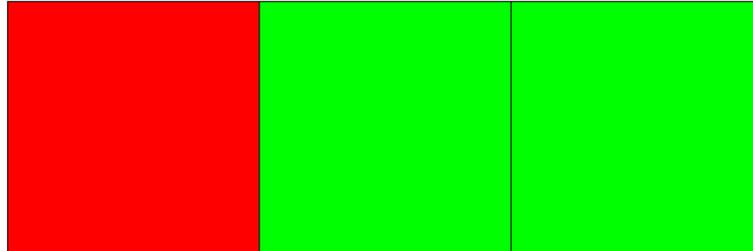


Ex_CHE_MECH_eq_CB23_14

The model is a simple domain with 2 types of waters which are identified by 1 (red) and 2 (green).



| | |
|---|------------------|
|  | _Constant 0 0 0 |
| | 0.11 0 0 1 0 0 0 |
| | 0 0 .. |
|  | _Constant 0 0 0 |
| | 0.11 0 0 2 0 0 0 |
| | 0 0 .. |



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 two types of water.

The chemical system corresponds to carbonates.

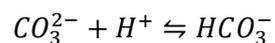
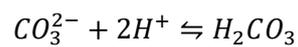
Lines 4 to 7 describe the chemical species with their chemical properties

Lines 13, 14, 16 and 17 describe the chemical equilibrium including the equilibrium constant.

Lines 19 and 20 include the matrix of components.

The chemical species are divided into primary (CO_3^{2-} and H^+) and secondary (H_2CO_3 and H_2CO_3^-). The user defines this and it is indicated in lines 27 to 31.

The equations are:



File: root_chem.dat

| File root_chem.dat | Line number for this case |
|-----------------------|---------------------------|
| 1 2 | 1 |
| | 2 |
| name_phase_liquid 1 4 | 3 |
| co3-2 5.4 0.0 -2.0 | 4 |
| h+ 4.78 0.24 1.0 | 5 |
| h2co3 0.0 0.0 0.0 | 6 |
| hco3- 5.4 0.0 -1.0 | 7 |
| | 8 |
| 2 | 9 |
| | 10 |
| 0 | 11 |
| | 12 |
| 1. 2. -1. 0. 0 | 13 |
| 2.08449e-17 | 14 |
| | 15 |
| 1. 1. 0. -1. 0 | 16 |
| 4.72063e-11 | 17 |
| | 18 |
| 1. 0. 1. 1. | 19 |
| 0. 1. 2. 1. | 20 |
| | 21 |
| 1 | 22 |
| 1 | 23 |
| 1 | 24 |
| 1 | 25 |
| | 26 |
| 1 | 27 |
| 2 | 28 |
| | 29 |
| 3 | 30 |
| 4 | 31 |

File: root_chem_ini.dat

| File root_chem_ini.dat | Line number for this case |
|---|---------------------------|
| 2 | 1 |
| 1 1.07e-06 1.04e-07 7.12E-004 2.78E-003 | 2 |
| 2 1.14e-06 1.08e-07 7.24E-004 3.2E-003 | 3 |

