

Analysis and simulation of a two phase flow model with phase apparition/disappearance

Application to gas migration in underground nuclear waste repository

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Unsaturated two phase flow

Saturated flow

Construction of a saturated/unsaturated model

Analysis and simulation

Context

- ▶ Production of hydrogen in the storage

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- ▶ Problem of the gas phase apparition/disappearance

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- ▶ Production of hydrogen in the storage
- ▶ Problem of the gas phase apparition/disappearance
 - ▶ 2 kinds of flow : saturated (liquid) et unsaturated (liquid/gas)

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- ▶ Problem of the gas phase apparition/disappearance
 - ▶ 2 kinds of flow : saturated (liquid) et unsaturated (liquid/gas)
- ▶ Saturated/unsaturated global formulation ?

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- ▶ 2 phases : liquid (incompressible) and gas (compressible)

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- ▶ 2 phases : liquid (incompressible) and gas (compressible)
- ▶ 2 components : water and hydrogen

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- ▶ 2 components : water and hydrogen
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- ▶ Generalized Darcy law for each phase

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- ▶ Isothermal flow

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- ▶ Isothermal flow
- ▶ **Additional assumption : no water vapor**

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Unsaturated flow equations

The unsaturated flow is described by :

$$\Phi \frac{\partial S_l}{\partial t} + \text{div} \left(\mathbf{q}_l - \frac{1}{G} \mathbf{J} \right) = \mathcal{F}^w / \rho_l^{std}$$

$$\Phi \frac{\partial}{\partial t} (C_h S_l p_g + C_v p_g S_g) + \text{div} (C_h p_g \mathbf{q}_l + C_v p_g \mathbf{q}_g + \mathbf{J}) = \mathcal{F}^h / \rho_g^{std}$$

with usual primary variables : (p_l, S_l) ou (p_l, p_g) .

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with usual primary variables : (p_l, S_l) ou (p_l, p_g) .

Where we denote fluxes : $\mathbf{q}_l = -\mathbb{K} \frac{kr_l}{\mu_l} (\nabla p_l - (\rho_l^{std} + C_h \rho_g^{std} p_g) \mathbf{g})$,

$$\mathbf{q}_g = -\mathbb{K} \frac{kr_g}{\mu_g} (\nabla p_g - C_v \rho_g^{std} p_g \mathbf{g}) ,$$

$$\mathbf{J} = -\frac{\Phi S_l F}{C_h p_g + F} D_l^h C_h \nabla p_g ,$$

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$$\mathbf{J} = -\frac{\Phi S_l F}{C_h p_g + F} D_l^h C_h \nabla p_g ,$$

and constants :

$$C_h = \frac{H(T)M^h}{\rho_g^{std}} , C_v = \frac{M^h}{RT \rho_g^{std}} , G = \frac{\rho_l^{std}}{\rho_g^{std}} , F = \frac{M^h \rho_l^{std}}{M^w \rho_g^{std}} .$$

Saturated flow

- ▶ Liquid saturated flow : $S_l \equiv 1$ and p_g non definite

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 - ▶ Classical Darcy law for liquid flow (water + dissolved hydrogen)

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- ▶ We denote $R_s = \frac{\rho_l^h}{\rho_g^{std}}$, The (saturated) flow of the solution (water + dissolved hydrogen) is described by :

$$\begin{aligned}\operatorname{div} \left(\mathbf{q}_l - \frac{1}{G} \mathbf{J} \right) &= \mathcal{F}^w / \rho_l^{std} \\ \Phi \frac{\partial R_s}{\partial t} + \operatorname{div} \left(R_s \mathbf{q}_l + \mathbf{J} \right) &= \mathcal{F}^h / \rho_g^{std}\end{aligned}$$

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- ▶ Usual primary variables : (p_l, R_s)

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How to globally describe saturated and unsaturated flows ?

Construction of a saturated/unsaturated model

Choice of suitable variables

- ▶ Usual primary variables

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Choice of suitable variables

- ▶ Usual primary variables
 - ▶ unsaturated : pressure/pressure or pressure/saturation

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Choice of suitable variables

- ▶ Usual primary variables
 - ▶ unsaturated : pressure/pressure or pressure/saturation
 - ▶ saturated : pressure/concentration
- ▶ Introduction of a new variable

$$X = R_s S_l + C_v p_g S_g$$

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- ▶ (p_l, X) is well definite in the 2 states of flow (saturated/unsaturated)

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$$X = R_s S_l + C_v p_g S_g$$

- ▶ (p_l, X) is well definite in the 2 states of flow (saturated/unsaturated)
- ▶ State of flow characterization
 - unsaturated : $X > C_h(p_l + p_c(0))$
 - saturated : $X \leq C_h(p_l + p_c(0))$

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 - unsaturated : $X > C_h(p_l + p_c(0))$
 - saturated : $X \leq C_h(p_l + p_c(0))$
 $X \equiv R_s$

Construction of a saturated/unsaturated model

Choice of suitable variables

Unsaturated :

usual primary
variables
 (p_l, S_l) and
 (p_l, p_g)

$$\Phi \frac{\partial S_l}{\partial t} + \text{div} \left(\mathbf{q}_l - \frac{1}{G} \mathbf{J} \right) = \mathcal{F}^w / \rho_l^{std}$$

$$\Phi \frac{\partial X}{\partial t} + \text{div} \left(R_s \mathbf{q}_l + C_v p_g \mathbf{q}_g + \mathbf{J} \right) = \mathcal{F}^h / \rho_g^{std}$$

Saturated :

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Formulation in (p_l, X)

- ▶ The saturated/unsaturated flow may be described with primary variables (p_l, X) by only one couple of equations :

$$\Phi \frac{\partial}{\partial t} (X - GS_g) + \operatorname{div} \left((G + R_s) \mathbf{q}_l + C_v p_g \mathbf{q}_g \right) = G \frac{\mathcal{F}^w}{\rho_l^{std}} + \frac{\mathcal{F}^h}{\rho_g^{std}}$$
$$\Phi \frac{\partial X}{\partial t} + \operatorname{div} \left(R_s \mathbf{q}_l + C_v p_g \mathbf{q}_g + \mathbf{J} \right) = \frac{\mathcal{F}^h}{\rho_g^{std}}$$

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- ▶ 1st equation is parabolic/elliptic in p_l ,
2nde equation is parabolic in X .

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Existence of solutions

- We consider the simplified formulation :

$$\left\{ \begin{array}{l} \Phi \frac{\partial S_l}{\partial t} + \operatorname{div}(\mathbf{q}_l + \mathbf{0}) = \mathcal{F}^w / \rho_l^{std} \\ \Phi \frac{\partial X}{\partial t} + \operatorname{div}(R_s \mathbf{q}_l + C_v p_g \mathbf{q}_g + \mathbf{J}) = \mathcal{F}^h / \rho_g^{std} \end{array} \right.$$

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- ▶ We can show the following existence result :

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- ▶ We can show the following existence result :

Suppose $r_{min} \leq R_s \leq r_{max}$ and $p_l \geq 0$ and assume that initial and Dirichlet conditions are enough regular.
Then there is a weak solution to the simplified formulation.

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- ▶ We consider the simplified formulation :

$$\begin{cases} \Phi \frac{\partial S_l}{\partial t} + \operatorname{div}(\mathbf{q}_l + \mathbf{0}) = \mathcal{F}^w / \rho_l^{std} \\ \Phi \frac{\partial X}{\partial t} + \operatorname{div}(R_s \mathbf{q}_l + C_v p_g \mathbf{q}_g + \mathbf{J}) = \mathcal{F}^h / \rho_g^{std} \end{cases}$$

- ▶ We can show the following existence result :

Suppose $r_{min} \leq R_s \leq r_{max}$ and $p_l \geq 0$ and assume that initial and Dirichlet conditions are enough regular.

Then there is a weak solution to the simplified formulation.

- ▶ A well chosen variable change allows to apply the Alt-Luckhaus theorem in order to prove existence of a solution.

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Numerical test : a simple configuration

$$\phi^w \cdot \mathbf{n} = 0$$

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$$\phi^w \cdot \mathbf{n} = 0$$

$$\phi^h \cdot \mathbf{n} = Q_{in}^h$$



$$X = X_{out}$$

$$p_l = p_{l,out}$$

$$\phi^w \cdot \mathbf{n} = 0$$

$$\phi^h \cdot \mathbf{n} = 0$$



► Boundary conditions :

- Injection of pure gas on left side
- Impervious condition on top and bottom side
- Pure water ($X_{out} = 0$) at fixed pressure on right side

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Numerical test : a simple configuration

$$\phi^w \cdot \mathbf{n} = 0$$

$$\phi^h \cdot \mathbf{n} = 0$$

$$\phi^w \cdot \mathbf{n} = 0$$

$$\phi^h \cdot \mathbf{n} = Q_{in}^h$$



$$X = X_{out}$$

$$p_l = p_{l,out}$$

$$\phi^w \cdot \mathbf{n} = 0$$

$$\phi^h \cdot \mathbf{n} = 0$$



- ▶ Boundary conditions :
 - ▶ Injection of pure gas on left side
 - ▶ Impervious condition on top and bottom side
 - ▶ Pure water ($X_{out} = 0$) at fixed pressure on right side
- ▶ Initial conditions :
stationary state without injection ($Q_{in}^h = 0$)

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- ▶ Van Genuchten-Mualem model for capillary pressure and relative permeabilities
- ▶ Fixed temperature, $T = 303 K$

Porous medium parameters			Fluid characteristics		
Parameter	Value		Parameter	Value	
k	$5 \cdot 10^{-20}$	m^2	D_l^h	$3 \cdot 10^{-9}$	m^2/s
Φ	0.15	(-)	μ_l	$1 \cdot 10^{-3}$	$Pa \cdot s$
P_r	$2 \cdot 10^6$	Pa	μ_g	$9 \cdot 10^{-6}$	$Pa \cdot s$
n	1.49	(-)	$H(T = 303K)$	$7.65 \cdot 10^{-6}$	$mol/Pa/m^3$
S_{lr}	0.4	(-)	M_l	10^{-2}	kg/mol
S_{gr}	0	(-)	M_g	$2 \cdot 10^{-3}$	kg/mol
			ρ_l^{std}	10^3	kg/m^3
			ρ_g^{std}	$8 \cdot 10^{-2}$	kg/m^3

Parameter	Value	
L_x	200	m
L_y	20	m
Q^h	$1.5 \cdot 10^{-5}$	$m/year$
$pl_{,out}$	10^6	Pa
T_{simul}	$5 \cdot 10^5$	$years$

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- ▶ Fully implicit time discretization of the space/time pde system

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- ▶ Spatial discretization of the linear pde with a MHFE method

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- ▶ Bi-conjugate gradient stabilized method to inverse each block

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- ▶ Blockwise Gauss-Seidel method to solve the 2 coupled linear systems
- ▶ Bi-conjugate gradient stabilized method to inverse each block
- ▶ Implementation with the modular code Cast3m

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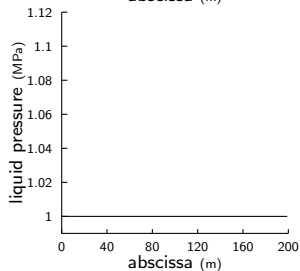
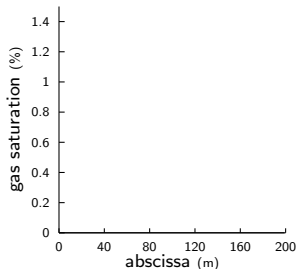
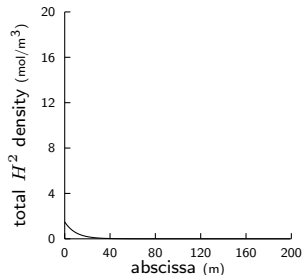
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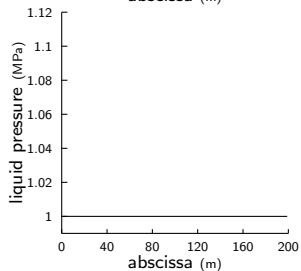
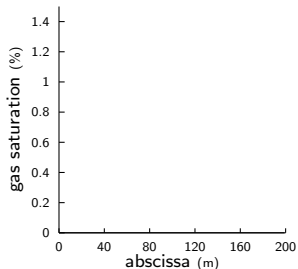
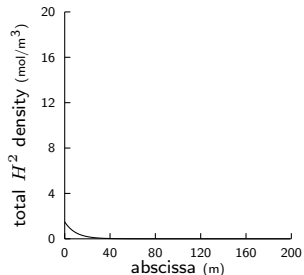
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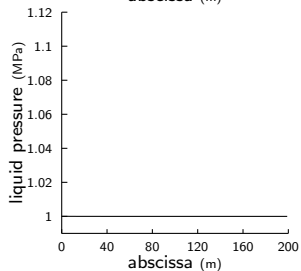
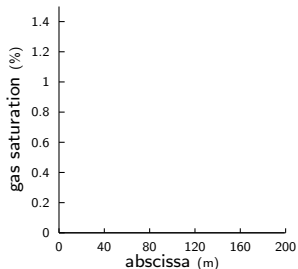
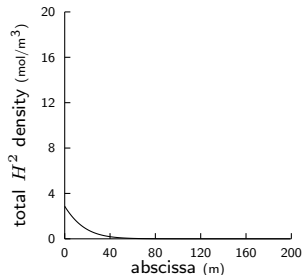
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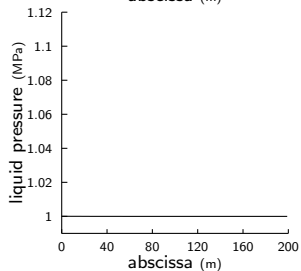
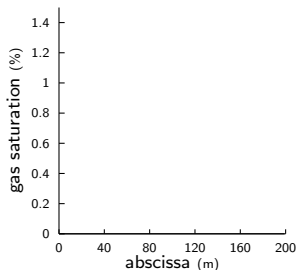
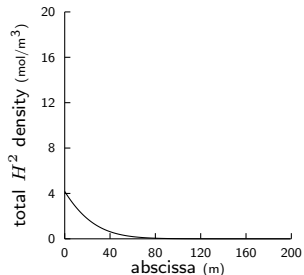
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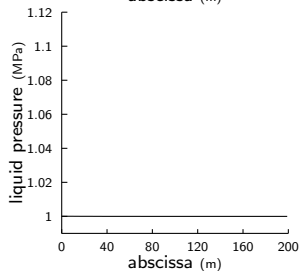
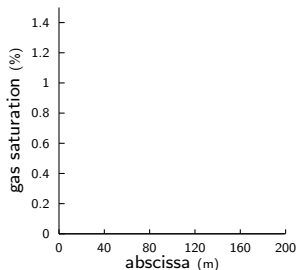
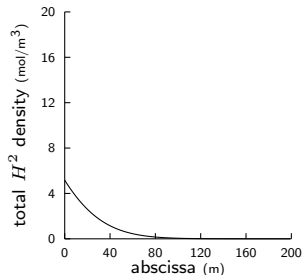
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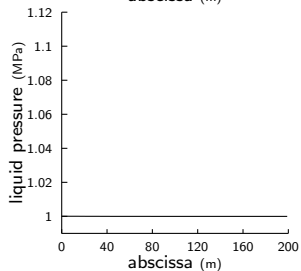
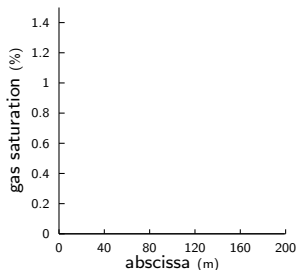
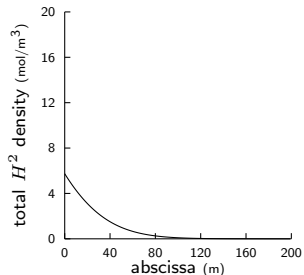
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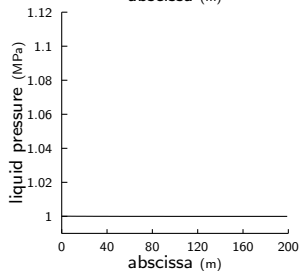
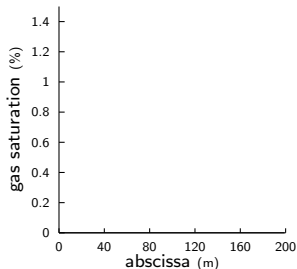
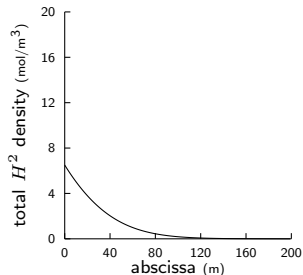
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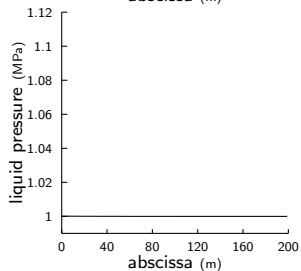
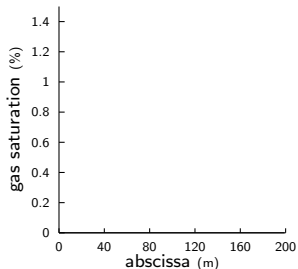
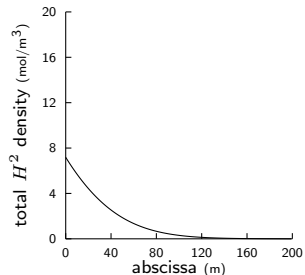
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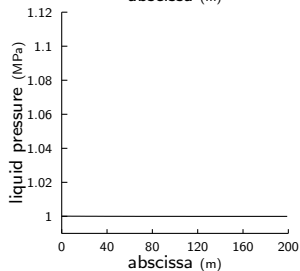
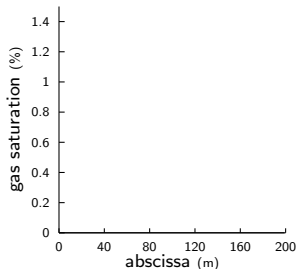
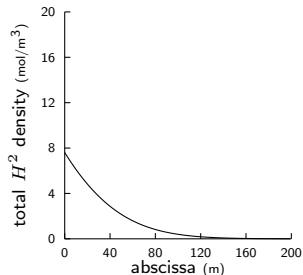
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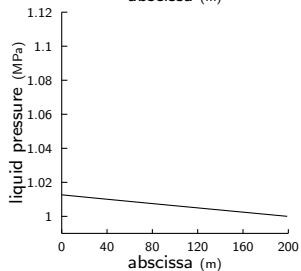
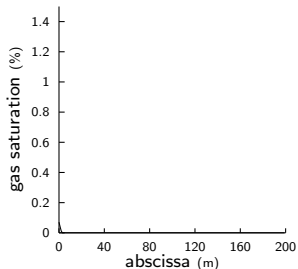
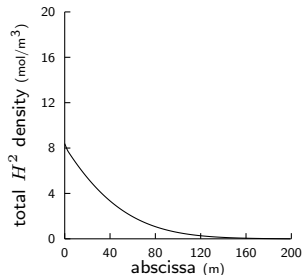
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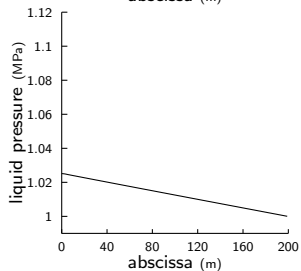
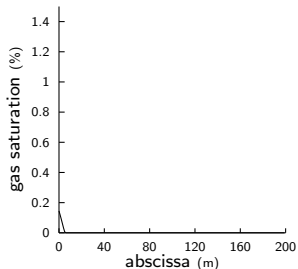
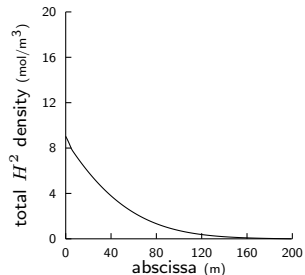
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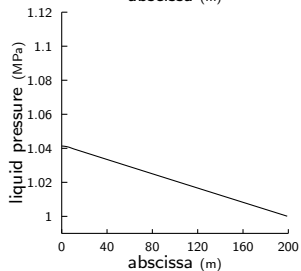
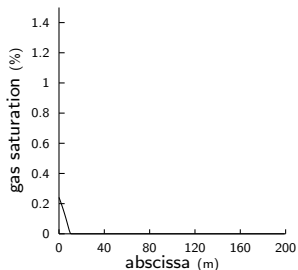
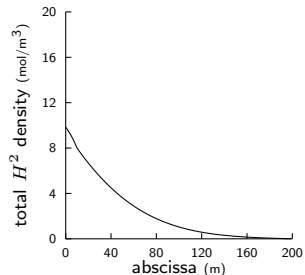
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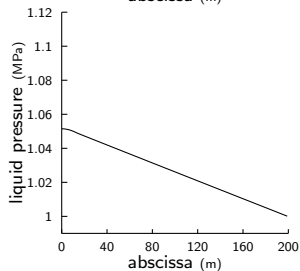
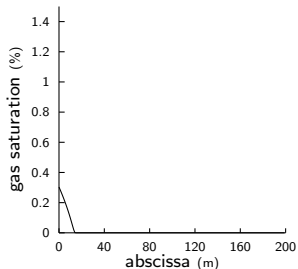
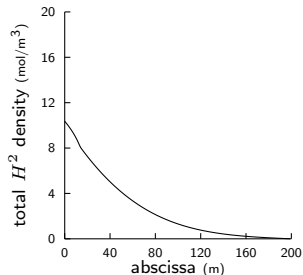
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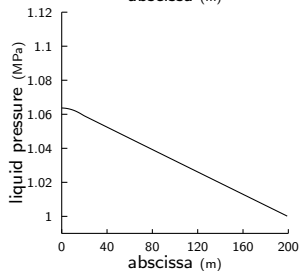
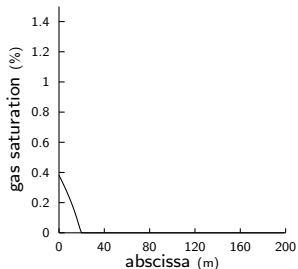
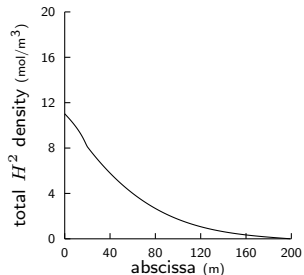
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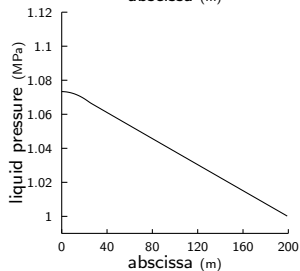
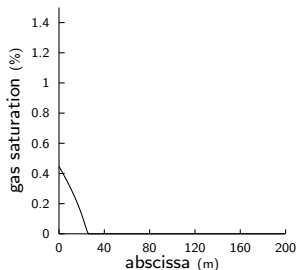
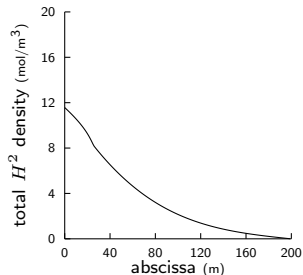
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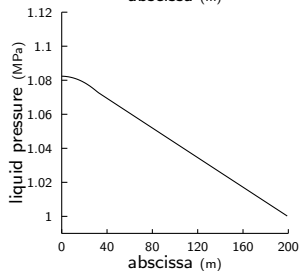
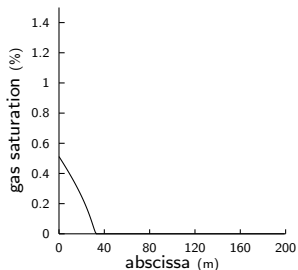
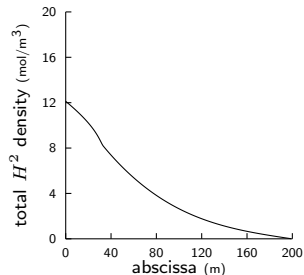
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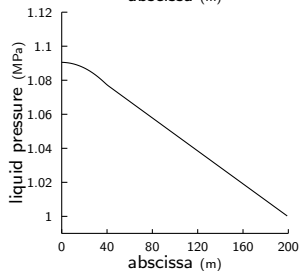
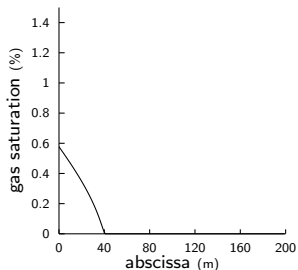
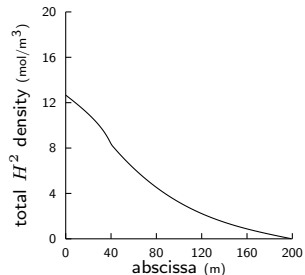
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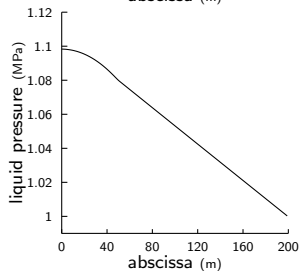
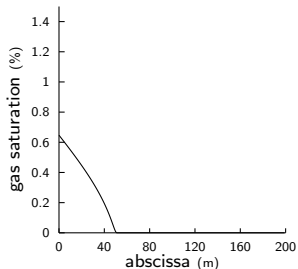
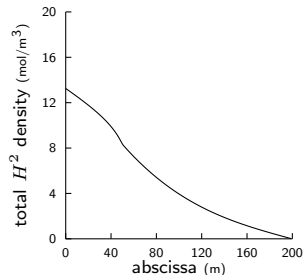
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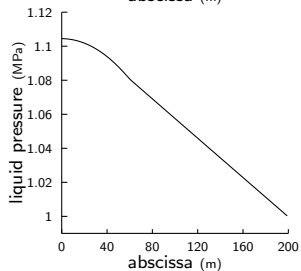
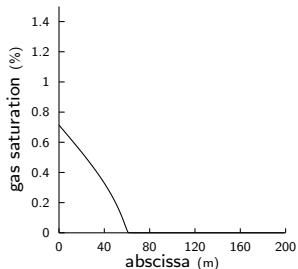
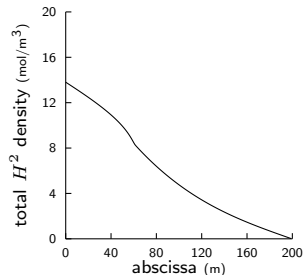
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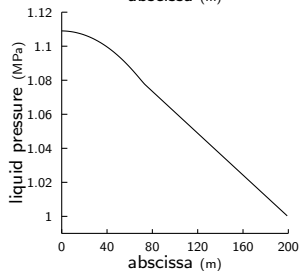
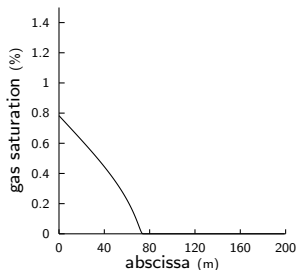
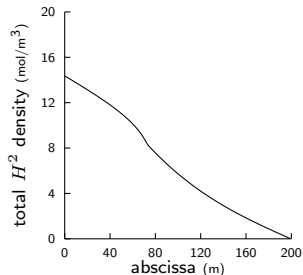
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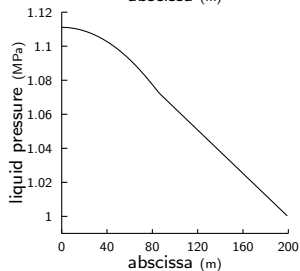
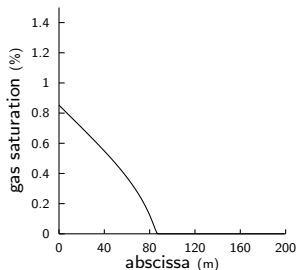
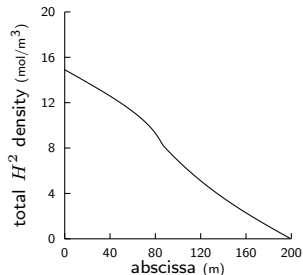
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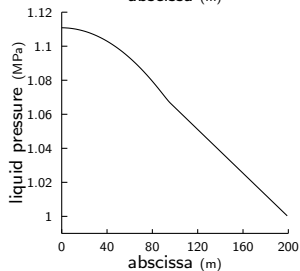
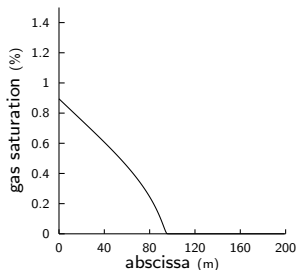
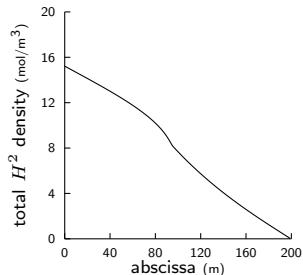
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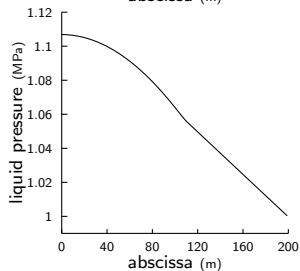
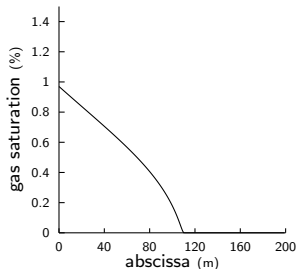
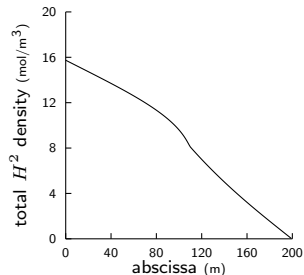
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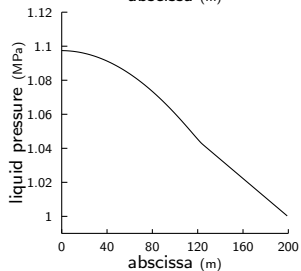
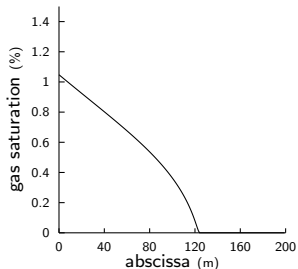
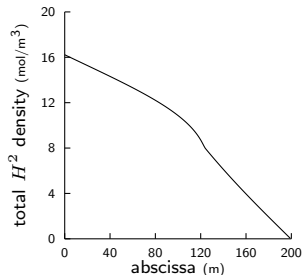
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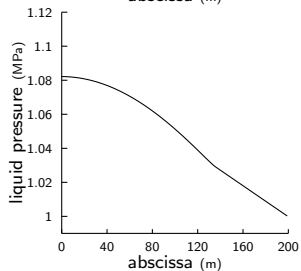
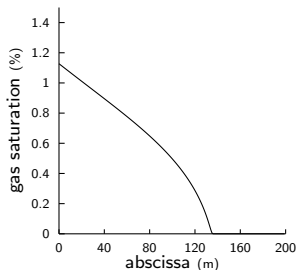
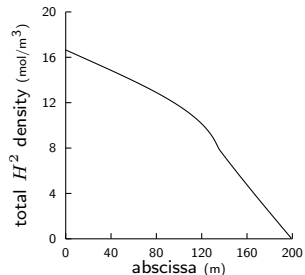
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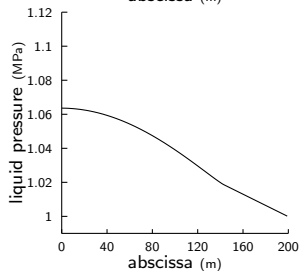
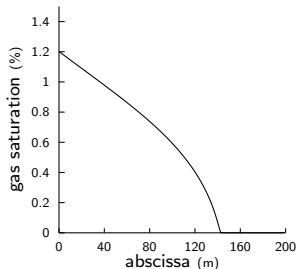
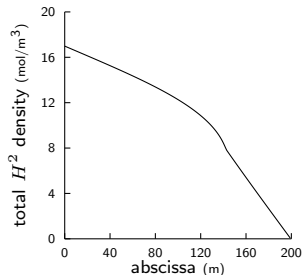
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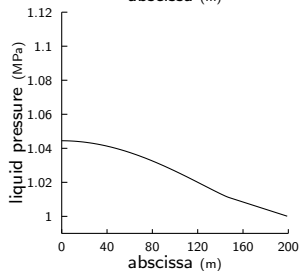
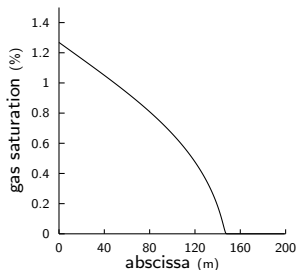
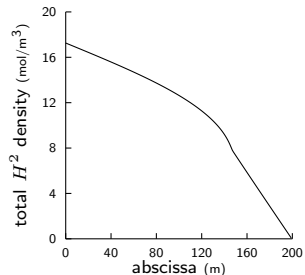
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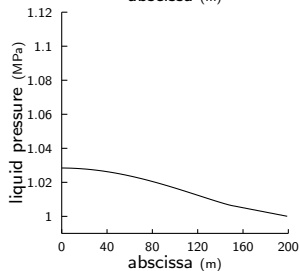
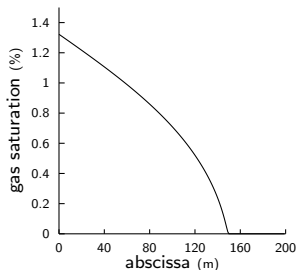
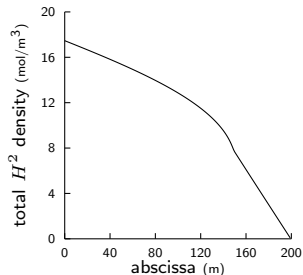
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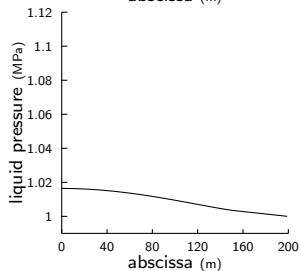
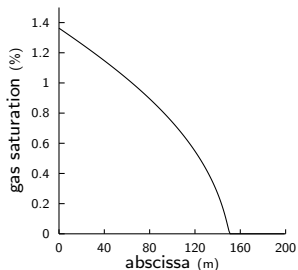
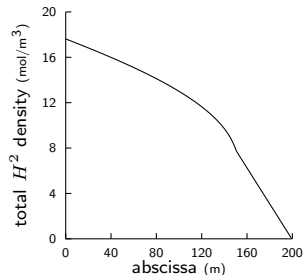
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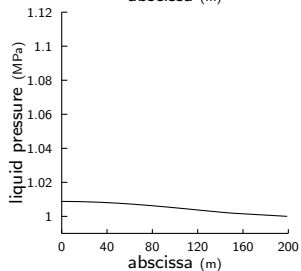
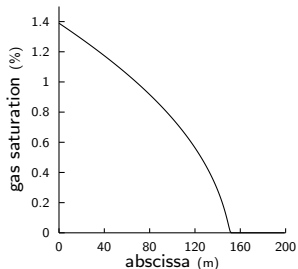
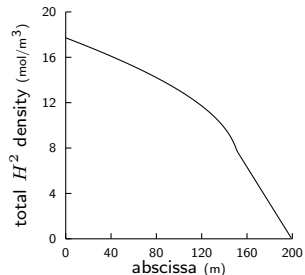
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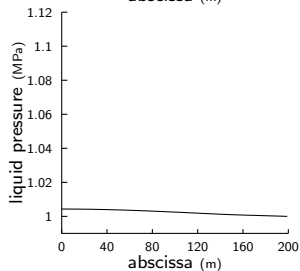
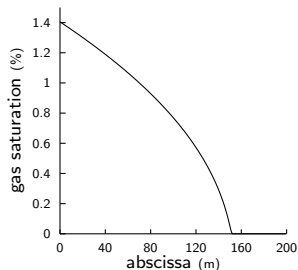
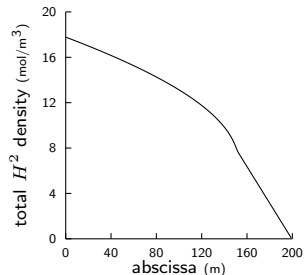
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References

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- ▶ SMAÏ, F. (-) A model of multiphase flow and transport in porous media applied to gas migration in underground nuclear waste repository. *submitted*

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