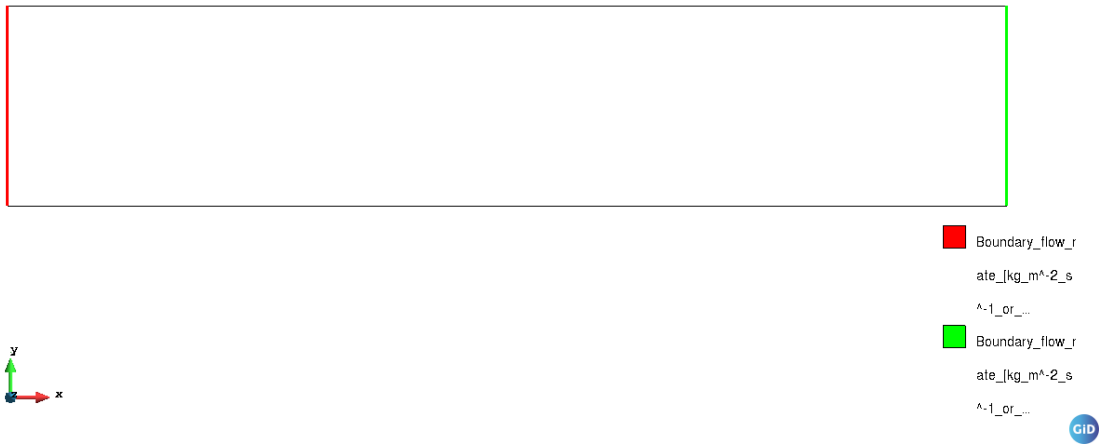
prueba_o2_CHE_MECH_bc_CB23_14.gid

The model is a simple domain with 2 boundary conditions.



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 oxygen transport in the form of gas and dissolved.

Lines 3 to 7 describe the chemical species with their chemical properties

Lines 13 and 14 describe the chemical equilibrium including the equilibrium constant.

Line 16 include the matrix of components.

The chemical species are divided into primary ($O_2(l)$) and secondary ($O_2(g)$). The user defines this and it is indicated in lines 18, 19, 21, 23

The equation is:

$$O_2(l) \leftrightharpoons O_2(g)$$

This chemical equation corresponds to the dissolution of oxygen in water and it is ruled by Henry's law. In this case, equation is:

$$K_H = \frac{c_{O_2(l)}}{c_{O_2(g)}} = 3.2 \times 10^{-5}(-)$$

Where the oxygen in the gas is considered the product of the reaction.

File: root_chem.dat

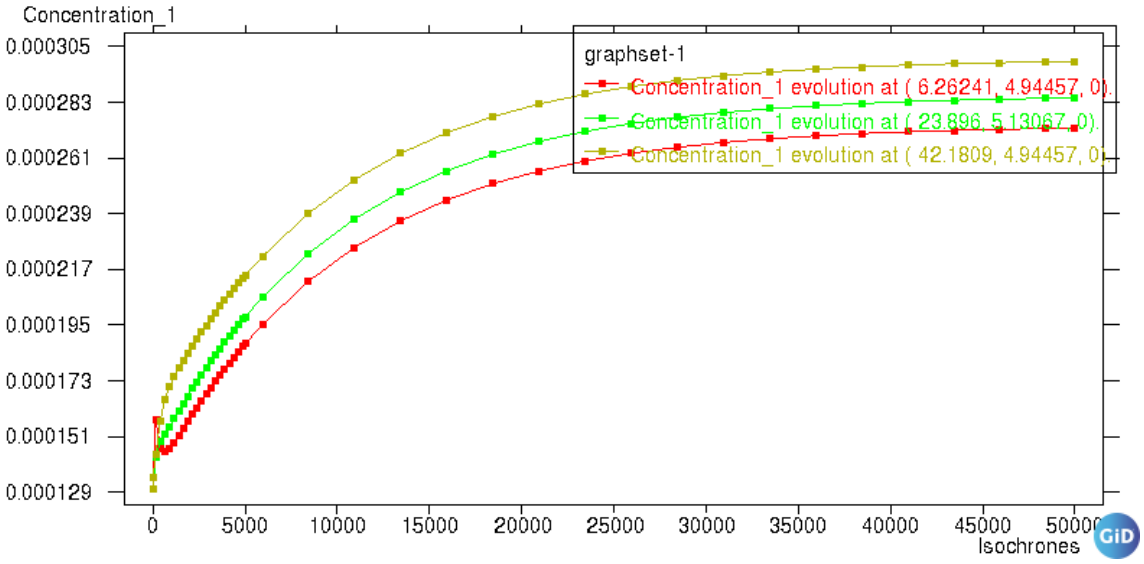
File root_chem.dat	Line number for this case
2 1	1
	2
name_phase_liquid 1 1	3
O2_l 5.4 0.0 1.0	4
	5
name_phase_gas 2 1	6
O2_g 0.0 0.0 0.0	7
	8
1	9
	10
0	11
	12
1. -1. 0	13
3.2e-5	14
	15
1. 1.	16
	17
1	18
2	19
	20
1	21
	22
2	23

File: root_chem_ini.dat

File root_chem_ini.dat	Line number for this case
2	1
1 0.00013 3.75 mol/kg l (water), mol/kg g (air)	2
2 0.00027 7.5	3

From the right side, oxygen is injected with the water at a higher concentration. The oxygen penetrates in the system until the new equilibrium is achieved.

Oxygen in dissolution for 3 points at different distances, mol/kg liquid (water):



Oxygen in gas for 3 points at different distances, mol/kg gas (air):