Numerical Simulation by Homogenization of Multiphase Flow in Heterogenous Porous Media

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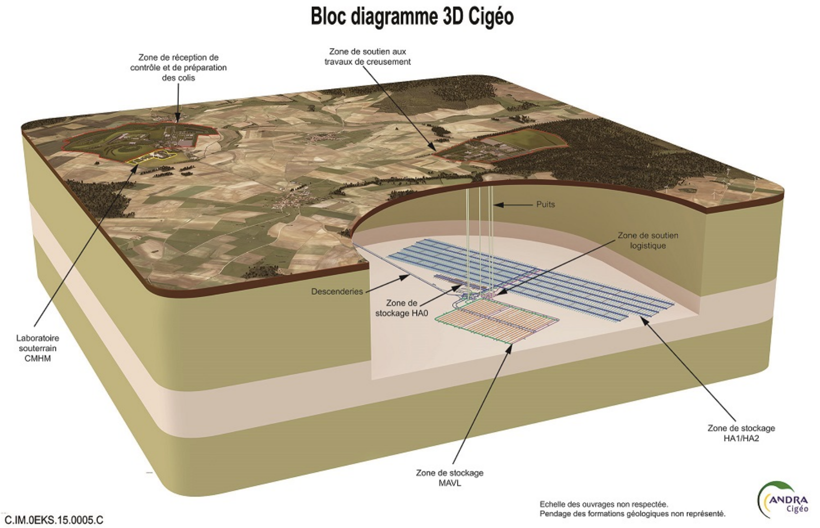
Outline

Introduction



Introduction

- Numerical modelling of gas migration and two-phase flow through engineered and geological barriers for a deep repository for radioactive waste.
- French Research Group **MoMaS** (PACEN/CNRS ANDRA, BRGM, CEA, EDF, IRSN): http://www.gdrmomas.org/
- Euratom FP7 Project **FORGE** (Fate Of Repository Gases): http://www.bgs.ac.uk/forge/home.html

Goal:

Couple DuMu^X to solve the coupled and non-linear system describing miscible compressible two phase flow in heterogeneous porous media and an upscaling strategy.

DuMu^X

http://dune-project.org/

[1] DuMu^X, DUNE for Multi-{Phase, Component, Scale, Physics, ...} flow and transport in porous media. DuMu^X web-page : http://www.dumux.org.

Introduction

References

B. Amaziane, M. El Ossmani, M. Jurak, *Numerical simulation of gas migration through engineered and geological barriers for a deep repository for radioactive waste*, Computat. and Visualiz. in Science **15**:1, (2012), 3–20.

E. Ahusborde, B. Amaziane, M. Jurak, *Three-dimensional numerical simulation by upscaling of gas migration through engineered and geological barriers for a deep repository for radioactive waste*, Geological Society Special Publication, **415**:1 (2015) 123–141.

B. Amaziane, S. Antontsev, L. Pankratov, A. Piatnitski, *Homogenization of immiscible compressible two-phase flow in porous media : application to gas migration in a nuclear waste repository*, SIAM J. Multiscale Model. Simul., **8**:5 (2010) 2023-2047.

B. Amaziane, L. Pankratov, A. Piatnitski, *An improved homogenization result for immiscible compressible two–phase flow in porous media*, Networks and Heterogeneous Media (NHM), **12**:1 (2017), 147–171.

Two-phase miscible compressible flow equations

Notation: The index $\alpha \in \{l, g\}$ refers to the phase (liquid and gas), while the superscript $c \in \{H_2O, H_2\}$ refers to the component.

- Generalized Darcy-Muskat's law

$$\boldsymbol{U}_\alpha = -\frac{k_{r\alpha}(S_\alpha)}{\mu_\alpha} K \left(\nabla P_\alpha - \rho_\alpha \mathbf{g}\right).$$

- Mass conservation law for each component

$$\frac{\partial}{\partial t}(\Phi \sum_\alpha \rho_\alpha X_\alpha^c S_\alpha) + \sum_\alpha \nabla \cdot (\rho_\alpha X_\alpha^c \boldsymbol{U}_\alpha + \mathbf{J}_\alpha^c) - \sum_\alpha Q_\alpha^c = 0. \quad (1)$$

- Diffusive fluxes

$$\mathbf{J}_\alpha^c = -\Phi \rho_\alpha S_\alpha \frac{1}{\tau^2} D_\alpha^c \nabla X_\alpha^c. \quad (2)$$

Two-phase miscible compressible flow equations

- Capillary pressure law : Van Genuchten-Mualem model

$$P_g - P_l = P_c(S_l), \tag{3}$$

with

$$S_{le} = \frac{S_l - S_{lr}}{1 - S_{lr} - S_{gr}}, \tag{4}$$

$$P_c(S_l) = P_r(S_{le}^{-1/m} - 1)^{1/n}, \tag{5}$$

$$k_{rl}(S_l) = \sqrt{S_{le}}[1 - (1 - S_{le}^{1/m})^m]^2, \tag{6}$$

$$k_{rg}(S_l) = \sqrt{1 - S_{le}}(1 - S_{le}^{1/m})^{2m}. \tag{7}$$

- Henry law

$$C_l^{H_2} = H_{H_2}(T)P_g^{H_2}, \quad C_l^{H_2} = \frac{X_l^{H_2}\rho_l}{M_{H_2}}. \tag{8}$$

Description of the benchmark

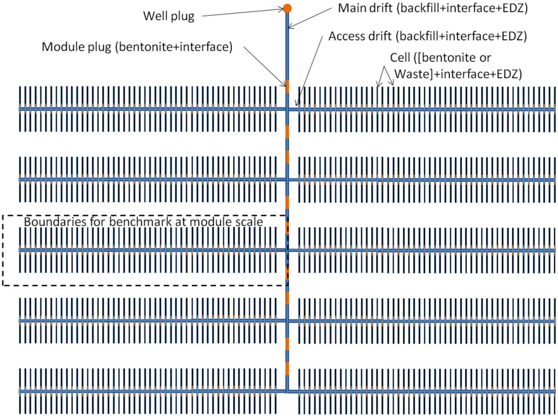


Figure: Schematic representation of a repository for HLW.

Description of the benchmark

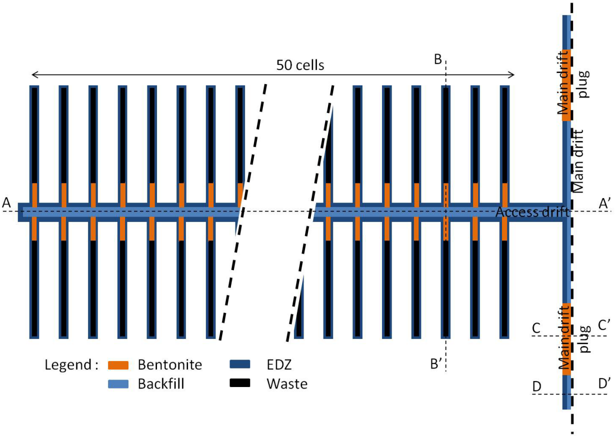


Figure: Schematic representation of the module to be simulated. Definition of the A-A', B-B' cross sections.

Description of the benchmark

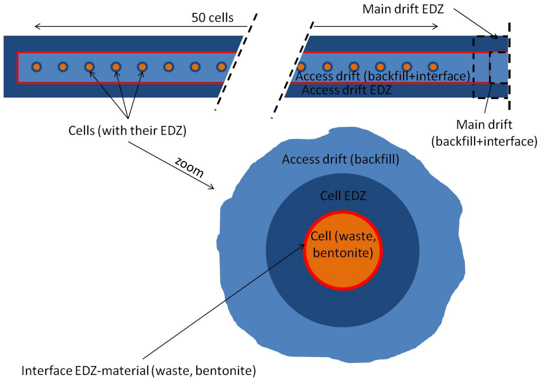


Figure: Schematic representation of the A-A' vertical cross section.

Description of the benchmark

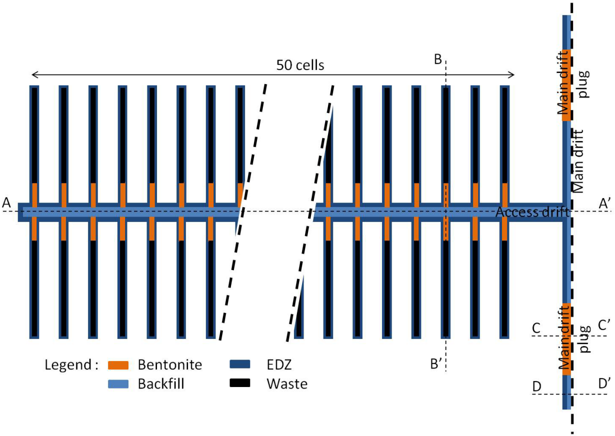


Figure: Schematic representation of the module to be simulated. Definition of the A-A', B-B' cross sections.

Description of the benchmark

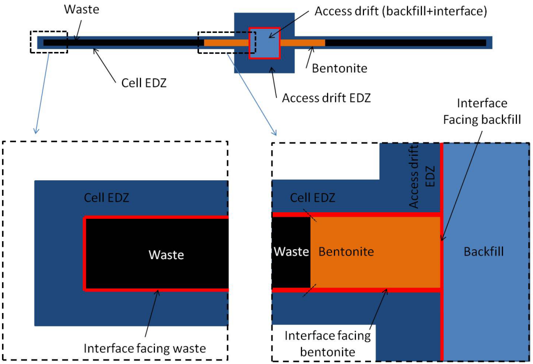


Figure: Schematic representation of the B-B' vertical cross section.

Physical parameters

Parameter	Materials		
	Interface facing plug	Interface facing waste	Interface facing backfill and edz
K $[m^2]$	$5 \cdot 10^{-18}$	10^{-12}	10^{-15}
Porosity $[\%]$	30	100	40
Van Genuchten parameters			
n [-]	4	4	4
Pr [Pa]	10^4	10^4	10^4
Tortuosity	1	1	1

Parameter	Materials			
	Backfills	Bentonite	EDZ	COX
K $[m^2]$	$5 \cdot 10^{-17}$	10^{-20}	$5 \cdot 10^{-18}$	10^{-20}
Porosity $[\%]$	40	35	15	15
Van Genuchten parameters				
n [-]	1.5	1.6	1.5	1.5
Pr [Pa]	$2 \cdot 10^6$	$1.6 \cdot 10^7$	$1.5 \cdot 10^6$	$1.5 \cdot 10^7$
Tortuosity	2	4.5	2	2

Table: Physical parameters.

Initial conditions and source term

At the initial moment the pressures are discontinuous.

Variables	Materials				
	Interfaces	Backfills	Bentonite plugs	EDZ	Geological Medium
S_l	$S_l = 0.05$	$S_l = 0.7$	$S_l = 0.7$	$S_l = 1$	$S_l = 1$
P_g, P_l	$P_g = 0.1MPa,\ P_l = P_g - P_c(S_l)$			$P_l = P_g = 5MPa$	

The source term:

- Implemented as Neumann boundary condition.
- $Q = 100$ mol/year for $t < 10000$ years; $Q = 0$ for $t > 10000$ years.

Finite volume scheme & Upscaling

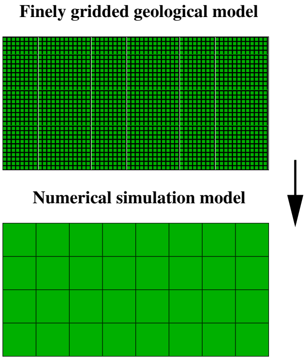
- Home-made code in C++ for the upscaling.
- Simulator : **DuMu**^{X}, DUNE for Multi-{Phase, Component, Scale, Physics, ...} flow and transport in porous media (http://www.dumux.org).
  - Model used : **2p2c** module which implements two-phase flow with two components.
  - Coupled fully-implicit approach.
  - Spatial discretization: vertex-centred finite volume approach.
  - Time discretization: implicit Euler scheme.
  - Mesh generator used: Gmsh + conversion into Dune Grid Format (DGF).

Scale up of the benchmark

Complete benchmark model can be represented only on a very fine grid. By means of upscaling we need to represent all model data on a coarser simulation grid. We upscale:

- Porosity $\Phi(\mathbf{x})$ and absolute permeability $K(\mathbf{x})$;
- Capillary pressure $P_c(\mathbf{x}, S)$ and relative permeability curves $kr_\alpha(\mathbf{x}, S)$;
- Tortuosity coefficient $\tau(\mathbf{x})$.

The upscaling is based on a local capillary equilibrium hypothesis. Heterogeneous quantities are replaced by homogeneous, effective ones.



Upscaling of permeability and porosity

Let the upscaling REV be denoted by V.
We have to solve in V the following steady-state Darcy's flow problem for $i = 1,2,3$:

$$-\nabla \cdot (K(\mathbf{x})\nabla P_i) = 0 \quad \text{in } V,$$
$$P_i = x_i \quad \text{on } \partial V.$$

where x_i is the i-th coordinate. Then we calculate the mean flux

$$< K\nabla P_i >= \frac{1}{\text{vol}(V)} \int_V K(\mathbf{x})\nabla P_i(\mathbf{x}) d\mathbf{x},$$

and the effective absolute permeability K^h is given by $\mathbb{K}^h \mathbf{e}_i =< K\nabla P_i >$.
The effective porosity Φ^h is computed such that pore volume is exactly conserved between the fine and coarses scales:

$$\Phi^h = \frac{1}{\text{vol}(V)} \int_V \Phi(\mathbf{x}) d\mathbf{x}.$$

Amaziane, B., Koebbe, J. (2006). JHomogenizer: A computational tool for upscaling permeability for flow in heterogeneous porous media. Computational Geosciences, 10(4), 343-359.

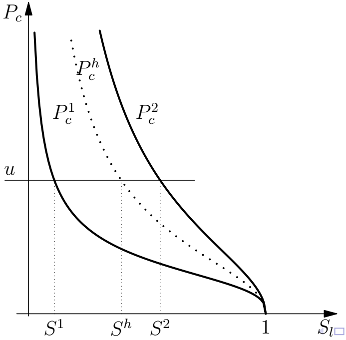
Bourgeat, A., Jurak, M. (2010). A two level scaling-up method for multiphase flow in porous media; numerical validation and comparison with other methods. Computational Geosciences, 14(1), 1-14.

Effective capillary pressure

- For given capillary pressure level u, we calculate the local saturation distribution $S^0(\mathbf{x})$ given by the local capillary equilibrium:

$$u = P_c^1(S_1) = \cdots = P_c^n(S_n), \quad S^h = \int_V \Phi(\mathbf{x}) S^0(\mathbf{x}) d\mathbf{x} / \Phi^h.$$

- Effective capillary pressure is then $P_c^h(S^h) = u$.



Effective relative permeability

- For given effective S^h, we calculate $P_c^h(S^h)$ and corresponding local saturation distribution $S^0(\mathbf{x})$.
- The effective relative permeability function $kr_\alpha^h(S^h)_i$, in the space direction i, is defined by the formula:

$$kr_\alpha^h(S^h)_i = \frac{1}{\mathrm{vol}(V)} \int_V K(\mathbf{x}) kr_\alpha(\mathbf{x}, S^0(\mathbf{x})) \nabla P_i \cdot \mathbf{e}_i d\mathbf{x} / \mathbb{K}_{i,i},$$

where P_i satisfies

$$-\nabla \cdot (K(\mathbf{x}) kr_\alpha(\mathbf{x}, S(\mathbf{x})) \nabla P_i) = 0 \quad \text{in } V,$$
$$P_i = x_i \quad \text{on } \partial V.$$

Effective tortuosity

- For given effective S^h calculate $P_c^h(S^h)$ and corresponding local saturation distribution $S^0(\mathbf{x})$.
- The effective tortuosity function $\tau_\alpha^h(S^h)_i$, in the space direction i, is defined for the effective saturation S^h and the phase α by:

$$\frac{\Phi^h S_\alpha^h}{\tau_\alpha^h(S^h)_i^2} = \frac{1}{\mathrm{vol}(V)} \int_V \Phi(\mathbf{x}) \frac{S_\alpha(\mathbf{x})}{\tau(\mathbf{x})^2} \nabla \xi_i^\alpha \cdot \mathbf{e}_i d\mathbf{x},$$

where ξ_i satisfies

$$-\nabla \cdot (\Phi(\mathbf{x}) \frac{S_\alpha(\mathbf{x})}{\tau(\mathbf{x})^2} \nabla \xi_i^\alpha) = 0 \quad \text{in } V,$$

$$\xi_i^\alpha = x_i \quad \text{on } \partial V.$$

Upscaling for the benchmark

- U1. Elimination of the Interfaces:
  - EDZ+Interface $\rightarrow$ homogeneous block
  - Backfill+Interface $\rightarrow$ homogeneous block
  - MainDriftPlug+Interface $\rightarrow$ homogeneous block

Upscaling for the benchmark

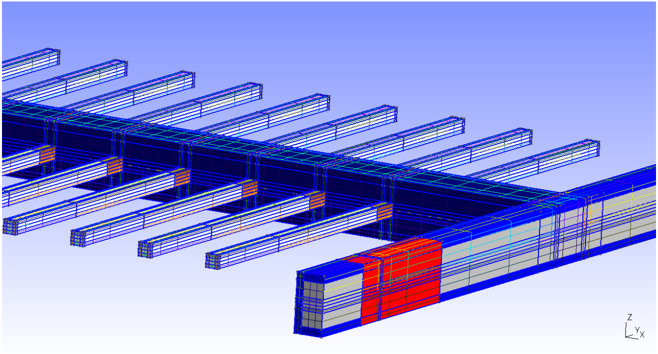


Figure: U1 grid: 510 112 elements.

Upscaling for the benchmark

- U1. Elimination of the Interfaces:
  - EDZ+Interface $\rightarrow$ homogeneous block
  - Backfill+Interface $\rightarrow$ homogeneous block
  - MainDriftPlug+Interface $\rightarrow$ homogeneous block
- U2. Intermediate Upscaling:
  - Canister+Interface+EDZ $\rightarrow$ homogeneous block
  - Plug+Interface+EDZ $\rightarrow$ homogeneous block
  - Backfill+Interface+EDZ $\rightarrow$ homogeneous block
  - MainDriftPlug+Interface $\rightarrow$ homogeneous block

Upscaling for the benchmark

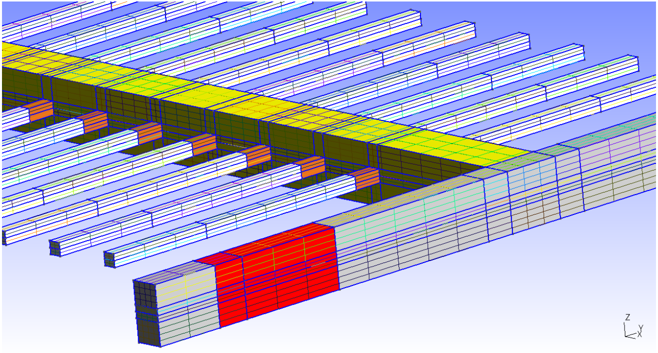


Figure: U2 grid: 247 620 elements.

Upscaling for the benchmark

- U1. Elimination of the Interfaces:
  - EDZ+Interface $\rightarrow$ homogeneous block
  - Backfill+Interface $\rightarrow$ homogeneous block
  - MainDriftPlug+Interface $\rightarrow$ homogeneous block
- U2. Intermediate Upscaling:
  - Canister+Interface+EDZ $\rightarrow$ homogeneous block
  - Plug+Interface+EDZ $\rightarrow$ homogeneous block
  - Backfill+Interface+EDZ $\rightarrow$ homogeneous block
  - MainDriftPlug+Interface $\rightarrow$ homogeneous block
- U3. Full Upscaling:
  - Canister+Plug+Interface+EDZ+GM $\rightarrow$ homogeneous block
  - Backfill+Interface+EDZ $\rightarrow$ homogeneous block
  - MainDriftPlug+Interface $\rightarrow$ homogeneous block

Upscaling for the benchmark

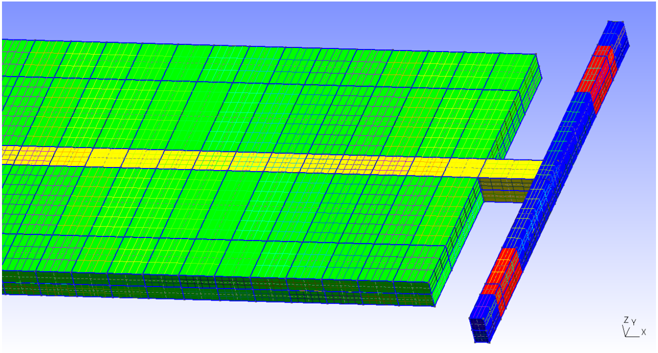
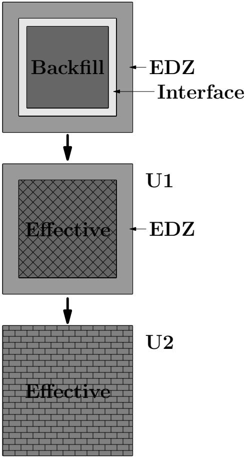


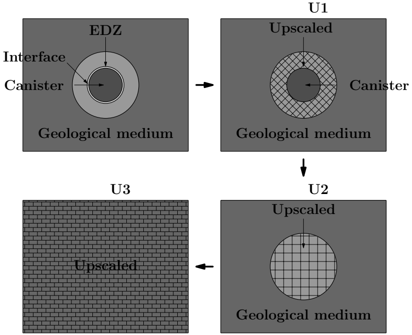
Figure: U3 grid: 27 776 elements.

Upscaling near the drifts

- U1. Elimination of Interfaces:
  Backfill+Interface → homogeneous block
- U2. Intermediate upscaling:
  Backfill+Interface+EDZ →
  homogeneous block
- U3. Full upscaling:
  The same.



Upscaling near the canisters



- U1. EDZ+Interface → homogeneous block
- U2. Canister+Interface+EDZ → homogeneous block
- U3. Canister+Plug+Interface+EDZ+GM → homogeneous block

Output results

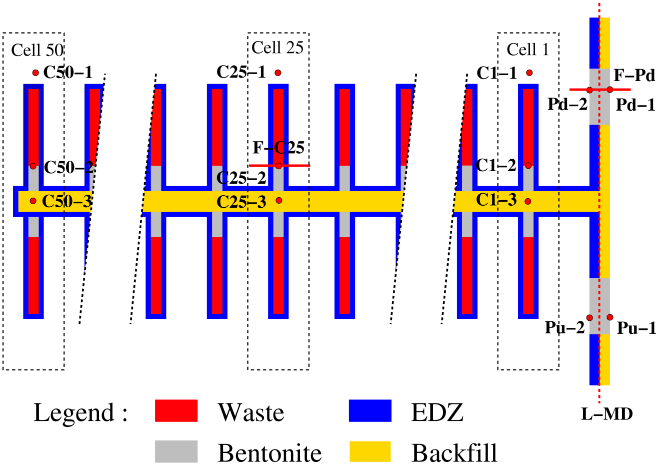


Figure: Definition of the points where results have been extracted, of the line L-MD and of the surfaces F-C25 and F-Pd.

Results for model U2 : Fluxes

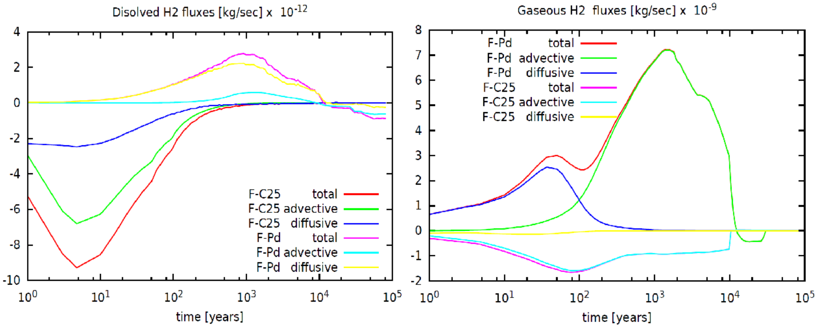


Figure: Dissolved hydrogen fluxes (Left) and Gaseous hydrogen fluxes (Right).

- Gaseous hydrogen total fluxes are three orders of magnitude larger than the dissolved hydrogen total fluxes.
- In gaseous phase, the advective fluxes dominate diffusive fluxes by several order of magnitudes, while in the liquid phase they are comparable.

Results for model U2 : Data in points

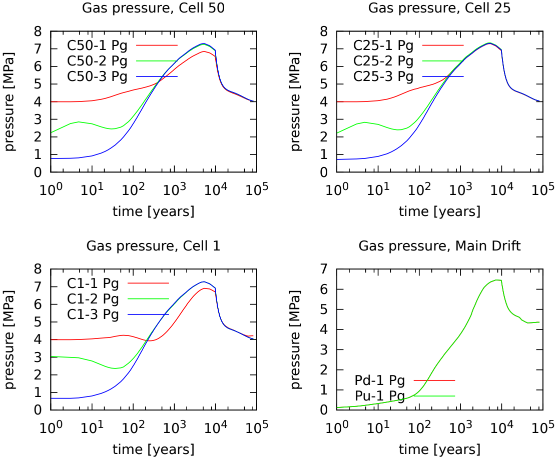


Figure: Gas pressure in points.

- The pressure maximum is about $7MPa$.

Results for model U2 : Data on line L-MD

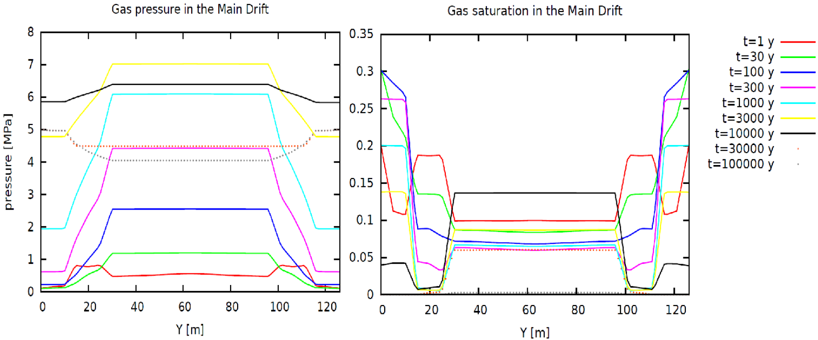


Figure: Gas pressure (left) and gas saturation (right) in the Main drift.

- Pressurisation of the Main Drift, which does not exceed 7 MPa, and return to the equilibrium which is not completely done even after 100,000 years.
- The Main Drift plugs are almost fully resaturated after 1,000 years.

Comparison between U2 and U3 models

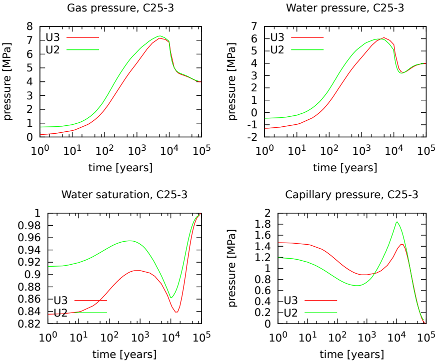


Figure: Solution in the point P-C25-3 for models U3 and U2.

	CPU time
Model U3	4 hours (8 proc)
Model U2	1 month (24 proc)

Table: CPU time for models U3 and U2.

Gas pressure and saturation

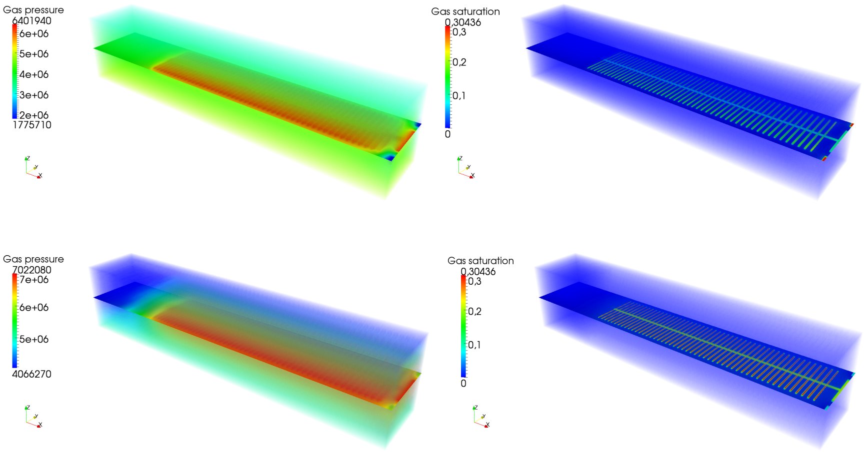


Figure: Gas pressure and saturation at t=1000y (top) and t=10000y (bottom) for the U2 model.

Comparison with other participants

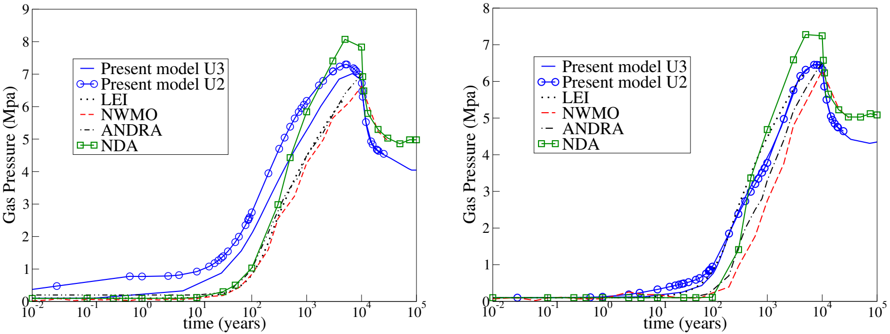


Figure: Comparison of the gas pressure for the points P-C50-3 (left) and P-Pd-1 (right).

Conclusion and acknowledgements

- The maximum pressure in the module will be about 7 MPa.
- The advection is the main way of hydrogen transport.
- Transport of hydrogen dissolved in water is about three orders of magnitude less significant than the transport of gaseous hydrogen.
- This work was partially supported by the **Euratom FP7 Project FORGE** under grant agreement 230357 and the **GnR MoMaS** (PACEN/CNRS, ANDRA, BRGM,CEA, EDF, IRSN) France, their supports are gratefully acknowledged.