# Two-Phase Flow Numerical Modeling : Application to a Geological Nuclear Waste Disposal

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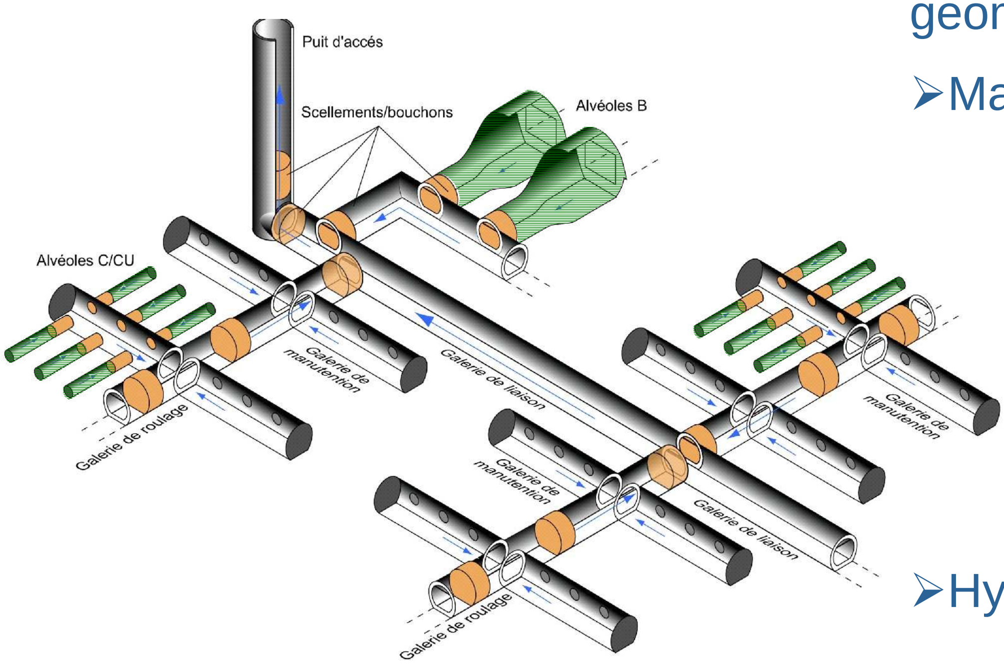
# OUTLINE

- ➢Industrial context : Nuclear waste storage
- ➢A classical two-phase flow model
- ➢An example of application : modeling of a disposal cell for an intermediate level long-lived waste (Benchmark Couplex Gaz 1 submitted by Andra)
  - ✓ Presentation of the problem
  - ✓ Numerical methods :
    - Classical FE Scheme : Discretization and results
    - Hybrid Finite Volume method : overview and first results
- ➢A first 3D study : modeling of a modulus of High level long-lived waste (Benchmark Couplex Gaz 2 submitted by Andra)
  - ➢ Results
  - ➢ Perspectives
- ➢Conclusions

# Industrial context : Underground waste storage




**Scheme for an underground mined repository**

- ➢A fully coupled THMC problem on a complex geometry !
- ➢Main reasons of two-phase flow modelling :
  - ✓Presence of initially unsaturated media (plugs, sealing …)
  - ✓Ventilation of the galleries
  - ✓Thermal drying
  - ✓Hydrogen production due to corrosion of steel components (containers, casing)
- ➢Hydraulic specificities :
  - ✓High level of capillary pressure (50 Mpa) and high level of gas pressure (due to corrosion)
  - ✓Saturation closed to one in the geological media

# A classical two-phase flow model

✓ 2 components ($H_2$ and $H_2O$) in 2 phases (liquid and gas)

✓ Capillary relation $P_c = f(S_l) = P_g - P_l$

✓ Mass conservation for water and hydrogen :

$$\frac{\partial}{\partial t}(m_c) + Div\left(F_l^c + F_g^c\right) = Q_c \quad c = H_2, H_2O$$

✓ Transport equations :

- Darcy's law for each phase

$$\begin{cases} F_l = -\dfrac{k.k_r^l(S_l)}{\mu_l}(\nabla P_l - \rho_l \mathbf{g}) \\ F_g = -\dfrac{k.k_r^g(S_g)}{\mu_g}\left(\nabla P_g - \rho_g \mathbf{g}\right) \end{cases}$$

- Diffusion law linking component velocities in each mixture (Fick's Law)

$$\frac{F_g^{H_2O}}{\rho_g^{H_2O}} + \frac{F_g^{H_2}}{\rho_g^{H_2}} = -F_g \nabla C_g \qquad \frac{F_l^{H_2O}}{\rho_l^{H_2O}} + \frac{F_l^{H_2}}{\rho_l^{H_2}} = -F_l \nabla C_l$$

- Dissolution (Henry's Law) $\dfrac{\rho_l^{H_2}}{M_{H_2}^{ol}} \leq \dfrac{P_g^{H_2}}{K_H}$
- Vaporization (equilibrium equation)

# Main modelisation difficulties

✓ Injection of gas in a saturated porous media
- Geological media initially saturated : what is the initial concentration of hydrogen or air in the liquid ?
- High level of gas pressure

✓ Presence of multiple barriers
- Very high level of heterogeneities of the different materials
- Initial level of saturation very dependant of the material

✓ Huge non linearities
- Capillary and Relative permeabilities functions (influencing type of equations and front shape)

**Ex. for relative permeabilities**

$$k_{rel}^{l} = \sqrt{S_l}\left(1-\left(1-S_l^{1/m}\right)^m\right)^2$$ (Van Genuchten)

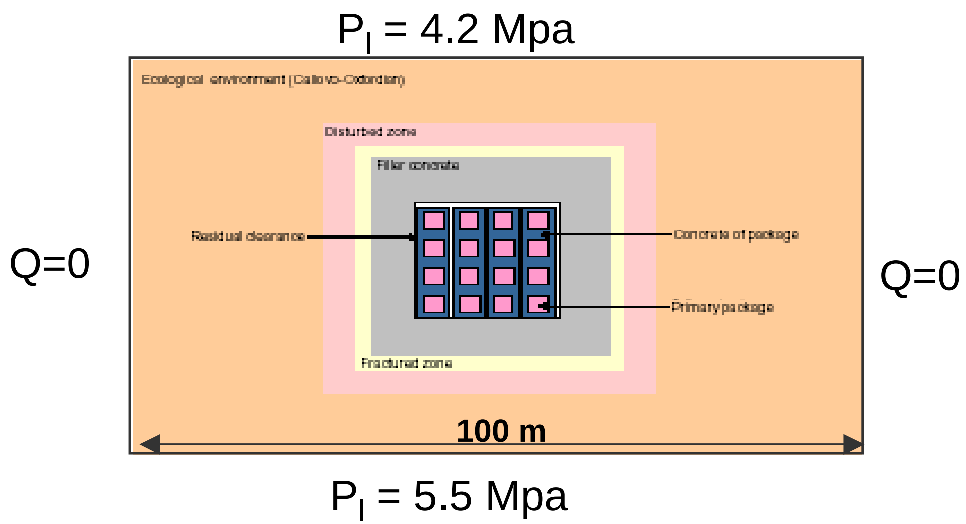
$$k_{rel}^{l} = S_l^{A} S_l^{B+1/\lambda}$$ (Brooks&Corey)

$$k_{rel}^{l} = S_l^{3}$$ (cubic)

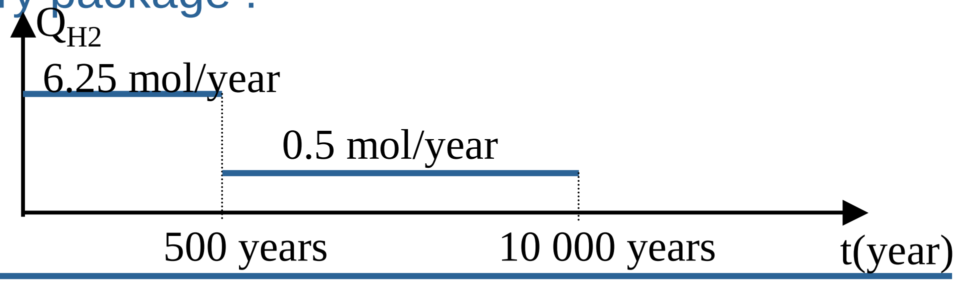
$$\frac{\partial(\phi\rho_l S_l)}{\partial t} + Div\left(\frac{k.k_r^l(S_l)}{\mu_l}(\nabla P_l)\right) = Q$$

# COUPLEX-GAZ I (Andra 2007): Exercice definition (1/2)

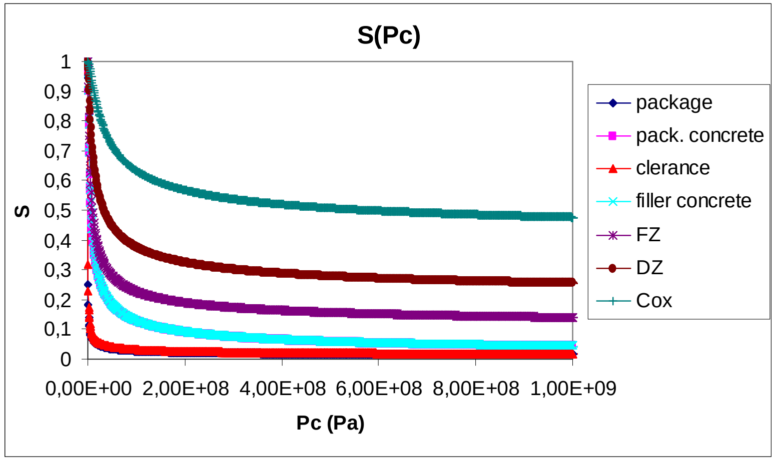
Modeling of a disposal cell for an intermediate level long-lived waste :

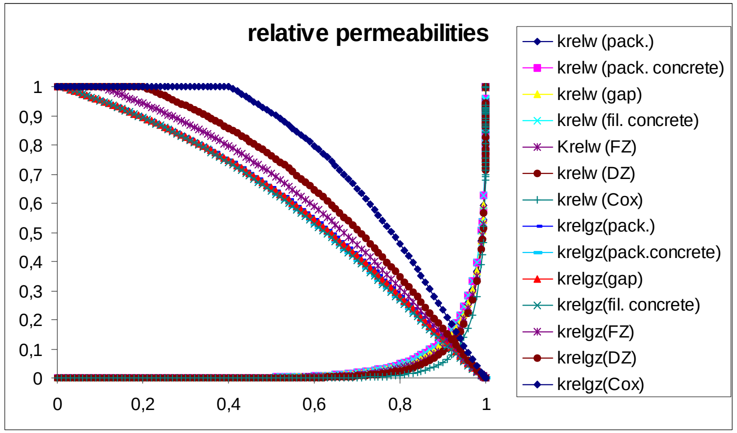



- Anisotropic problem (in the clay $K_H \neq K_v$ )
- Total hydrogen Flux for each primary package :



# COUPLEX-GAZ I : caracteristic curves – Van Genuchten Mualem model



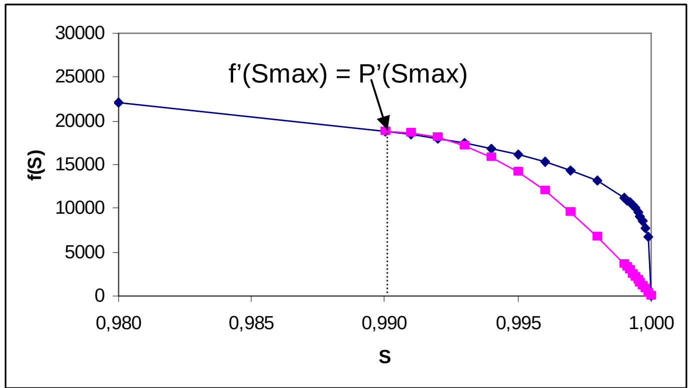

$$S_l = \frac{1 - S_{wres}}{\left(\left(\frac{P_c}{P_r}\right)^n + 1\right)^m} + S_{wres}$$

$$k_{rel}^l = \sqrt{S_{we}}\left(1 - \left(1 - S_{we}^{\ 1/m}\right)^m\right)^2 \qquad k_{rel}^g = \sqrt{\left(1 - S_{we}\right)}\left(1 - S_{we}^{\ 1/m}\right)^{2m}$$

Singularities for S = 1 :

$$\frac{\partial S(Pc)}{\partial Pc} = 0 \qquad \frac{\partial k_r^g(S_w)}{\partial S_w} = \infty \qquad \frac{\partial k_r^w(S_w)}{\partial S_w} = \infty$$

2nd order polynomial C1 Interpolation for S > Smax (ex. Smax = 0,99)



## COUPLEX-GAZ I : Exercice definition (2/2)

✓ Couplex's initial conditions : high contrast of saturation and capillary pressure

| | $S^{init}$ | $Pc^{init}$ | K |
|---|---|---|---|
| Filler concrete | 0,7 | 3 Mpa | $10^{-18}$ m$^2$ |
| Concrete of package | 0,6 | 4,4 Mpa | $10^{-19}$ m$^2$ |
| clearance | 0,1 | 6 Mpa | $10^{-12}$ m$^2$ |
| Primary package | 0,2 | 0,8 Mpa | $10^{-15}$ m$^2$ |

- In the clay (healthy, disturbed or fractured) :

  S = 1

  Hydrostatic liquid pressure

  ✓ Actually, we consider a small gas pressure : Pg= 1atm (corresponding to a initial concentration of hydrogen in liquid)

# COUPLEX-GAZ I : Numerical method (FE)

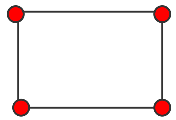
- **Couplex Gaz modelisation's tool (www.code-aster.org)**

✓ Choice of the unknowns : Pc and Pg

- In our formulation, we write $\frac{\rho_l^{H_2}}{M_{H_2}^{ol}} = \frac{P_g^{H_2}}{K_H}$
- In saturated area : $S_l = 1$

Variable transformation : $\hat{P}_g = \frac{K_H}{M_{H_2}^{ol}} \rho_l^{H_2}$ $\Rightarrow Pc = \hat{P}_g - P_l \leq 0$

✓ A Classical Finite Element method :



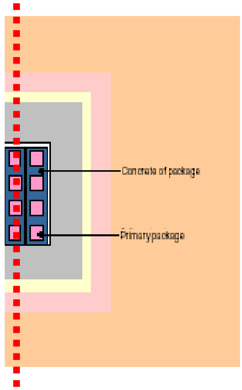
- Finite Elements with Q1 elements
- Lumping of the mass matrix :

Non diagonal mass matrix => maximum principle not verified => Oscillations

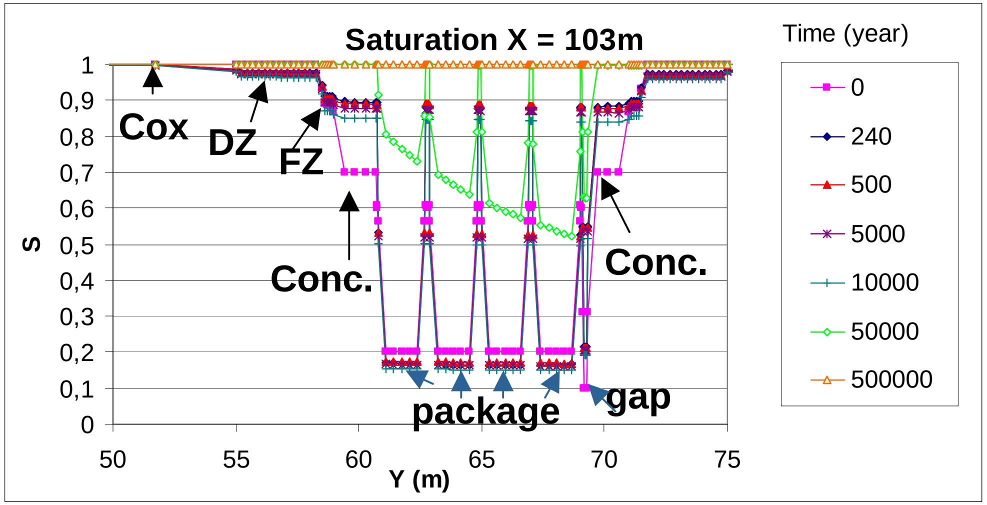
**Integration points at the vertex of the elements**

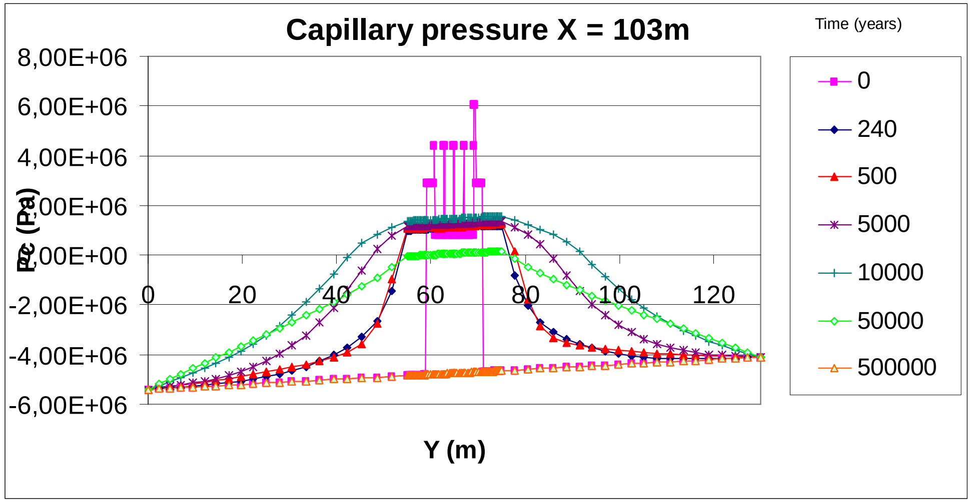
- Time discretization = Implicite Euler
- Newton method for non linear resolution

# COUPLEX-GAZ I : Gas saturation and capillary pressure profiles – X = 103 m




➢Vertical cross section




➢**<u>3 steps :</u>**

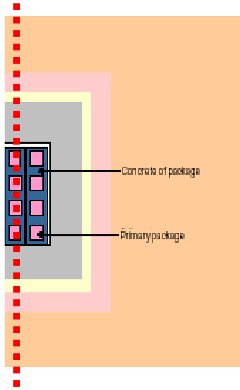
**1- capillary equilibrium (t<200 years)**

**2- Small desaturation by gas production (t< 10 000 years)**

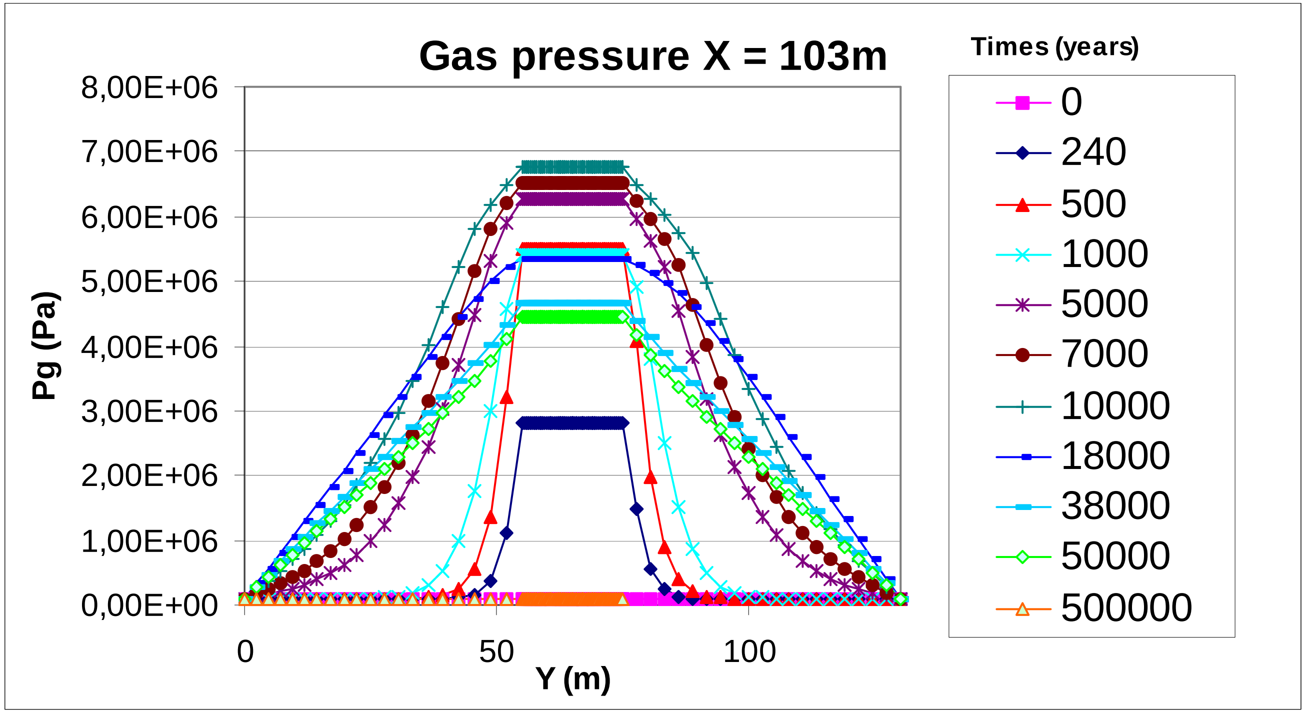
**3- The gas disappears gradually**

➢**Complete saturation at 60 000 years !**

# COUPLEX-GAZ I : Gas pressure – X = 103 m




➢Vertical cross section



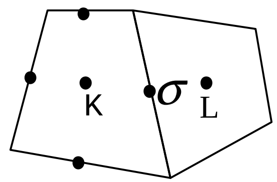

**Maximal Gas Pressure of 6,75 Mpa at 10 000 years– The pressure remains constant in the engineered area**

# COUPLEX-GAZ I : Using of a Hybrid Finite Volume scheme (1/4)

**REF :** ***Eymard R., Gallouët T., Herbin R. « A new finite volume scheme for anisotropic diffusion problems on general grids : convergence analysis » (CRAS 2007 – vol 344 – num 6)***

- On an elliptic problem $-\nabla.(\Lambda \nabla u) = f$
  - ✓ Volumic integration : $-\sum_{\sigma \in \varepsilon_K} F_{K,\sigma} = \int_K f$ with $F_{K,\sigma} \approx \int_\sigma \Lambda \nabla u.\mathbf{n}_{K\sigma}.d\sigma$
  - ✓ Flow calculation

$$F_{K,\sigma} = m_\sigma \Lambda_K \left[ \left( \alpha_K \frac{u_\sigma - u_K}{d_{K\sigma}} \right) + (\nabla_D u)_K \left( \mathbf{n}_{K\sigma} - \alpha_K \frac{\mathbf{x}_\sigma - \mathbf{x}_K}{d_{K\sigma}} \right) \right]$$




Coercivity term

To determine

We remove what we added

- Computation of discrete flow :
  - ✓ Flow $$(\nabla_D u)_K = \mathbf{M}_K . \sum_{\sigma \in \varepsilon_K} m_\sigma \left( \mathbf{n}_{K\sigma} - \alpha_K \frac{\mathbf{x}_\sigma - \mathbf{x}_K}{d_{K\sigma}} \right) (u_\sigma - u_K)$$
  - ✓ Consistence $$\mathbf{M}_K^{-1} = \sum_{\sigma \in \varepsilon_K} m_\sigma \left( \mathbf{n}_{K\sigma} \otimes (\mathbf{x}_\sigma - \mathbf{x}_K) - \frac{\alpha_K}{d_{K\sigma}} (\mathbf{x}_\sigma - \mathbf{x}_K) \otimes (\mathbf{x}_\sigma - \mathbf{x}_K) \right)$$
  - ✓ finally $$F_{K,\sigma} = \sum_{\sigma'} (\mathbf{C}_K)_{\sigma,\sigma'} (u_{\sigma'} - u_K)$$

# COUPLEX-GAZ I : Using of a Hybrid Finite Volume scheme (2/4)

## ▪Hybrid Finite Volume for two phase flow modeling

- ✓ Mass conservation for the two constituents

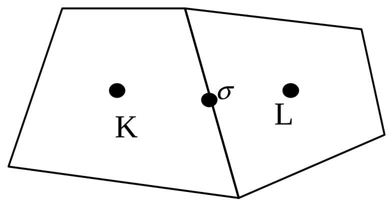
$$\frac{A_K}{\Delta t}\left(m_K^p - m_K^{p-}\right) - \sum_{\sigma}\sum_{\sigma'} k_\sigma^p \left(\mathbf{C}_K\right)_{\sigma,\sigma'}\left(u_{\sigma'}^p - u_K^p\right) = 0$$

- ✓ Flow continuity

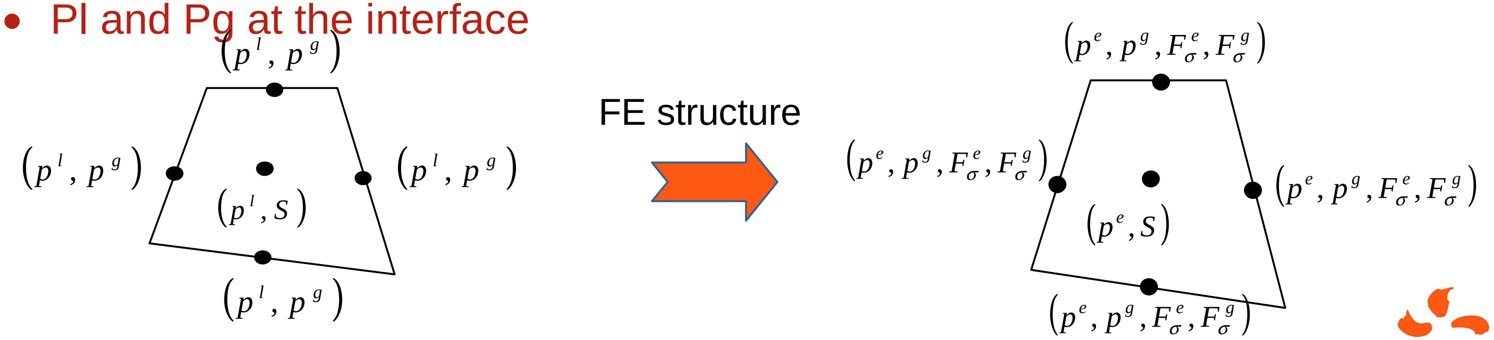
$$\sum_{\sigma}\sum_{\sigma'}\left(\mathbf{C}_K\right)_{\sigma,\sigma'}\left(u_{\sigma'}^p - u_K^p\right) + \sum_{\sigma}\sum_{\sigma'}\left(\mathbf{C}_L\right)_{\sigma,\sigma'}\left(u_{\sigma'}^p - u_L^p\right) = 0$$

- ✓ Upstream flow

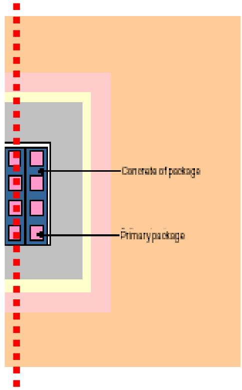
$$if\ F_{K,\sigma}^p \le 0$$
$$k_\sigma^p = k^p\left(u_K^p\right)$$
$$\text{else}$$
$$k_\sigma^p = k^p\left(u_L^p\right)$$



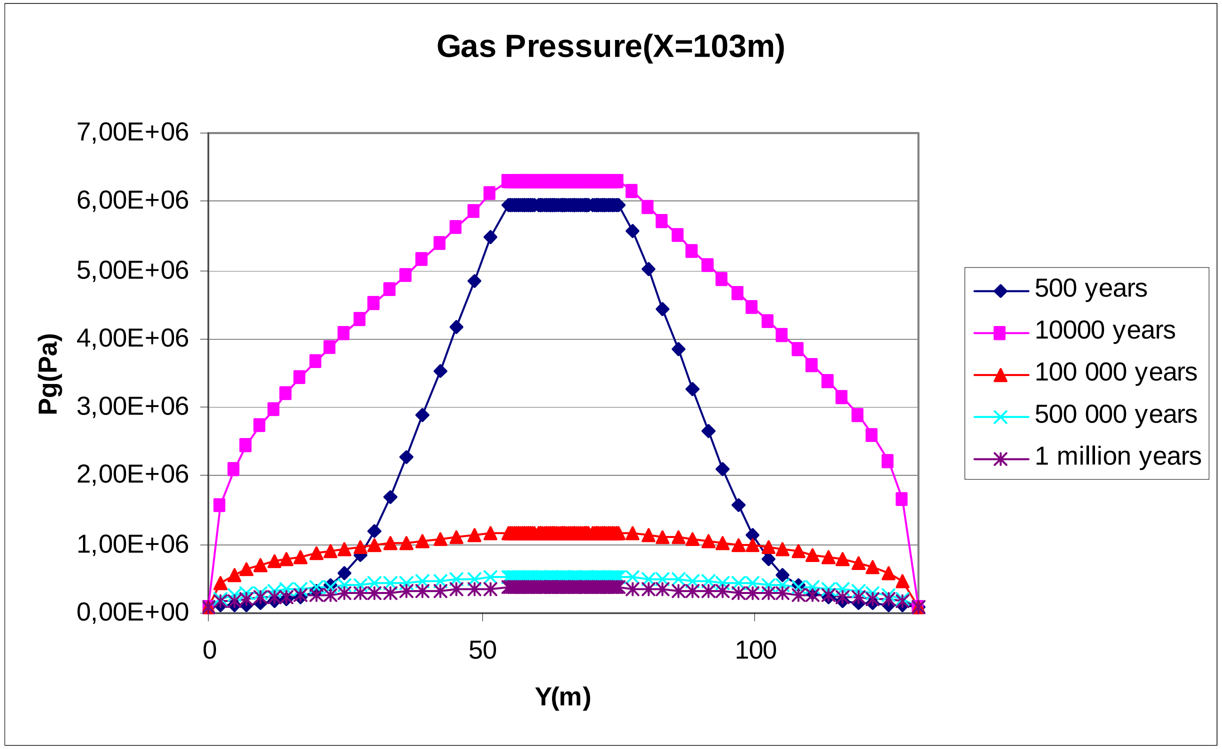

- ✓ Unkowns :
  - P,S at the center,
  - Pl and Pg at the interface



# COUPLEX-GAZ I : Using of a Hybrid Finite Volume scheme (3/4)




- Vertical cross section

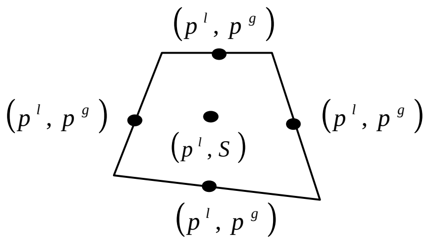



**Not exactly the same case (no gravity and isotropic permeability), but closed results**

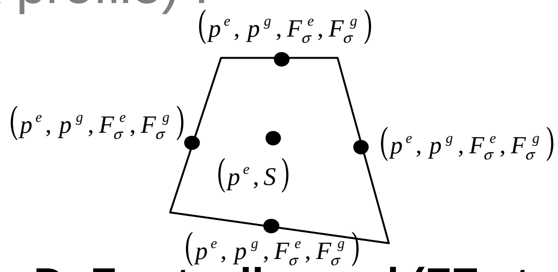
# COUPLEX-GAZ I : Using of a Hybrid Finite Volume scheme (4/4)

➢ In this test, Hybrid Finite Volume method allows us :

- ✓ A better initial saturation condition (S is an unknown instead of Pc)
- ✓ Good performance (better matrix profile) :




**DoF normaly required**



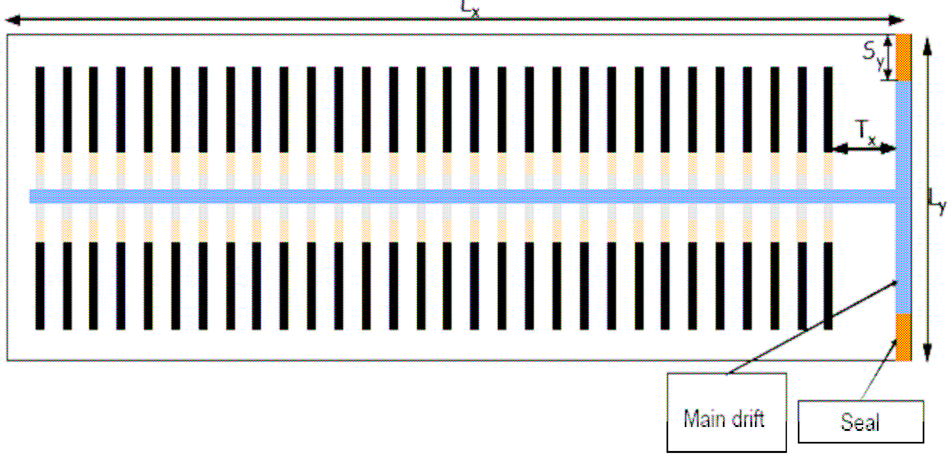

**DoF actually used (FE structure)**

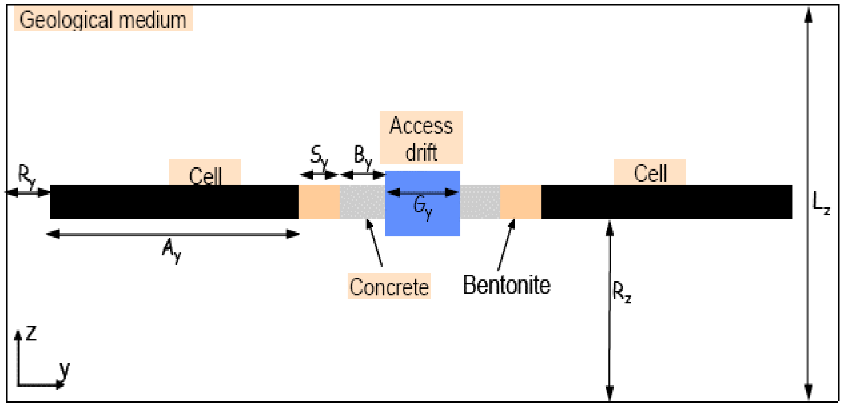
| | FE | HFV |
|---|---|---|
| Max nb of iterations per time step | 43 | 10 |
| Total nb of Newton iterations | 5230 | 5220 |
| Average nb of iterations per time step | 12 | 3 |
| Total CPU Times | 24 | 26 |

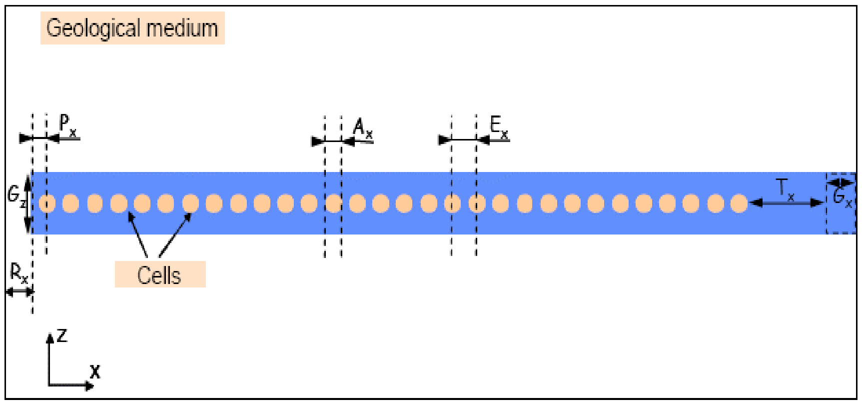
➡ **Promising method (sushis developments)…**

# A 3D application : Couplex 2 (1/3)

## 3D Modeling of a modulus of High level long-lived waste :

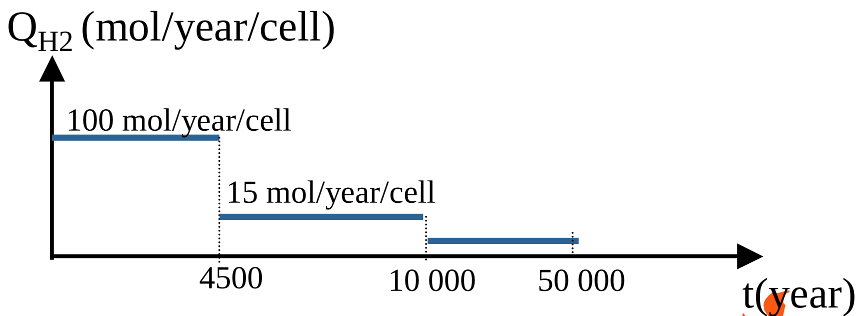


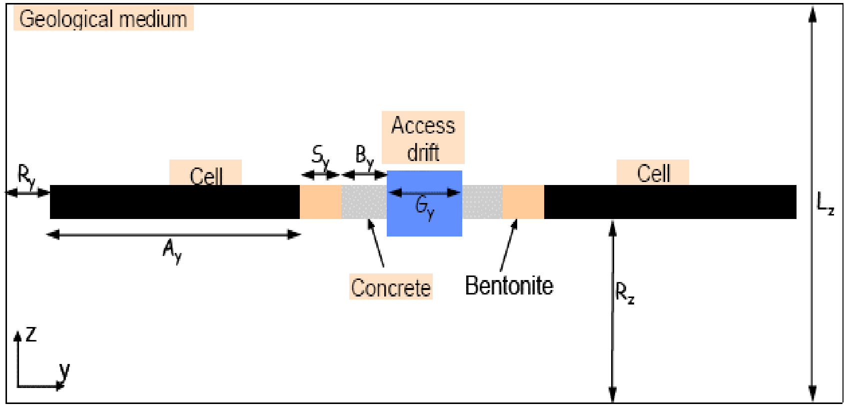




Lenght of modulus : Ly= 100m
Width of the modulus : 30m

## Gas production around each cell :



# A 3D application : Couplex 2 (2/3)



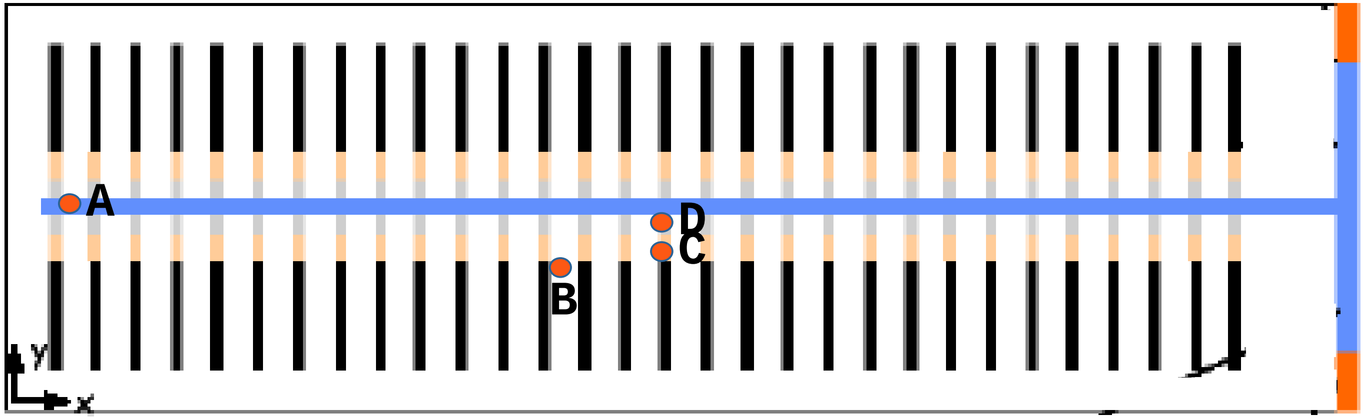

- Initial conditions :
  - ✓In the geological media :
    S=1; Hydrostatic liquid pressure
  - ✓In plugs and drifts :
    S=0,7; Pg = 1atm
- Material datas :
  - ✓Mualem/Van Genuchten model

Numerical scheme : Classical FE scheme (sequential computation)

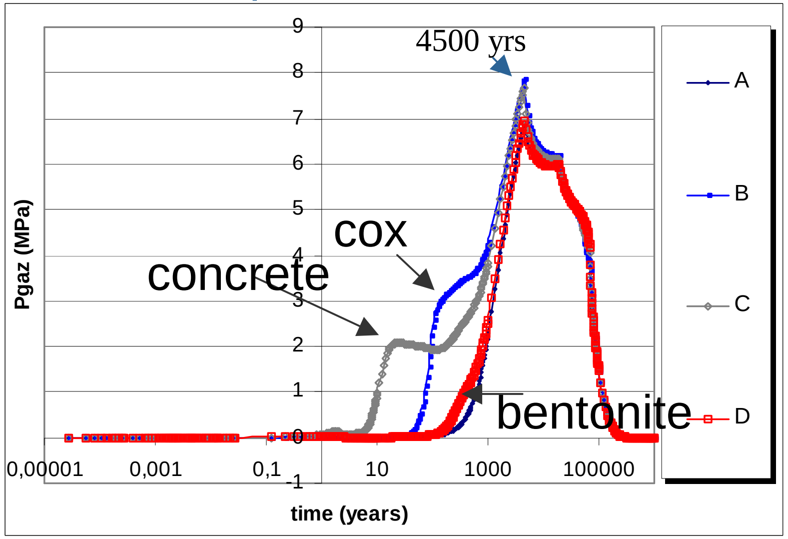
Mesh : 115 000 elements – 160 000 nodes – 287 000 equations

*Performances : CPU time : 100 hours for simulation of 500 000 years*

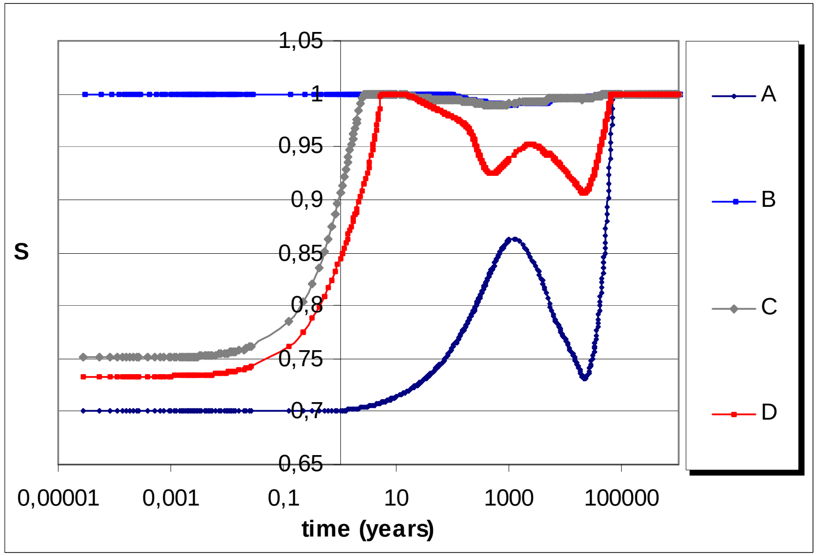
# A 3D application : Couplex 2 (3/3)




## Gas pressure evolution




## Saturation evolution



# Conclusions

- ➢Description of a coupled two-phase flow model :
  - ✓ Model of gas transfer in porous media
  - ✓ 2 phases, 2 constituents
  - ✓ Diffusion in gas and liquid mixture
- ➢Application to industrial studies (undeground waste storage modeling ):

▪**Benchmark Couplex 1 (2D - intermediate level long-lived waste )**

- ✓ Treated with a classical FE method
- ✓ Partially treated with a promising Hybrid Finite volume method

▪**Benchmark Couplex 3 (3D - High level long-lived waste )**

- ✓ First results obtained with a sequential FE method and a coarse mesh
- ✓ To be continued with a parallelism strategy
- ✓ To be continued with Hybrid Finite volume method (Sushi Method – PHD O. Angelini)