397e-04	1.397e-04
Cl	5.219e-04	5.219e-04
K	2.993e-04	2.993e-04
Mg	2.057e-04	2.057e-04
Na	1.048e-03	1.048e-03
S(6)	4.997e-05	4.997e-05

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

pH = 6.800
pe = 6.661

Specific Conductance (µS/cm, 15°C)	= 147
Density (g/cm³)	= 0.99927
Volume (L)	= 1.00086
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 2.143e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 1.203e-03
Total CO2 (mol/kg)	= 1.203e-03
Temperature (°C)	= 14.50
Electrical balance (eq)	= 5.557e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 15.85
Iterations	= 6
Total H	= 1.110133e+02
Total O	= 5.550968e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.661e-07	1.585e-07	-6.780	-6.800	-0.020	0.00
OH-	2.886e-08	2.744e-08	-7.540	-7.562	-0.022	-4.65
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.03
C(4)	1.203e-03					
HCO3-	8.574e-04	8.161e-04	-3.067	-3.088	-0.021	23.73
CO2	3.423e-04	3.425e-04	-3.466	-3.465	0.000	33.90
MgHCO3+	1.617e-06	1.538e-06	-5.791	-5.813	-0.022	5.13
CaHCO3+	1.012e-06	9.640e-07	-5.995	-6.016	-0.021	9.21
NaHCO3	4.863e-07	4.865e-07	-6.313	-6.313	0.000	1.80
CO3-2	2.309e-07	1.895e-07	-6.637	-6.722	-0.086	-6.45
CaCO3	3.049e-08	3.051e-08	-7.516	-7.516	0.000	-14.64
MgCO3	2.565e-08	2.566e-08	-7.591	-7.591	0.000	-17.08
NaCO3-	2.137e-09	2.032e-09	-8.670	-8.692	-0.022	-2.25
(CO2)2	1.489e-09	1.490e-09	-8.827	-8.827	0.000	67.81
Ca	1.397e-04					
Ca+2	1.380e-04	1.132e-04	-3.860	-3.946	-0.086	-18.27
CaHCO3+	1.012e-06	9.640e-07	-5.995	-6.016	-0.021	9.21
CaSO4	7.269e-07	7.273e-07	-6.138	-6.138	0.000	7.04
CaCO3	3.049e-08	3.051e-08	-7.516	-7.516	0.000	-14.64
CaOH+	1.246e-10	1.185e-10	-9.904	-9.926	-0.022	(0)
CaHSO4+	6.946e-13	6.606e-13	-12.158	-12.180	-0.022	(0)
Cl	5.219e-04					
Cl-	5.219e-04	4.962e-04	-3.282	-3.304	-0.022	17.66
H(0)	1.887e-30					
H2	9.437e-31	9.442e-31	-30.025	-30.025	0.000	28.62
K	2.993e-04					
K+	2.992e-04	2.844e-04	-3.524	-3.546	-0.022	8.62
KSO4-	6.807e-08	6.479e-08	-7.167	-7.188	-0.021	33.77
Mg	2.057e-04					
Mg+2	2.029e-04	1.667e-04	-3.693	-3.778	-0.085	-21.38
MgHCO3+	1.617e-06	1.538e-06	-5.791	-5.813	-0.022	5.13
MgSO4	1.157e-06	1.158e-06	-5.937	-5.936	0.000	5.37
MgCO3	2.565e-08	2.566e-08	-7.591	-7.591	0.000	-17.08
MgOH+	1.501e-09	1.429e-09	-8.824	-8.845	-0.021	(0)
Na	1.048e-03					
Na+	1.048e-03	9.967e-04	-2.980	-3.001	-0.022	-2.11
NaHCO3	4.863e-07	4.865e-07	-6.313	-6.313	0.000	1.80
NaSO4-	1.920e-07	1.828e-07	-6.717	-6.738	-0.021	14.06
NaCO3-	2.137e-09	2.032e-09	-8.670	-8.692	-0.022	-2.25
NaOH	2.733e-21	2.735e-21	-20.563	-20.563	0.000	(0)
O(0)	2.873e-36					
O2	1.437e-36	1.437e-36	-35.843	-35.842	0.000	29.45
S(6)	4.997e-05					
SO4-2	4.783e-05	3.920e-05	-4.320	-4.407	-0.086	12.83
MgSO4	1.157e-06	1.158e-06	-5.937	-5.936	0.000	5.37
CaSO4	7.269e-07	7.273e-07	-6.138	-6.138	0.000	7.04
NaSO4-	1.920e-07	1.828e-07	-6.717	-6.738	-0.021	14.06
KSO4-	6.807e-08	6.479e-08	-7.167	-7.188	-0.021	33.77

```
   HSO4-          5.104e-10   4.853e-10    -9.292    -9.314    -0.022     39.42
   CaHSO4+        6.946e-13   6.606e-13   -12.158   -12.180    -0.022     (0)

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

  Phase               SI** log IAP   log K(287 K,   1 atm)

  Anhydrite         -4.19     -8.35   -4.17  CaSO4
  Aragonite         -2.39    -10.67   -8.28  CaCO3
  Calcite           -2.25    -10.67   -8.42  CaCO3
  CO2(g)            -2.13     -3.47   -1.33  CO2
  Dolomite          -4.24    -21.17  -16.93  CaMg(CO3)2
  Gypsum            -3.76     -8.35   -4.59  CaSO4:2H2O
  H2(g)            -26.95    -30.02   -3.07  H2
  H2O(g)            -1.78     -0.00    1.78  H2O
  Halite            -7.87     -6.31    1.56  NaCl
  O2(g)            -33.03    -35.84   -2.81  O2
  Sylvite           -7.70     -6.85    0.85  KCl

**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 18.
------------------------------------

      Solution 38 #LF38 Estrada RQ
      temp  45.9
      pH    6.4
      pe    4
      redox pe
      units mg/l
      Alkalinity  542.5 as Ca.5CO3.5
      Cl    152.8
      S(6)  11
      Na    162.9
      Mg    14.5
      K     21.8
      Ca    53.3
      END
------------------------------------------
Beginning of initial solution calculations.
------------------------------------------

Initial solution 38.

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

      Elements           Molality       Moles

      Alkalinity        6.167e-03   6.167e-03
      Ca                1.331e-03   1.331e-03
      Cl                4.314e-03   4.314e-03
      K                 5.581e-04   5.581e-04
      Mg                5.970e-04   5.970e-04
      Na                7.093e-03   7.093e-03
      S(6)              1.146e-04   1.146e-04

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

                                     pH  =   6.400
                                     pe  =   4.000
      Specific Conductance (µS/cm,  46°C)  = 1622
                          Density (g/cm³)  =   0.99045
```

Volume (L)	= 1.01063
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 1.285e-02
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 1.032e-02
Total CO2 (mol/kg)	= 1.032e-02
Temperature (°C)	= 45.90
Electrical balance (eq)	= 7.964e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 3.64
Iterations	= 8
Total H	= 1.110186e+02
Total O	= 5.553347e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	4.415e-07	3.981e-07	-6.355	-6.400	-0.045	0.00
OH-	1.211e-07	1.071e-07	-6.917	-6.970	-0.053	-3.67
H2O	5.551e+01	9.996e-01	1.744	-0.000	0.000	18.20
C(4)	1.032e-02					
HCO3-	6.039e-03	5.383e-03	-2.219	-2.269	-0.050	25.74
CO2	4.153e-03	4.165e-03	-2.382	-2.380	0.001	35.45
CaHCO3+	7.447e-05	6.652e-05	-4.128	-4.177	-0.049	10.30
MgHCO3+	2.890e-05	2.562e-05	-4.539	-4.591	-0.052	5.90
NaHCO3	1.699e-05	1.704e-05	-4.770	-4.768	0.001	1.80
CaCO3	1.960e-06	1.966e-06	-5.708	-5.706	0.001	-14.54
CO3-2	1.378e-06	8.697e-07	-5.861	-6.061	-0.200	-4.70
(CO2)2	5.857e-07	5.874e-07	-6.232	-6.231	0.001	70.90
MgCO3	4.059e-07	4.071e-07	-6.392	-6.390	0.001	-17.10
NaCO3-	3.074e-07	2.727e-07	-6.512	-6.564	-0.052	0.13
Ca	1.331e-03					
Ca+2	1.245e-03	7.853e-04	-2.905	-3.105	-0.200	-17.86
CaHCO3+	7.447e-05	6.652e-05	-4.128	-4.177	-0.049	10.30
CaSO4	9.526e-06	9.555e-06	-5.021	-5.020	0.001	8.10
CaCO3	1.960e-06	1.966e-06	-5.708	-5.706	0.001	-14.54
CaOH+	3.688e-10	3.272e-10	-9.433	-9.485	-0.052	(0)
CaHSO4+	3.978e-11	3.529e-11	-10.400	-10.452	-0.052	(0)
Cl	4.314e-03					
Cl-	4.314e-03	3.822e-03	-2.365	-2.418	-0.053	18.36
H(0)	1.842e-24					
H2	9.210e-25	9.237e-25	-24.036	-24.034	0.001	28.59
K	5.581e-04					
K+	5.577e-04	4.938e-04	-3.254	-3.306	-0.053	9.59
KSO4-	3.234e-07	2.883e-07	-6.490	-6.540	-0.050	34.43
Mg	5.970e-04					
Mg+2	5.595e-04	3.558e-04	-3.252	-3.449	-0.197	-22.31
MgHCO3+	2.890e-05	2.562e-05	-4.539	-4.591	-0.052	5.90
MgSO4	8.128e-06	8.152e-06	-5.090	-5.089	0.001	6.44
MgCO3	4.059e-07	4.071e-07	-6.392	-6.390	0.001	-17.10
MgOH+	2.115e-08	1.892e-08	-7.675	-7.723	-0.048	(0)
Na	7.093e-03					
Na+	7.073e-03	6.289e-03	-2.150	-2.201	-0.051	-0.53
NaHCO3	1.699e-05	1.704e-05	-4.770	-4.768	0.001	1.80
NaSO4-	2.365e-06	2.108e-06	-5.626	-5.676	-0.050	13.38
NaCO3-	3.074e-07	2.727e-07	-6.512	-6.564	-0.052	0.13
NaOH	6.717e-20	6.737e-20	-19.173	-19.172	0.001	(0)
O(0)	1.956e-38					
O2	9.781e-39	9.810e-39	-38.010	-38.008	0.001	31.72
S(6)	1.146e-04					
SO4-2	9.427e-05	5.910e-05	-4.026	-4.228	-0.203	16.36
CaSO4	9.526e-06	9.555e-06	-5.021	-5.020	0.001	8.10
MgSO4	8.128e-06	8.152e-06	-5.090	-5.089	0.001	6.44
NaSO4-	2.365e-06	2.108e-06	-5.626	-5.676	-0.050	13.38
KSO4-	3.234e-07	2.883e-07	-6.490	-6.540	-0.050	34.43
HSO4-	4.213e-09	3.738e-09	-8.375	-8.427	-0.052	41.27
CaHSO4+	3.978e-11	3.529e-11	-10.400	-10.452	-0.052	(0)

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

Phase	SI**	log IAP	log K(319 K, 1 atm)	
Anhydrite	-2.81	-7.33	-4.52	CaSO4
Aragonite	-0.67	-9.17	-8.50	CaCO3
Calcite	-0.48	-9.17	-8.68	CaCO3
CO2(g)	-0.70	-2.38	-1.68	CO2
Dolomite	-1.13	-18.67	-17.55	CaMg(CO3)2
Gypsum	-2.73	-7.33	-4.61	CaSO4:2H2O
H2(g)	-20.90	-24.03	-3.13	H2
H2O(g)	-1.01	-0.00	1.01	H2O
Halite	-6.20	-4.62	1.59	NaCl
O2(g)	-35.00	-38.01	-3.01	O2
Sylvite	-6.72	-5.72	1.00	KCl

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

End of simulation.

Reading input data for simulation 19.

```
Solution 39 #LF39 Disimo
temp  14.3
pH    6.6
pe    4
redox pe
units mg/l
Alkalinity  68.6  as Ca.5CO3.5
Cl    19.8
S(6)  4.8
Na    26.1
Mg    4.4
K     8.2
Ca    4.6
END
```

Beginning of initial solution calculations.

Initial solution 39.

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

Elements	Molality	Moles
Alkalinity	7.792e-04	7.792e-04
Ca	1.148e-04	1.148e-04
Cl	5.586e-04	5.586e-04
K	2.097e-04	2.097e-04
Mg	1.810e-04	1.810e-04
Na	1.135e-03	1.135e-03
S(6)	4.997e-05	4.997e-05

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

pH = 6.600
pe = 4.000
Specific Conductance (µS/cm, 14°C) = 141
Density (g/cm³) = 0.99930
Volume (L) = 1.00084
Activity of water = 1.000

```
                Ionic strength (mol/kgw)  =   2.022e-03
                     Mass of water (kg)  =   1.000e+00
                  Total carbon (mol/kg)  =   1.273e-03
                     Total CO2 (mol/kg)  =   1.273e-03
                       Temperature (°C)  =  14.30
                Electrical balance (eq)  =   4.991e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  14.84
                              Iterations  =   7
                                 Total H  = 1.110132e+02
                                 Total O  = 5.550974e+01
```

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	2.630e-07	2.512e-07	-6.580	-6.600	-0.020	0.00
OH-	1.788e-08	1.702e-08	-7.748	-7.769	-0.021	-4.66
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.03
C(4)	1.273e-03					
HCO3-	7.766e-04	7.401e-04	-3.110	-3.131	-0.021	23.71
CO2	4.940e-04	4.942e-04	-3.306	-3.306	0.000	33.89
MgHCO3+	1.296e-06	1.234e-06	-5.887	-5.909	-0.021	5.12
CaHCO3+	7.541e-07	7.190e-07	-6.123	-6.143	-0.021	9.20
NaHCO3	4.789e-07	4.791e-07	-6.320	-6.320	0.000	1.80
CO3-2	1.308e-07	1.079e-07	-6.884	-6.967	-0.084	-6.49
CaCO3	1.431e-08	1.432e-08	-7.844	-7.844	0.000	-14.64
MgCO3	1.289e-08	1.289e-08	-7.890	-7.890	0.000	-17.08
(CO2)2	3.077e-09	3.079e-09	-8.512	-8.512	0.000	67.79
NaCO3-	1.303e-09	1.241e-09	-8.885	-8.906	-0.021	-2.29
Ca	1.148e-04					
Ca+2	1.134e-04	9.355e-05	-3.945	-4.029	-0.084	-18.28
CaHCO3+	7.541e-07	7.190e-07	-6.123	-6.143	-0.021	9.20
CaSO4	6.062e-07	6.064e-07	-6.217	-6.217	0.000	7.03
CaCO3	1.431e-08	1.432e-08	-7.844	-7.844	0.000	-14.64
CaOH+	6.490e-11	6.180e-11	-10.188	-10.209	-0.021	(0)
CaHSO4+	9.146e-13	8.709e-13	-12.039	-12.060	-0.021	(0)
Cl	5.586e-04					
Cl-	5.586e-04	5.318e-04	-3.253	-3.274	-0.021	17.65
H(0)	9.973e-25					
H2	4.986e-25	4.989e-25	-24.302	-24.302	0.000	28.62
K	2.097e-04					
K+	2.097e-04	1.996e-04	-3.678	-3.700	-0.021	8.61
KSO4-	4.804e-08	4.578e-08	-7.318	-7.339	-0.021	33.76
Mg	1.810e-04					
Mg+2	1.787e-04	1.476e-04	-3.748	-3.831	-0.083	-21.37
MgHCO3+	1.296e-06	1.234e-06	-5.887	-5.909	-0.021	5.12
MgSO4	1.029e-06	1.030e-06	-5.987	-5.987	0.000	5.36
MgCO3	1.289e-08	1.289e-08	-7.890	-7.890	0.000	-17.08
MgOH+	8.210e-10	7.830e-10	-9.086	-9.106	-0.021	(0)
Na	1.135e-03					
Na+	1.135e-03	1.081e-03	-2.945	-2.966	-0.021	-2.12
NaHCO3	4.789e-07	4.791e-07	-6.320	-6.320	0.000	1.80
NaSO4-	2.099e-07	2.001e-07	-6.678	-6.699	-0.021	14.05
NaCO3-	1.303e-09	1.241e-09	-8.885	-8.906	-0.021	-2.29
NaOH	1.839e-21	1.840e-21	-20.735	-20.735	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-47.358	-47.358	0.000	29.43
S(6)	4.997e-05					
SO4-2	4.808e-05	3.962e-05	-4.318	-4.402	-0.084	12.79
MgSO4	1.029e-06	1.030e-06	-5.987	-5.987	0.000	5.36
CaSO4	6.062e-07	6.064e-07	-6.217	-6.217	0.000	7.03
NaSO4-	2.099e-07	2.001e-07	-6.678	-6.699	-0.021	14.05
KSO4-	4.804e-08	4.578e-08	-7.318	-7.339	-0.021	33.76
HSO4-	8.132e-10	7.743e-10	-9.090	-9.111	-0.021	39.39
CaHSO4+	9.146e-13	8.709e-13	-12.039	-12.060	-0.021	(0)

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

Phase	SI**	log IAP	log K(287 K, 1 atm)	
Anhydrite	-4.27	-8.43	-4.16	CaSO4
Aragonite	-2.72	-11.00	-8.28	CaCO3
Calcite	-2.58	-11.00	-8.42	CaCO3
CO2(g)	-1.97	-3.31	-1.33	CO2
Dolomite	-4.87	-21.79	-16.93	CaMg(CO3)2
Gypsum	-3.84	-8.43	-4.59	CaSO4:2H2O
H2(g)	-21.23	-24.30	-3.07	H2
H2O(g)	-1.79	-0.00	1.79	H2O
Halite	-7.80	-6.24	1.56	NaCl
O2(g)	-44.55	-47.36	-2.81	O2
Sylvite	-7.82	-6.97	0.84	KCl

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

End of simulation.

Reading input data for simulation 20.

```
      Solution 39 #Nasc. Golf
      temp  13.4
      pH    6.64
      pe    4
      redox pe
      units mg/l
      Alkalinity  35    as Ca.5CO3.5
      Cl    15.0
      S(6)  3.2
      Na    20
      Mg    0.42
      K     8.1
      Ca    2.7
      Si    52.1 as SiO2
      END
```

Beginning of initial solution calculations.

Initial solution 39.

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

Elements	Molality	Moles
Alkalinity	3.976e-04	3.976e-04
Ca	6.737e-05	6.737e-05
Cl	4.232e-04	4.232e-04
K	2.072e-04	2.072e-04
Mg	1.728e-05	1.728e-05
Na	8.701e-04	8.701e-04
S(6)	3.332e-05	3.332e-05
Si	8.672e-04	8.672e-04

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

```
                                    pH  =   6.640
                                    pe  =   4.000
      Specific Conductance (µS/cm,  13°C)  = 91
                          Density (g/cm³)  =   0.99942
                               Volume (L)  =   1.00075
                      Activity of water  =   1.000
```

Ionic strength (mol/kgw)	= 1.183e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 6.341e-04
Total CO2 (mol/kg)	= 6.341e-04
Temperature (°C)	= 13.40
Electrical balance (eq)	= 3.592e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 16.85
Iterations	= 6
Total H	= 1.110163e+02
Total O	= 5.551148e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	2.375e-07	2.291e-07	-6.624	-6.640	-0.016	0.00
OH-	1.795e-08	1.728e-08	-7.746	-7.762	-0.017	-4.74
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.03
C(4)	6.341e-04					
HCO3-	3.968e-04	3.822e-04	-3.401	-3.418	-0.016	23.59
CO2	2.368e-04	2.369e-04	-3.626	-3.625	0.000	33.85
CaHCO3+	2.321e-07	2.236e-07	-6.634	-6.650	-0.016	9.14
NaHCO3	1.927e-07	1.928e-07	-6.715	-6.715	0.000	1.80
CO3-2	6.926e-08	5.965e-08	-7.160	-7.224	-0.065	-6.68
MgHCO3+	6.612e-08	6.365e-08	-7.180	-7.196	-0.016	5.07
CaCO3	4.825e-09	4.826e-09	-8.316	-8.316	0.000	-14.64
MgCO3	7.033e-10	7.035e-10	-9.153	-9.153	0.000	-17.08
(CO2)2	6.836e-10	6.837e-10	-9.165	-9.165	0.000	67.69
NaCO3-	5.257e-10	5.061e-10	-9.279	-9.296	-0.016	-2.44
Ca	6.737e-05					
Ca+2	6.687e-05	5.758e-05	-4.175	-4.240	-0.065	-18.33
CaSO4	2.642e-07	2.643e-07	-6.578	-6.578	0.000	6.98
CaHCO3+	2.321e-07	2.236e-07	-6.634	-6.650	-0.016	9.14
CaCO3	4.825e-09	4.826e-09	-8.316	-8.316	0.000	-14.64
CaOH+	4.332e-11	4.171e-11	-10.363	-10.380	-0.016	(0)
CaHSO4+	3.557e-13	3.425e-13	-12.449	-12.465	-0.016	(0)
Cl	4.232e-04					
Cl-	4.232e-04	4.074e-04	-3.374	-3.390	-0.017	17.59
H(0)	8.377e-25					
H2	4.189e-25	4.190e-25	-24.378	-24.378	0.000	28.62
K	2.072e-04					
K+	2.071e-04	1.994e-04	-3.684	-3.700	-0.017	8.56
KSO4-	3.329e-08	3.207e-08	-7.478	-7.494	-0.016	33.71
Mg	1.728e-05					
Mg+2	1.714e-05	1.477e-05	-4.766	-4.831	-0.065	-21.37
MgSO4	7.167e-08	7.169e-08	-7.145	-7.145	0.000	5.31
MgHCO3+	6.612e-08	6.365e-08	-7.180	-7.196	-0.016	5.07
MgCO3	7.033e-10	7.035e-10	-9.153	-9.153	0.000	-17.08
MgOH+	8.167e-11	7.871e-11	-10.088	-10.104	-0.016	(0)
Na	8.701e-04					
Na+	8.698e-04	8.376e-04	-3.061	-3.077	-0.016	-2.21
NaHCO3	1.927e-07	1.928e-07	-6.715	-6.715	0.000	1.80
NaSO4-	1.141e-07	1.099e-07	-6.943	-6.959	-0.016	13.97
NaCO3-	5.257e-10	5.061e-10	-9.279	-9.296	-0.016	-2.44
NaOH	1.447e-21	1.447e-21	-20.840	-20.839	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-47.520	-47.520	0.000	29.34
S(6)	3.332e-05					
SO4-2	3.283e-05	2.825e-05	-4.484	-4.549	-0.065	12.56
CaSO4	2.642e-07	2.643e-07	-6.578	-6.578	0.000	6.98
NaSO4-	1.141e-07	1.099e-07	-6.943	-6.959	-0.016	13.97
MgSO4	7.167e-08	7.169e-08	-7.145	-7.145	0.000	5.31
KSO4-	3.329e-08	3.207e-08	-7.478	-7.494	-0.016	33.71
HSO4-	5.139e-10	4.948e-10	-9.289	-9.306	-0.016	39.29
CaHSO4+	3.557e-13	3.425e-13	-12.449	-12.465	-0.016	(0)
Si	8.672e-04					
H4SiO4	8.669e-04	8.671e-04	-3.062	-3.062	0.000	53.24

H3SiO4-	3.749e-07	3.610e-07	-6.426	-6.443	-0.016	27.57
H2SiO4-2	5.539e-14	4.770e-14	-13.257	-13.322	-0.065	(0)

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

Phase	SI**	log IAP	log K(286 K, 1 atm)	
Anhydrite	-4.63	-8.79	-4.16	CaSO4
Aragonite	-3.19	-11.46	-8.27	CaCO3
Calcite	-3.05	-11.46	-8.41	CaCO3
Chalcedony	0.63	-3.06	-3.69	SiO2
Chrysotile	-14.47	19.22	33.69	Mg3Si2O5(OH)4
CO2(g)	-2.31	-3.63	-1.32	CO2
Dolomite	-6.60	-23.52	-16.92	CaMg(CO3)2
Gypsum	-4.20	-8.79	-4.59	CaSO4:2H2O
H2(g)	-21.31	-24.38	-3.07	H2
H2O(g)	-1.81	-0.00	1.81	H2O
Halite	-8.03	-6.47	1.56	NaCl
O2(g)	-44.72	-47.52	-2.80	O2
Quartz	1.10	-3.06	-4.16	SiO2
Sepiolite	-8.36	7.71	16.08	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-10.95	7.71	18.66	Mg2Si3O7.5OH:3H2O
SiO2(a)	-0.25	-3.06	-2.81	SiO2
Sylvite	-7.93	-7.09	0.84	KCl
Talc	-9.67	13.10	22.77	Mg3Si4O10(OH)2

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

End of simulation.

Reading input data for simulation 21.

```
Solution 40 #Média cápsulas
temp  19.66
pH    5.87
pe    4
redox pe
units mg/l
Cl    5.29
S(6)  1.81
Na    8.60
Mg    0.44
K     19.97
Ca    0.59
Al    0.138
Fe    0.01134
END
```

Beginning of initial solution calculations.

Initial solution 40.

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

Elements	Molality	Moles
Al	5.115e-06	5.115e-06
Ca	1.472e-05	1.472e-05
Cl	1.492e-04	1.492e-04
Fe	2.031e-07	2.031e-07
K	5.107e-04	5.107e-04
Mg	1.810e-05	1.810e-05

Na	3.741e-04	3.741e-04
S(6)	1.884e-05	1.884e-05

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

pH	= 5.870
pe	= 4.000
Specific Conductance (µS/cm, 20°C)	= 65
Density (g/cm³)	= 0.99830
Volume (L)	= 1.00174
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 6.257e-04
Mass of water (kg)	= 1.000e+00
Total alkalinity (eq/kg)	= 8.247e-06
Temperature (°C)	= 19.66
Electrical balance (eq)	= 7.711e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 67.35
Iterations	= 3
Total H	= 1.110124e+02
Total O	= 5.550630e+01

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.386e-06	1.349e-06	-5.858	-5.870	-0.012	0.00
OH-	5.080e-09	4.938e-09	-8.294	-8.306	-0.012	-4.35
H2O	5.551e+01	1.000e+00	1.744	-0.000	0.000	18.05
Al	5.115e-06					
Al(OH)2+	3.326e-06	3.234e-06	-5.478	-5.490	-0.012	(0)
AlOH+2	1.007e-06	9.007e-07	-5.997	-6.045	-0.048	-27.58
Al(OH)4-	3.167e-07	3.079e-07	-6.499	-6.512	-0.012	(0)
Al(OH)3	2.350e-07	2.350e-07	-6.629	-6.629	0.000	(0)
Al+3	2.219e-07	1.738e-07	-6.654	-6.760	-0.106	-41.96
AlSO4+	8.787e-09	8.544e-09	-8.056	-8.068	-0.012	(0)
Al(SO4)2-	4.519e-12	4.394e-12	-11.345	-11.357	-0.012	(0)
AlHSO4+2	1.095e-15	9.785e-16	-14.960	-15.009	-0.049	(0)
Ca	1.472e-05					
Ca+2	1.468e-05	1.313e-05	-4.833	-4.882	-0.048	-18.23
CaSO4	3.739e-08	3.739e-08	-7.427	-7.427	0.000	7.28
CaOH+	1.662e-12	1.616e-12	-11.779	-11.792	-0.012	(0)
CaHSO4+	3.170e-13	3.082e-13	-12.499	-12.511	-0.012	(0)
Cl	1.492e-04					
Cl-	1.492e-04	1.451e-04	-3.826	-3.838	-0.012	17.89
FeCl+	3.731e-11	3.627e-11	-10.428	-10.440	-0.012	(0)
FeCl+2	5.296e-19	4.735e-19	-18.276	-18.325	-0.049	(0)
FeCl2+	3.749e-22	3.645e-22	-21.426	-21.438	-0.012	(0)
FeCl3	5.287e-27	5.288e-27	-26.277	-26.277	0.000	(0)
Fe(2)	2.030e-07					
Fe+2	2.024e-07	1.811e-07	-6.694	-6.742	-0.048	-22.51
FeSO4	4.864e-10	4.864e-10	-9.313	-9.313	0.000	25.01
FeCl+	3.731e-11	3.627e-11	-10.428	-10.440	-0.012	(0)
FeOH+	2.909e-11	2.829e-11	-10.536	-10.548	-0.012	(0)
FeHSO4+	4.372e-15	4.251e-15	-14.359	-14.372	-0.012	(0)
Fe(OH)2	1.112e-16	1.112e-16	-15.954	-15.954	0.000	(0)
Fe(OH)3-	2.986e-21	2.904e-21	-20.525	-20.537	-0.012	(0)
Fe(3)	9.887e-11					
Fe(OH)2+	9.165e-11	8.913e-11	-10.038	-10.050	-0.012	(0)
Fe(OH)3	6.715e-12	6.716e-12	-11.173	-11.173	0.000	(0)
FeOH+2	4.991e-13	4.463e-13	-12.302	-12.350	-0.049	(0)
Fe(OH)4-	3.752e-15	3.649e-15	-14.426	-14.438	-0.012	(0)
Fe+3	1.639e-16	1.284e-16	-15.785	-15.891	-0.106	(0)
FeSO4+	2.141e-17	2.082e-17	-16.669	-16.681	-0.012	(0)
FeCl+2	5.296e-19	4.735e-19	-18.276	-18.325	-0.049	(0)
Fe(SO4)2-	7.651e-21	7.438e-21	-20.116	-20.129	-0.012	(0)
FeCl2+	3.749e-22	3.645e-22	-21.426	-21.438	-0.012	(0)
FeHSO4+2	8.473e-23	7.570e-23	-22.072	-22.121	-0.049	(0)

Fe2(OH)2+4	1.053e-23	6.711e-24	-22.977	-23.173	-0.196	(0)
FeCl3	5.287e-27	5.288e-27	-26.277	-26.277	0.000	(0)
Fe3(OH)4+5	4.176e-31	2.064e-31	-30.379	-30.685	-0.306	(0)
H(0)	2.719e-23					
H2	1.360e-23	1.360e-23	-22.867	-22.866	0.000	28.61
K	5.107e-04					
K+	5.107e-04	4.964e-04	-3.292	-3.304	-0.012	8.82
KSO4-	5.441e-08	5.291e-08	-7.264	-7.276	-0.012	33.95
Mg	1.810e-05					
Mg+2	1.804e-05	1.615e-05	-4.744	-4.792	-0.048	-21.64
MgSO4	5.487e-08	5.488e-08	-7.261	-7.261	0.000	5.62
MgOH+	2.734e-11	2.660e-11	-10.563	-10.575	-0.012	(0)
Na	3.741e-04					
Na+	3.741e-04	3.637e-04	-3.427	-3.439	-0.012	-1.79
NaSO4-	3.020e-08	2.937e-08	-7.520	-7.532	-0.012	13.82
NaOH	1.796e-22	1.796e-22	-21.746	-21.746	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-48.402	-48.402	0.000	29.95
S(6)	1.884e-05					
SO4-2	1.865e-05	1.668e-05	-4.729	-4.778	-0.049	13.72
MgSO4	5.487e-08	5.488e-08	-7.261	-7.261	0.000	5.62
KSO4-	5.441e-08	5.291e-08	-7.264	-7.276	-0.012	33.95
CaSO4	3.739e-08	3.739e-08	-7.427	-7.427	0.000	7.28
NaSO4-	3.020e-08	2.937e-08	-7.520	-7.532	-0.012	13.82
AlSO4+	8.787e-09	8.544e-09	-8.056	-8.068	-0.012	(0)
HSO4-	2.008e-09	1.952e-09	-8.697	-8.710	-0.012	39.87
FeSO4	4.864e-10	4.864e-10	-9.313	-9.313	0.000	25.01
Al(SO4)2-	4.519e-12	4.394e-12	-11.345	-11.357	-0.012	(0)
CaHSO4+	3.170e-13	3.082e-13	-12.499	-12.511	-0.012	(0)
FeHSO4+	4.372e-15	4.251e-15	-14.359	-14.372	-0.012	(0)
AlHSO4+2	1.095e-15	9.785e-16	-14.960	-15.009	-0.049	(0)
FeSO4+	2.141e-17	2.082e-17	-16.669	-16.681	-0.012	(0)
Fe(SO4)2-	7.651e-21	7.438e-21	-20.116	-20.129	-0.012	(0)
FeHSO4+2	8.473e-23	7.570e-23	-22.072	-22.121	-0.049	(0)

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

Phase	SI**	log IAP	log K(292 K, 1 atm)	
Al(OH)3(a)	-0.30	10.85	11.15	Al(OH)3
Alunite	2.81	2.08	-0.73	KAl3(SO4)2(OH)6
Anhydrite	-5.44	-9.66	-4.22	CaSO4
Fe(OH)3(a)	-3.17	1.72	4.89	Fe(OH)3
Gibbsite	2.44	10.85	8.41	Al(OH)3
Goethite	2.53	1.72	-0.81	FeOOH
Gypsum	-5.08	-9.66	-4.58	CaSO4:2H2O
H2(g)	-19.78	-22.87	-3.09	H2
H2O(g)	-1.64	-0.00	1.64	H2O
Halite	-8.84	-7.28	1.57	NaCl
Hematite	7.03	3.44	-3.60	Fe2O3
Jarosite-K	-16.52	-25.31	-8.79	KFe3(SO4)2(OH)6
Melanterite	-9.24	-11.52	-2.28	FeSO4:7H2O
O2(g)	-45.55	-48.40	-2.85	O2
Sylvite	-8.02	-7.14	0.87	KCl

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

End of simulation.

Reading input data for simulation 22.

End of Run after 0.15 Seconds.
