

Two-phase flow in a heterogeneous porous media

A 2D geometry test case

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1 Notation

Symbol	meaning	dimension
\mathbf{q}_l	Darcy's velocitie for water	$m.s^{-1}$
\mathbf{q}_g	Darc's velocitie for gas	$m.s^{-1}$
K	the absolute permeability	m^2
k_{rl}	relative water permeability	-
k_{rg}	relative gas permeability	-
p_l	water pressure	Pa
p_g	gas pressure	Pa
p_g^w	partial pressure of water vapor in the gaz phase	Pa
p_g^h	partial pressure of hydrogen in the gaz phase	Pa
p_c	capillary pressure	Pa
g	gravity acceleration	$m.s^{-2}$
y	altitude	m
ϕ	porosity	-
S_l	water saturation of phase	-
S_g	gas saturation of phase	-
S_{lr}	residual water saturation	-
S_{gr}	residual gas saturation	-
p_r	parameter of Van Genuchten Law	Pa
n, m	coefficients of Van Genuchten Law $m = 1 - \frac{1}{n}$	-
ρ_l	density of the water	$kg.m^{-3}$
ρ_l	density of the gas	$kg.m^{-3}$
ρ_l^w	density of water in liquid phase	$kg.m^{-3}$
ρ_g^w	density of water vapor	$kg.m^{-3}$
ρ_l^h	density of dissolved hydrogen	$kg.m^{-3}$
ρ_g^h	density of hydrogen in the gas phase	$kg.m^{-3}$
M^h	molar mass of hydrogen	$kg.mol^{-1}$
M_g^w	molar mass of water vapor	$kg.mol^{-1}$
R	constant of ideal gases	$(j.mol^{-1}.K^{-1})$
T	the temperature	K
D_l^h	Diffusion coefficient of disolved hydrogen	$m^2.s^{-1}$
μ^w	viscosity of liquid phase	Pa.s
μ^g	viscosity of gas phase	Pa.s
τ	tortuosity	-
C_l^h	hydrogen concentration in water	$mol.m^{-3}$
H_h	solubility of hydrogen in water	$mol.Pa^{-1}.m^{-3}$

2 Introduction

Andra and MoMas proposed the Couplex-Gas Benchmark for simulating the migration of hydrogen produced by the corrosion of nuclear waste packages in an underground storage.

This is a system of two-phase (liquid-gas) flow with two components (hydrogen-water). We proposed in this paper a simplified exercise of this Benchmark which contain the same numerical difficulties. We will assume that water does not vaporize.

3 Physical Model

We first describe the equations and some simplifying hypotheses.

3.1 Fluid phases

- 2 phases : Liquid (incompressible) (l), Gas (compressible) (g)
- Darcy's law for each phase :

$$\mathbf{q}_i = -K(x) \frac{k_{ri}(S_i)}{\mu_i} (\nabla p_i - \rho_i g \nabla y) \quad i \in l, g.$$

- $S_l + S_g = 1$
- $p_c(S_l) = p_g - p_l$

The capillary pressure is expressed by the Van Genuchten model as follows :

- $p_c = p_r (S_{le}^{-1/m} - 1)^{1/n}$

Where $S_{le} = \frac{S_l - S_{lr}}{1 - S_{lr} - S_{gr}}$ is the effective saturation.

The relative water permeability and the relative gas permeability are expressed by the Mualem model as follows :

- $k_r^l = \sqrt{S_{le}} (1 - (1 - S_{le}^{1/m})^m)^2$
- $k_r^g = \sqrt{1 - S_{le}} (1 - S_{le}^{1/m})^{2m}$

3.2 Fluid components

- 2 components : Water (w), Hydrogen (h)
- $\rho_i = \rho_i^w + \rho_i^h, \quad i \in \{l, g\}$.

- We define mass concentration : $\chi_i^h = \frac{\rho_i^h}{\rho_i}$, $\chi_i^w = \frac{\rho_i^w}{\rho_i}$, $i \in \{l, g\}$.

We assume that the liquid phase may contain both components, while the gas phase contains only hydrogen, that is the water does not vaporize. In this situation we have

- $\rho_g^w = 0$, $\chi_g^h = 1$ and $\chi_g^w = 0$
- Ideal Gas

$$\star p_g^h = \frac{\rho_g^h}{M^h} RT.$$

3.3 Molecular diffusion flux in the liquid phase

- Molecular diffusion flux of hydrogen in the liquid phase $\mathbf{j}_l^h = -\phi S_l \rho_l D_l^h \nabla \chi_l^h$
- Molecular diffusion flux of water in the liquid phase $\mathbf{j}_l^w = -\phi S_l \rho_l D_l^w \nabla \chi_l^w$.

– With molecular diffusion coefficient

$$\star D_l^h = D_l^w = \left(\frac{1}{\tau^2}\right) 1.5710^{-14} \frac{T}{\mu^w(T)} \quad [m^2/s]$$

3.4 Conservation of mass for each component

- $\phi \frac{\partial}{\partial t} (S_l \rho_l^w) + \text{div}(\rho_l^w \mathbf{q}_l + \mathbf{j}_l^w) = 0$
- $\phi \frac{\partial}{\partial t} (S_l \rho_l^h + S_g \rho_g^h) + \text{div}(\rho_l^h \mathbf{q}_l + \rho_g^h \mathbf{q}_g + \mathbf{j}_l^h) = 0$
- Total flux for each component

$$\star \mathbf{F}^w = \rho_l^w \mathbf{q}_l + \mathbf{j}_l^w$$

$$\star \mathbf{F}^h = \rho_l^h \mathbf{q}_l + \rho_g^h \mathbf{q}_g + \mathbf{j}_l^h$$

3.5 Phase equilibrium

- Henry's law and the hydrogen concentration

$$\star M^h H(T) p_g^h = \rho_l^h,$$

- We define the concentration of hydrogen in water C_l^h by $C_l^h = H(T) p_g^h = \frac{\rho_l^h}{M^h}$.

3.6 Simulation Periods

The simulation will take place between moment $t_0 = 0$ and moment $t_{end} = 1000$ years.

4 A simplified 2D exercice

We consider a rectangle of dimension [200 m x 130 m] initially saturated into which we inject gazeous hydrogen at a given rate. This core sample is actually made of two different rock types (the concrete package and the Cox) with different capillary pressure and relative permeability curves. The hydrogen source S is located near the interface between the two materials in the rectangle representing rock type 1 as shown in Fig. 4.1.

4.1 Geometry

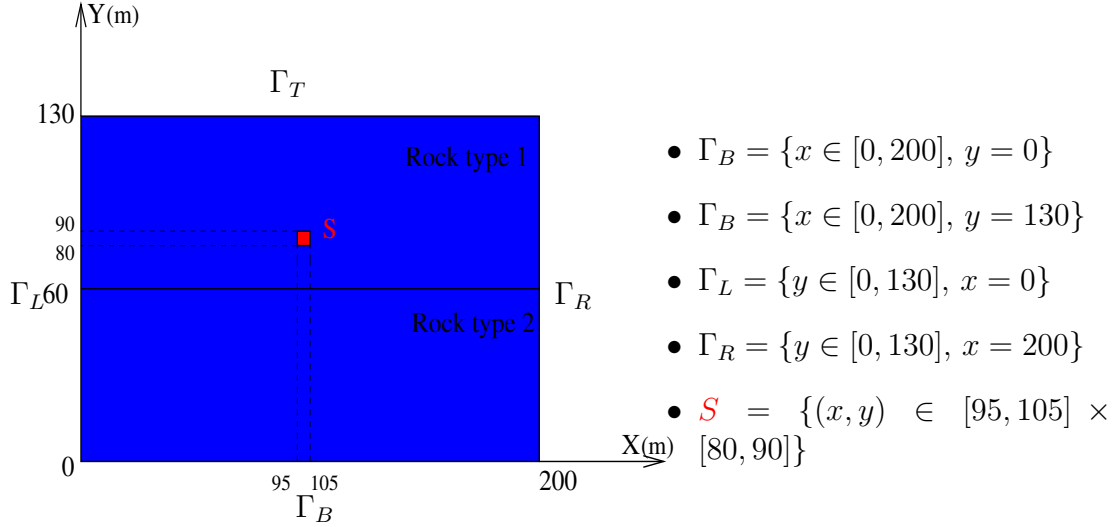


Figure 4.1: Geometry

4.2 Boundary conditions

We denote by \mathbf{n}_{Γ_L} and \mathbf{n}_{Γ_R} the unit outward pointing normal vectors respectively on Γ_L and Γ_R . We denote by $\mathbf{n}_{\partial S}$ the unit outward pointing normal vector on the boundary of S.

- $p_l = 4.2$ MPa, $S_l = 1$ on Γ_T .
- $p_l = 5.5$ MPa, $S_l = 1$ on Γ_B .
- $\mathbf{F}^w \cdot \mathbf{n}_{\Gamma_L} = 0$ and $\mathbf{F}^h \cdot \mathbf{n}_{\Gamma_L} = 0$
- $\mathbf{F}^w \cdot \mathbf{n}_{\Gamma_R} = 0$ and $\mathbf{F}^h \cdot \mathbf{n}_{\Gamma_R} = 0$
- $\mathbf{F}^w \cdot \mathbf{n}_{\partial S} = 0$ and $\mathbf{F}^h \cdot \mathbf{n}_{\partial S} = Q^h$.

4.3 Initial conditions

- $S_l = 1$.
- hydrostatic liquid pressure.
- $C_l^h = 0 \text{ mol.m}^{-3}$.

4.4 hydrogen flux

- $Q^h = 0.5210^{-10} \text{ kg/m}^2/\text{year}$ for $0 \leq t \leq 500$ years
- $Q^h = 0.2610^{-10} \text{ kg/m}^2/\text{year}$ for $500 < t \leq 530$ years
- $Q^h = 0 \text{ kg/m}^2/\text{year}$ for $530 < t \leq 10000$ years

5 Examples

We propose two test cases :

- Case 1 : Rock type 1 = COX, rock type 2 = Concrete package.
- Case 2 : Rock type 1 = Concrete package, rock type 2 = COX.

6 Physical parameters

The calculations are isotherm; temperature is set at 303 Kelvin throughout the simulation period.

Materials parameters	Concrete package	COX
$K[m^2]$	10^{-19}	10^{-21}
Porosity (ϕ)[%]	15	15
Two-phase flow parameters	Concrete package	COX
S_{gr} [%]	0	0
S_{lr} [%]	1	40
n [-]	1.54	1.49
$P_r[Pa]$	2.10^6	15.10^6
Tortuosity (τ)	2	2
Fluids parameters		
Viscosity of liquid phase μ_l	$10^{-3} Pa.s$	
Viscosity of gas phase μ_g	$9.10^{-6} Pa.s$	
Molar mass of hydrogen M_h	$2 g.mol^{-1}$	
Constant of ideal gases R	$8.314 J.mol^{-1}.K^{-1}$	
Solubility of hydrogen in water H_h	$7.65 10^{-6} mol.Pa^{-1}.m^{-3}$	
Masse volumique de l'eau ρ_l	$10^6 g.m^{-3}$	

7 Required results

7.1 Required conditions

- What are the unknown that you use?
- if $S_l = 1$ is impossible for numerical reasons, please specify intial and boundary conditions.
- Do you take into account an initial concentration of hydrogen? If yes, which one?
- Which treatment you use to regularize the curve of the capillary pressure when the saturation is maximum?

7.2 Required output

- Gaz-pressure, water pressure and gaz saturation profile in ($y = 50 m$, $y = 85 m$ and $x = 100 m$) at ($t = 0, 1, 10, 50, 100, 200, 500, 550, 800, 1000, 5000, 10000 year$).
- Gaz pressure in relation to time in the following points : $(90,85.5)$, $(100,55)$, $(100,70)$.
- Hydrogen flows (in mol/year) through the surface which contain the source : $(x = 85 m, 70 m \leq y \leq 100 m) \cup (x = 115 m, 70 m \leq y \leq 100m) \cup (y = 70 m, 85 m \leq x \leq 115 m) \cup (y = 100 m, 85 m \leq x \leq 115 m)$