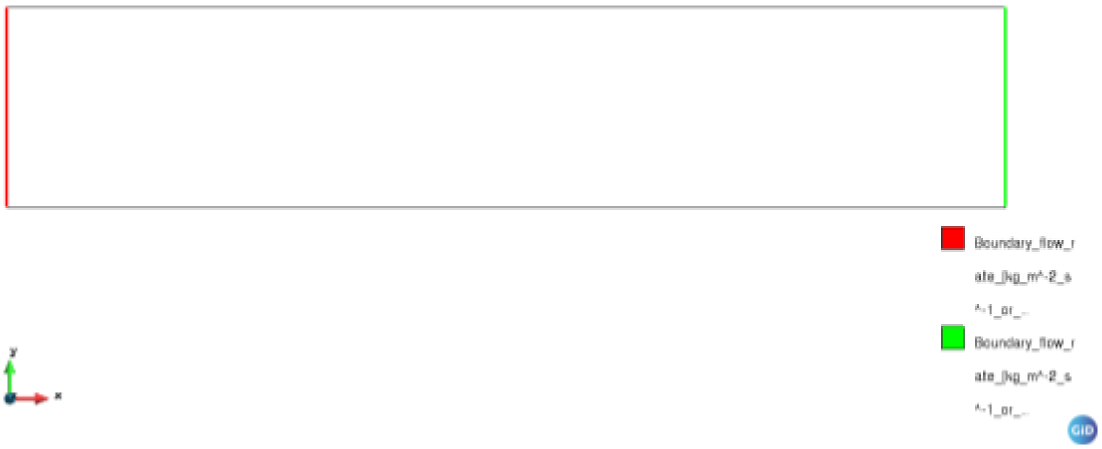
prueba_o2_CHE_MECH_bc_CB25_02_D.gid

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 4.06 mol/kg l (liquid), mol/kg g (gas)	2
2 0.00027 8.43	3

From the right side, oxygen is injected with the liquid at a higher concentration, while oxygen is consumed on the left side by the lower concentration imposed.

Solute types used in this model

Solute type 1. This corresponds to 0.00013 mol/kg (mol oxygen in kg of liquid) and 4.06 mol/kg (mol oxygen in kg of gas). These numbers satisfy the Stoichiometric Henry equation with a constant of 3.2e-5.

Solute type 2. This corresponds to 0.00027 mol/kg (mol oxygen in kg of liquid) and 8.43 mol/kg (mol oxygen in kg of gas). These numbers satisfy the Stoichiometric Henry equation with a constant of 3.2e-5.

While solute 2 type corresponds roughly to air with a 21% of oxygen, solute 1 corresponds to half of it.

Material properties

Intrinsic permeability: 1 e -18 m^2

Porosity 0.1

Van Genughten P0 = 1MPa, Lambda = 0.5

Boundary Conditions

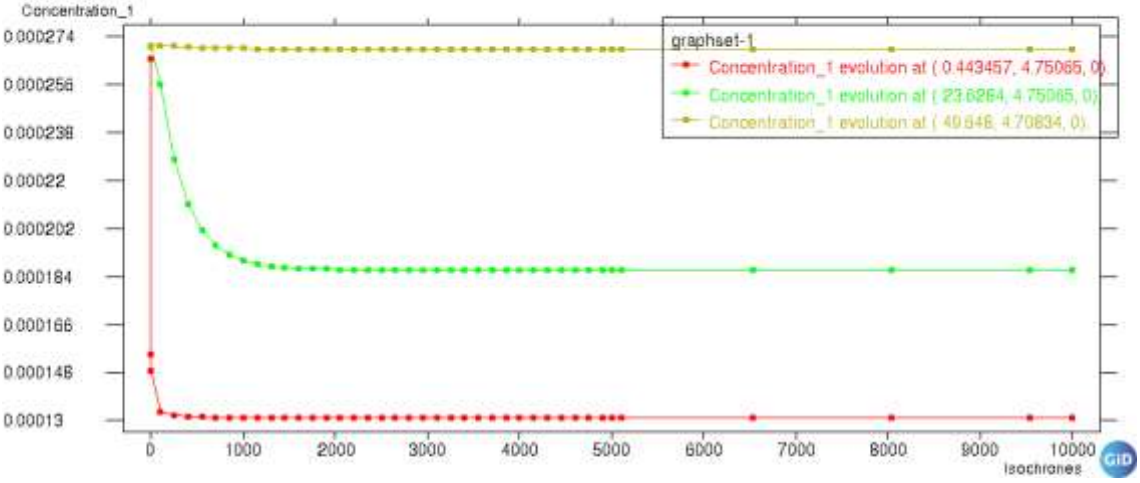
Inflow:
Gas pressure = 0.1 MPa
Gamma for gas = 100
Beta for gas = 0
Gas density = 1.18 kg/m^3
Solute type = 2 (concentrations in mol/kg)
Dissolved air concentration = 1.6 e-5 kg/kg
Liquid pressure = -0.05 MPa
Gamma for liquid = 100
Beta for liquid = 0.01
Liquid density = 1000 kg/m^3

Outflow:
Gas pressure = N/A (not applicable because gamma and beta for gas are zero)
Gamma for gas = 0
Beta for gas = 0
Gas density = 1.18 kg/m^3
Solute type = 1 (concentrations in mol/kg)
Dissolved air concentration = 1.6 e-5 kg/kg
Liquid pressure = -0.1 MPa
Gamma for liquid = 100
Beta for liquid = 0.01
Liquid density = 1000 kg/m^3

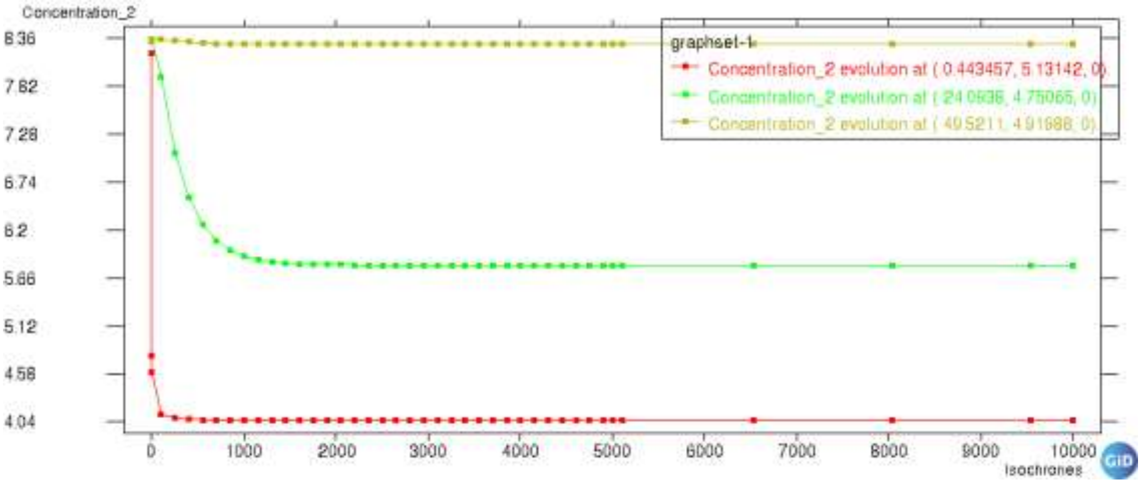
Oxygen concentration is prescribed through the concentration in the liquid phase and beta for liquid. Since equilibrium is established at each point, the concentration of oxygen in the gas equilibrates instantaneously with the dissolved concentration through the Henry's constant. For instance (in prueba_o2_CHE_MECH_bc_CB25_02_D.gid), at the injection point the concentration in the liquid is 0.00027 mol/kg and the concentration in the gas is 8.43 mol/kg.

For the air, that essentially would correspond to N_2, the idea is similar. However, the concentration is given as 1.6 e-5 kg/kg.

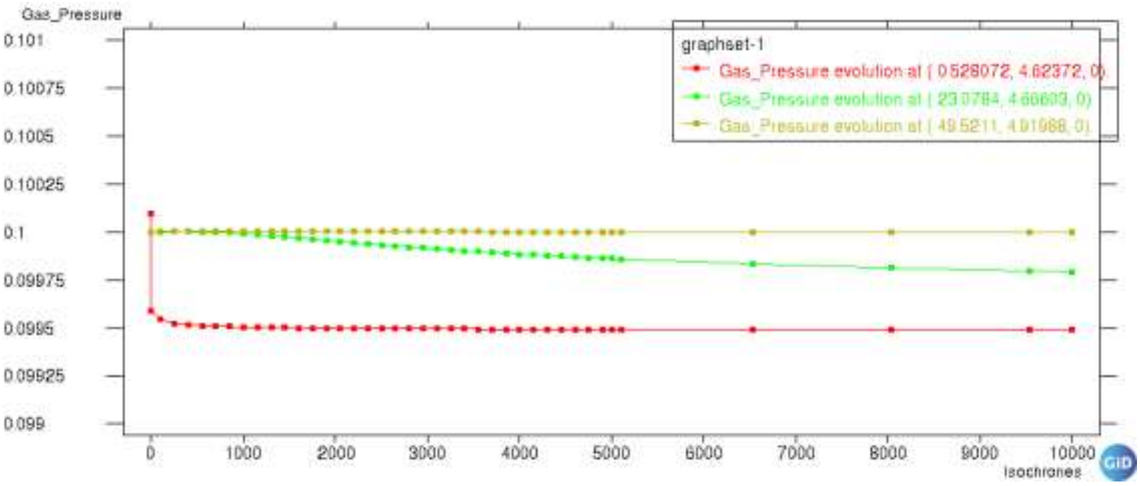
Oxygen in dissolution in water for 3 points at different distances, mol/kg liquid (water):



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



Gas pressure for 3 points



Gas composition and partial pressure of oxygen

Following the ideal gas law, the partial pressure of Oxygen is:

$$p_g^{o_2} = \frac{\rho_g^{o_2} R(T + 273.15)}{M^{o_2}} \quad (1)$$

The concentration can be transformed into density by the product:

$$\rho_g^{o_2} = \omega_g^{o_2} \rho_g = c_g^{o_2} M^{o_2} \rho_g \quad (2)$$

Where density is $[\rho] = \frac{\mathrm{kg}}{\mathrm{m}^3}$, molar concentration is $[c] = \frac{\mathrm{mol}}{\mathrm{kg}}$, mass fraction is $[\omega] = \frac{\mathrm{kg}}{\mathrm{kg}}$, and molar mass is $[M] = \frac{\mathrm{kg}}{\mathrm{mol}}$

Substituting (2) in (1) leads to:

$$p_g^{o_2} = \frac{\rho_g^{o_2} R(T + 273.15)}{M^{o_2}} = c_g^{o_2} M^{o_2} \rho_g \frac{R(T + 273.15)}{M^{o_2}}$$

Which can lead to:

$$p_g^{o_2} = c_g^{o_2} M^{o_2} \frac{p_g M^g}{R(T + 273.15)} \frac{R(T + 273.15)}{M^{o_2}} = c_g^{o_2} p_g M^g$$

Actually, this is equivalent to:

$$p_g^{o_2} = c_g^{o_2} p_g M^g = \chi_g^{o_2} p_g$$

Where $\left[\chi_g^{o_2}\right] = \frac{\mathrm{mol}}{\mathrm{mol}}$ is the molar fraction.

For the initial conditions, the following calculation can be done (assuming atmospheric gas pressure and constant molar mass of gas):

$$p_g^{o_2} = c_g^{o_2} p_g M^g = 4.06 \times 0.1 \times 0.028 = 0.011 \text{ MPa}$$

For the final conditions:

$$p_g^{o_2} = c_g^{o_2} p_g M^g = 8.43 \times 0.1 \times 0.028 = 0.024 \text{ MPa}$$

The volumetric content of oxygen in air is 21% which is close to the second value.

Solute 2 corresponds with an air with a concentration of 21% of oxygen.
