The model is a simple domain with 2 materials and 2 types of waters. The buffer (red) is initially unsaturated while the rock (green) is saturated. The type of waters are identified by 1 (red) and 4 (green).

Water inflows from the outer boundary of the rock, travels through it, and saturates the buffer. The buffer develops a pressure because it is a swelling material. The swelling is affected by the chemistry via the ionic strength, which is related to salinity.

The input file (*root*_chem.dat) according to the guide document is included below for this example.

The initial and boundary conditions can use the types of water included in another file (*root*_chem_ini.dat). This file contains the concentrations for all species for 4 types of water. Water number 3 is the one that contains higher salinity. Water 4 contains more salinity than waters 1 and 2.

The chemical system corresponds to sodium chloride and calcium chloride.

Lines 4 to 8 describe the chemical species with their chemical properties.

Lines 14, 15, 17 and 18 describe the chemical equilibrium including the equilibrium constants.

Lines 19, 20 and 21 include the matrix of components.

The chemical species are divided into primary (Na+, Cl- and Ca2+) and secondary (NaCl and CaCl2). The user defines this and it is indicated in lines 30 to 35.

The equations would be:

$$Na^+ + Cl^- \rightleftharpoons NaCl(aq)$$

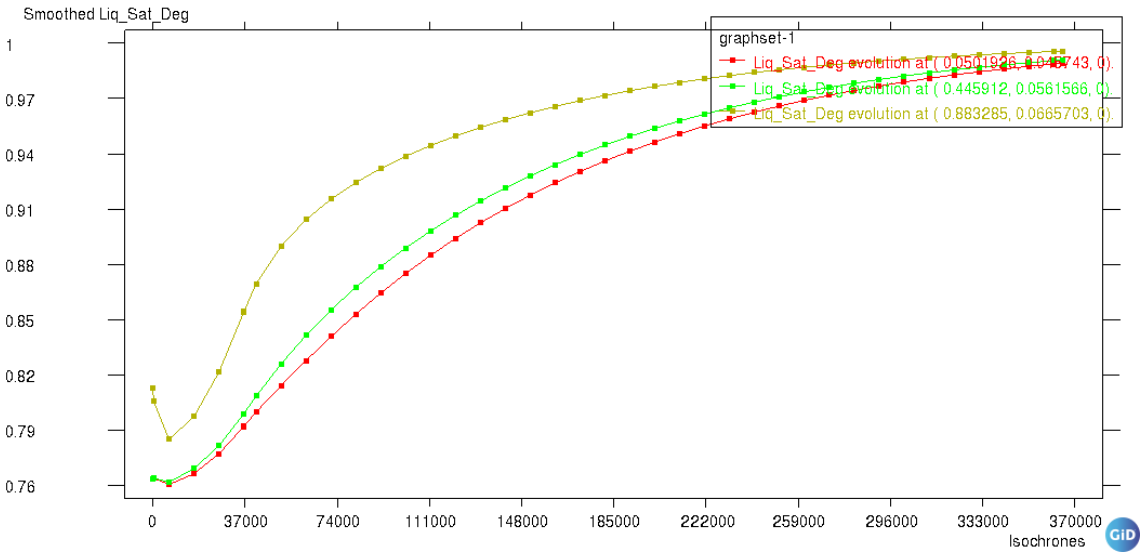
$$2Cl^- + Ca^{2+} \rightleftharpoons CaCl_2(aq)$$

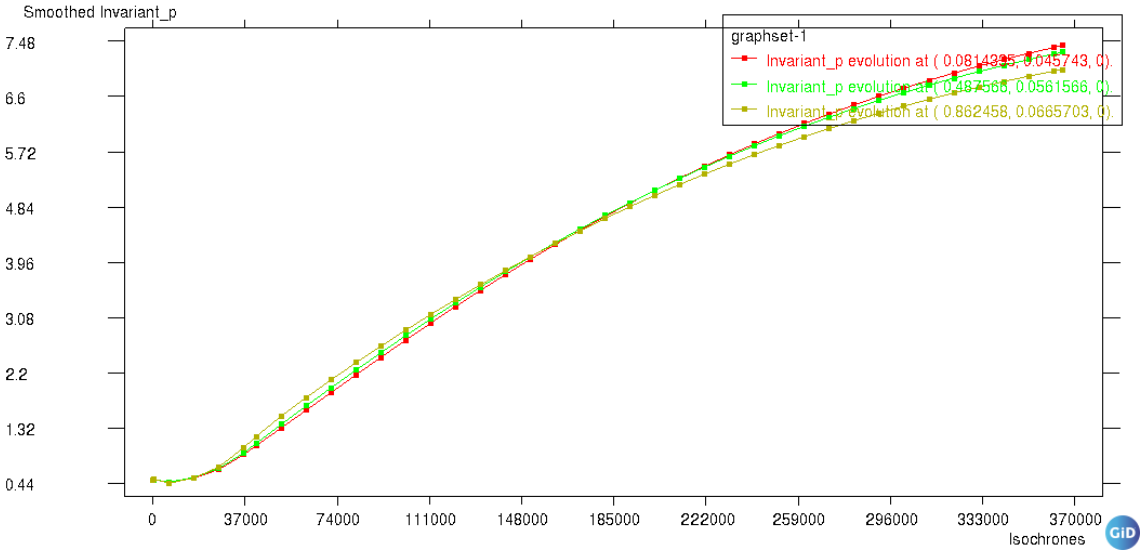
File: root_chem.dat

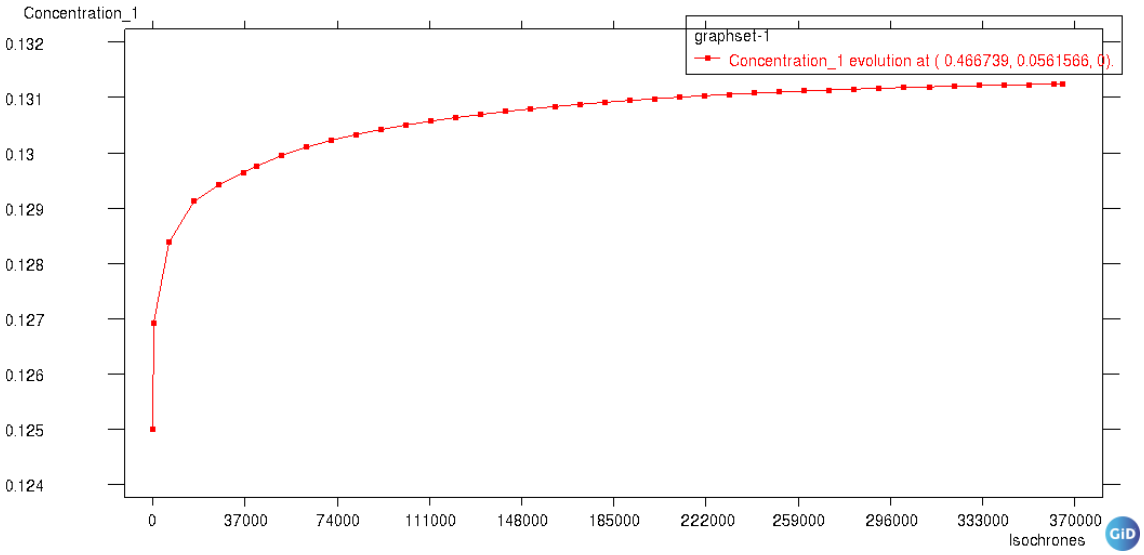
File root_chem.dat	Line number for this case
1 3	1
	2
name_phase_liquid 1 5	3
na+ 5.0 0.0 1.0	4
cl- 5.0 0.0 -1.0	5
ca2+ 5.0 0.0 2.0	6
nacl(aq) 5.0 0.0 0.0	7
cacl2(aq) 5.0 0.0 0.0	8
	9
2	10
	11
0	12
	13
1. 1. 0. -1. 0. 0	14
0.02618	15
	16
0. 2. 1. 0. -1. 0	17
0.1	18
	19
1. 0. 0. 1. 0.	20
0. 1. 0. 1. 2.	21
0. 0. 1. 0. 1.	22
	23
1	24
1	25
1	26
1	27
1	28
	29
1	30
2	31
3	32
	33
4	34
5	35

File: root_chem_ini.dat

File root_chem_ini.dat	Line number for this case
4	1
1 0.125 0.182 0.042 0.46 0.002	2
2 0.015 0.018 0.0016 0.046 0.0002	3
3 0.428 1.221 0.396 0.46 0.002	4
4 0.150 0.218 0.050 0.552 0.0024	5


Smoothed Liq_Sat_Deg
graphset-1
Liq_Sat_Deg evolution at (0.0501926, 0.045743, 0).
Liq_Sat_Deg evolution at (0.445912, 0.0561566, 0).
Liq_Sat_Deg evolution at (0.883285, 0.0665703, 0).
1
0.97
0.94
0.91
0.88
0.85
0.82
0.79
0.76
0
37000
74000
111000
148000
185000
222000
259000
296000
333000
370000
Isochrones


Smoothed Invariant_p
graphset-1
Invariant_p evolution at (0.0814235, 0.045743, 0).
Invariant_p evolution at (0.487566, 0.0561566, 0).
Invariant_p evolution at (0.862458, 0.0665703, 0).
7.48
6.6
5.72
4.84
3.96
3.08
2.2
1.32
0.44
0
37000
74000
111000
148000
185000
222000
259000
296000
333000
370000
Isochrones


Concentration_1
graphset-1
Concentration_1 evolution at (0.466739, 0.0561566, 0).
0.132
0.131
0.13
0.129
0.128
0.127
0.126
0.125
0.124
0
37000
74000
111000
148000
185000
222000
259000
296000
333000
370000
Isochrones