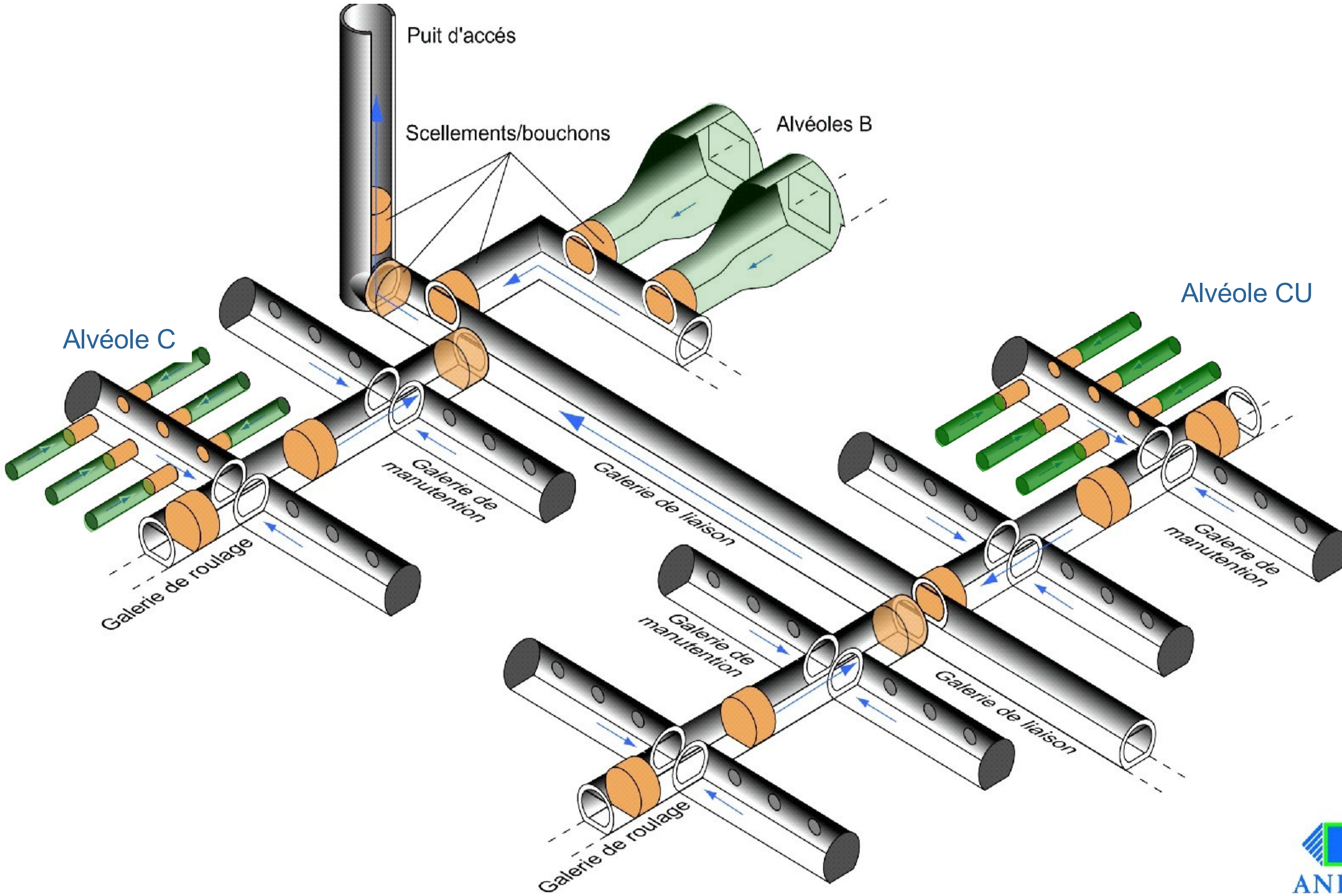
Thermo hydro mechanical coupling for underground waste storage simulations

Clément Chavant - Sylvie Granet – Roméo Frenande
EDF R&D

Outline

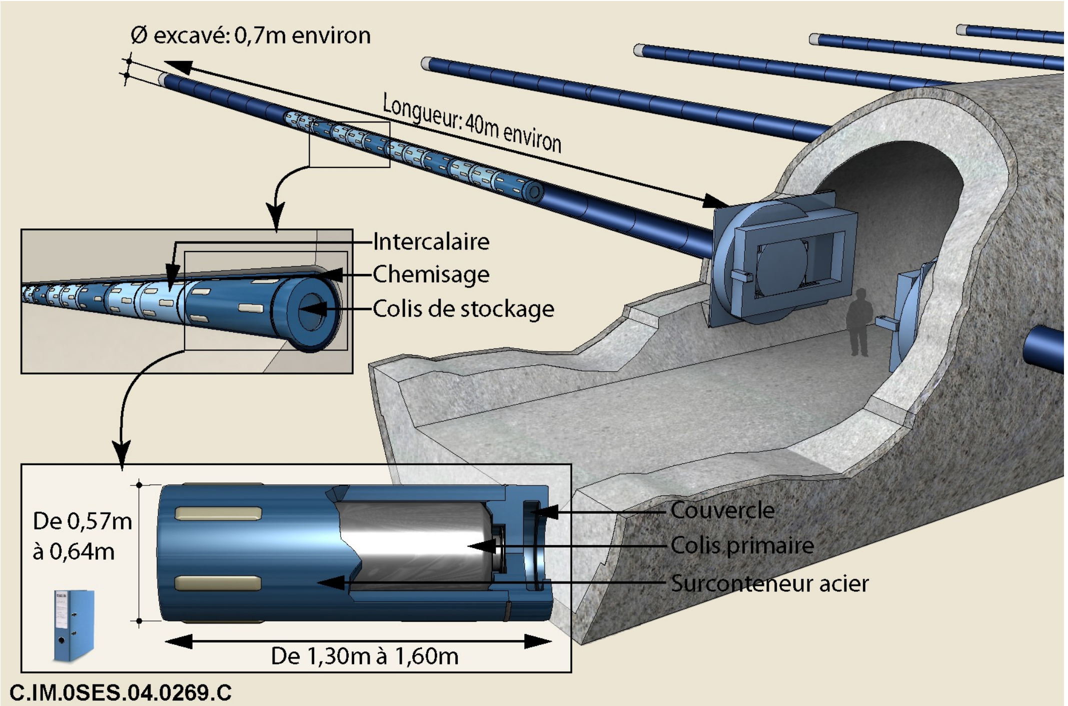
- Underground waste storage concepts
- Main phenomena and modelisation
- Coupling
- Numerical difficulties
- Spatial discretisation for flows and stresses
- Simulation of the excavation of a gallery

Underground waste storage concepts(1/3)

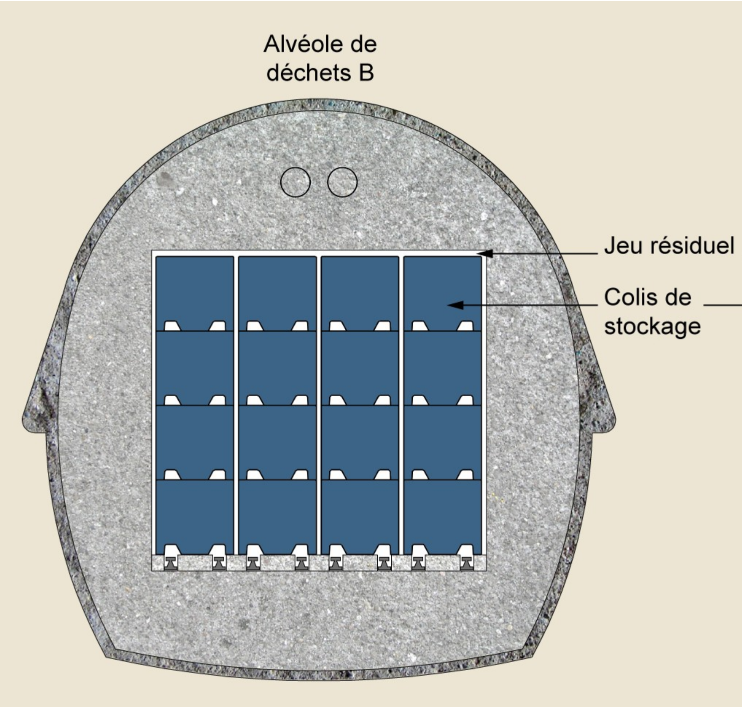


Underground waste storage concepts (2/3)

➢C waste Cell



➢B waste cell



Underground waste storage concepts (3/3)

- Complex geometry
- Heterogeneous materials
  - ✓ Rock at initial state or damaged rock
  - ✓ Concrete
  - ✓ Engineered barriers (sealing, cells closure)
  - ✓ Fill materials
  - ✓ Gaps
  - ✓ Steel : container liners
- Different physical behaviour
  - ✓ Mechanical, thermal , chemical, hydraulic

Main phenomena and modelisation (1/2)

➢ Flows

- ✓ 2 components (air or H_2 and water) in 2 phases (liquid and gaz)
- ✓ Transport equations :
  - Pressures Velocities

$$p_{gz}=p_{as}+p_{vp}$$
$$p_{lq}=p_w+p_{ad}$$

$$\frac{M_{gz}}{\rho_{gz}}=\left(1-C_{vp}\right)\frac{M_{as}}{\rho_{as}}+C_{vp}\frac{M_{vp}}{\rho_{vp}} \qquad \left(C_{vp}=\frac{p_{vp}}{p_{gz}}\right)$$

  - Darcy for each phase + diffusion + within each phase phase change (dissolution /vaporization)

$$\frac{M_{lq}}{\rho_{lq}}=\frac{K^{\mathrm{int}}.k^{rel}_{lq}(S_{lq})}{\mu_{lq}}\left(-\nabla p_{lq}+\rho_{lq}g\right)$$
$$\frac{M_{gz}}{\rho_{gz}}=\frac{K^{\mathrm{int}}.k^{rel}_{gz}(S_{lq})}{\mu_{gz}}\left(-\nabla p_{gz}+\rho_{gz}g\right)$$

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$$\frac{M_{vp}}{\rho_{vp}}-\frac{M_{as}}{\rho_{as}}=-F_{vp}\nabla C_{vp}$$
$$M_{ad}-M_w=-F_{ad}\nabla\rho_{ad}$$

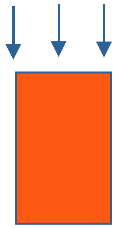
$$\frac{dp_{vp}}{\rho_{vp}}=\frac{dp_w}{\rho_w}+\left(h^m_{vp}-h^m_w\right)\frac{dT}{T}$$
$$\frac{\rho_{ad}}{M^{ol}_{ad}}=\frac{p_{ad}}{K_H}$$

  - Sorption curve

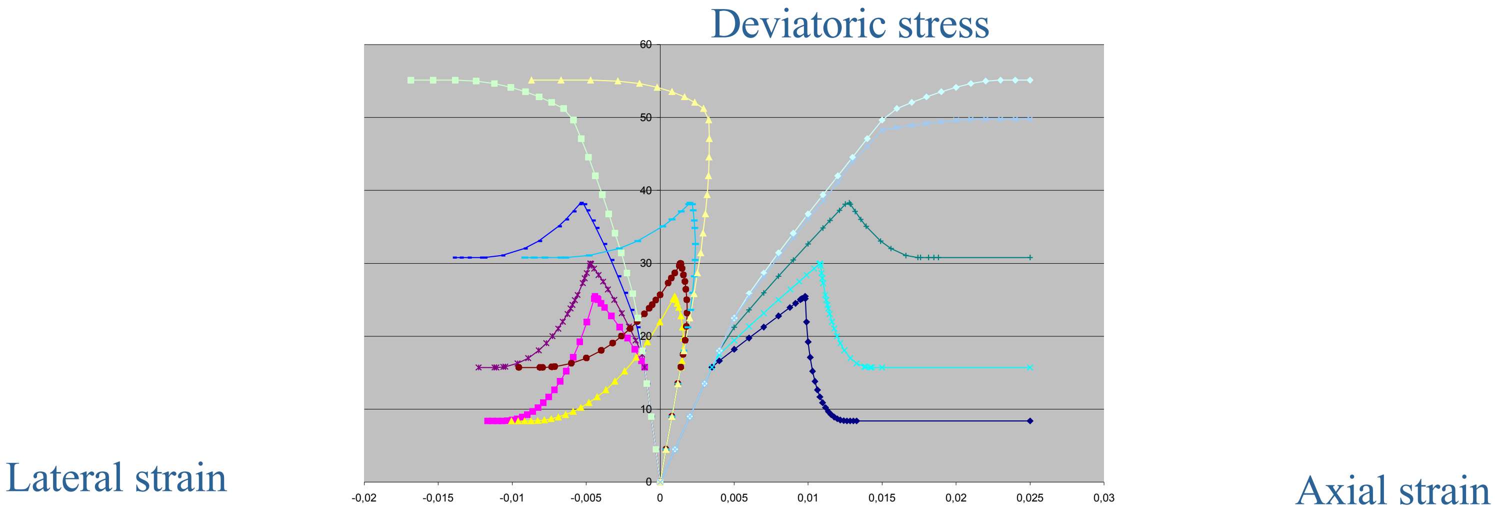
$$P_c=f\left(S_{lq}\right)=P_{gz}-P_{lq}$$

Main phenomena and modelisation (2/2)

➢Mechanical behaviour



- ✓Plastic and brittle behaviour or the rock
- ✓Dilatance effect at rupture stage



- ✓Swelling of Engineered materials .

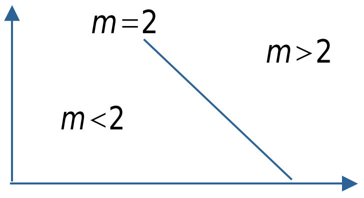
Numerical difficulties (1/3)

➤ For flows

- ✓ Non linear terms induce hyperbolic behaviour
  - Kind of equation :

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u^m}{\partial x^2} = 0$$

  - Stiff fronts can appear



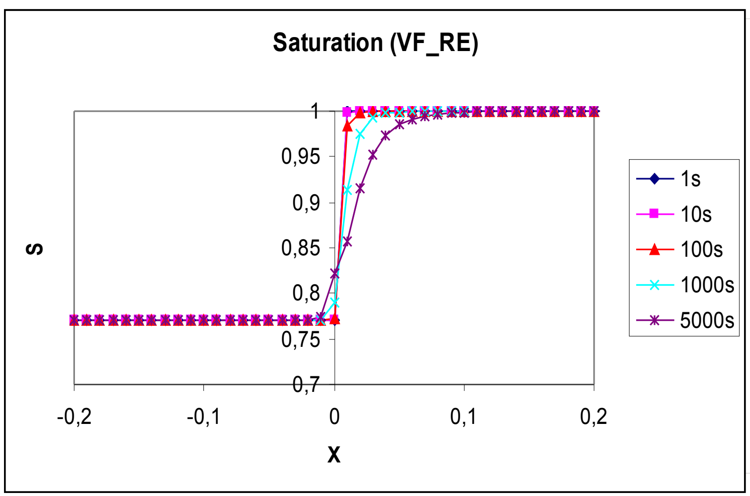
  - Big capillary effect -> No « mean » pressure

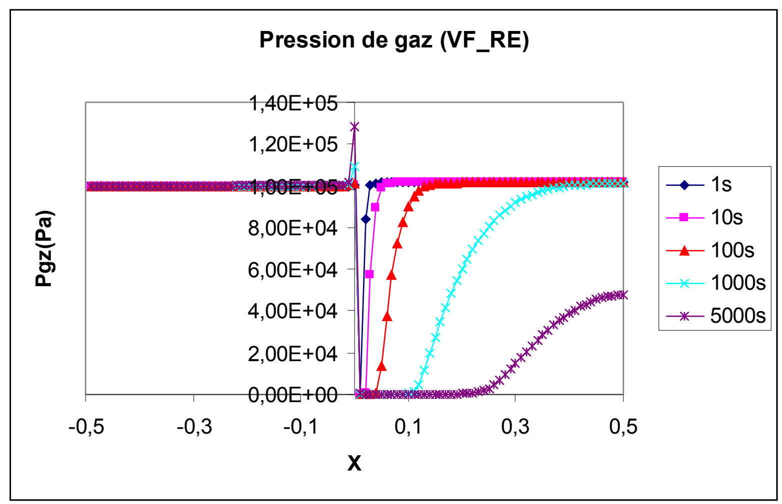
Numerical difficulties (2/3)

- Example of a desaturation problem
  - ✓ Initial state :

Sat=0,7 Porosity=0,3	Sat=1 Porosity=0,05

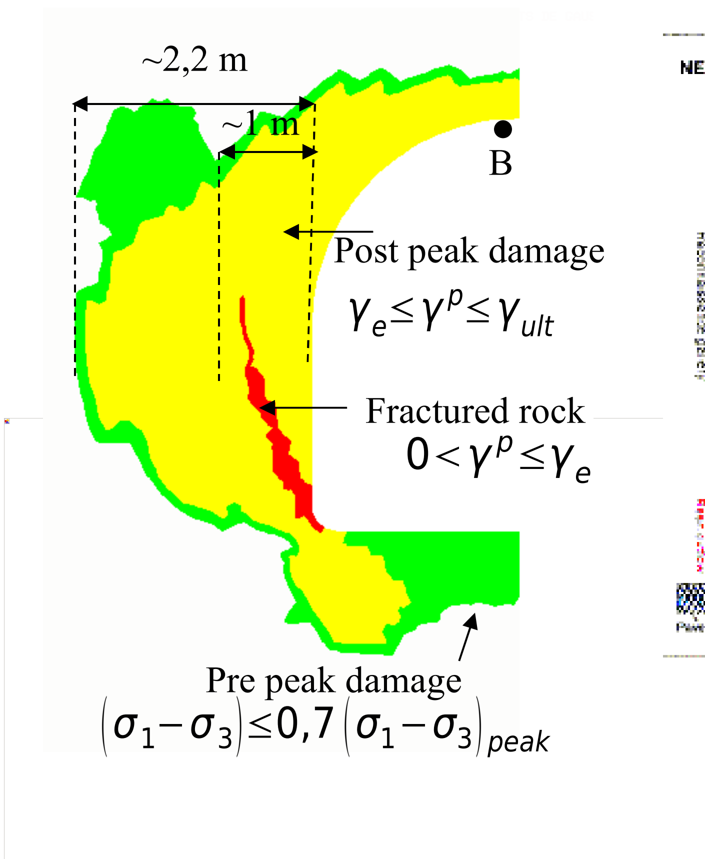
Near desaturation transition zone gas pressure tends to zero

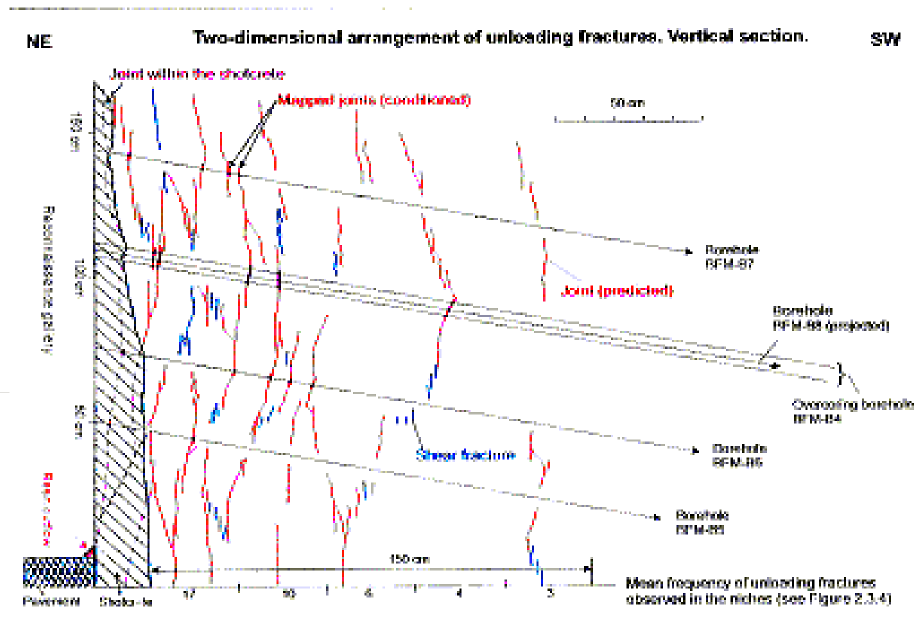




Numerical difficulties (3/3)

➢ Instabilities due to brittle behaviour





Incidence of flow on mechanical behaviour

- Standard notion of pore pressure
- Equivalent pore pressure definition for partially saturated media
  - Taking into account of interfaces in thermodynamic formulation

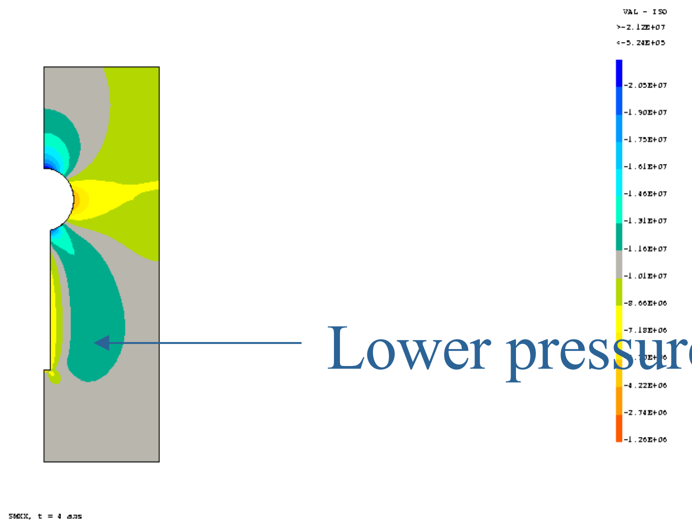
$$\pi = S_\alpha p^\alpha - \frac{2}{3}\int_{S_l}^{1} p_c(S)\,dS$$

Incidence material deformation on flow

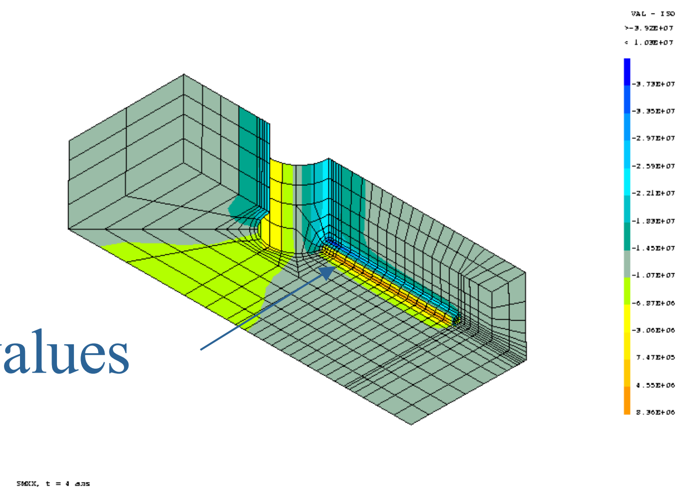
- Porosity change
- Straight increase of permeability with damage

Coupling (2/2)

- Thermal evolution -> Mechanic
  - ✓ Thermal expansion



Lower pressure values



- Thermal evolution -> flow
  - ✓ Changes in Viscosity, diffusivity coefficients
- Flow, mechanic -> thermal evolution
  - ✓ No effect

Numerical methods for flow

➢Choice of principal variables

✓ Capillary pressure/gas pressure

- Air mass balance ill conditioned for S=1

$$\phi \frac{\partial\left(\rho_a\left(1-S\right)\right)}{\partial t}-\nabla\left(\rho_a k_a\left(S\right)\nabla p_a\right)=0$$

✓ Saturation/water pressure

- Air mass balance becomes :

$$\phi\left(1-S\right)\frac{\partial p_e}{\partial t}+\phi\left(g\left(S\right)-p_e\right)\frac{\partial S}{\partial t}-\nabla\left[p_a h\left(S\right)\nabla S\right]-\nabla\left[p_a k_a\left(S\right)\nabla p_e\right]=0$$

$$P_c\left(S\right)\approx A\left(1-S\right)^{0.6} \qquad k_a\left(S\right)\approx\left(1-S\right)^3$$

$$\Rightarrow \quad g\left(S\right)\approx p_c \qquad h\left(S\right)\approx A\left(1-S\right)^{2,6} \quad \Rightarrow$$

At S=1

We have $\frac{\partial S}{\partial t}=0$

Numerical methods for flow and mechanic : spatial discretisation

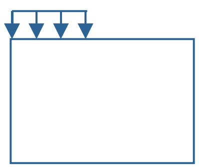
➢ Goals

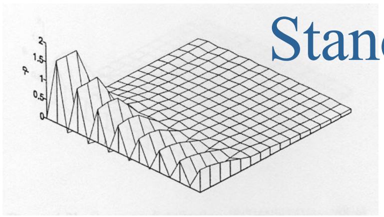
✓ A stable, monotone method for flow

✓ Easy to implement in a finite element code

➢ Method 1 :pressure and displacement EF P2/P1 lumped formulation

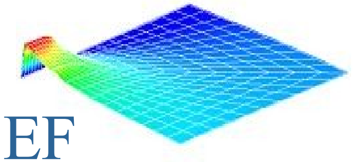
- OK for consolidation modelling



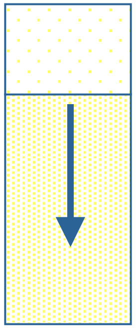


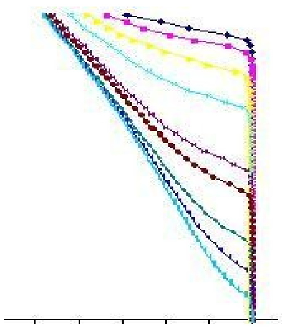
Standard EF

Lumped EF



- OK for desaturation test (Liakopoulos)





Saturation

Air Pressure

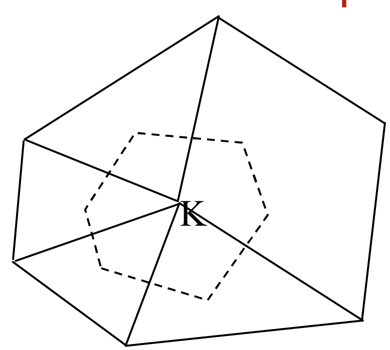
Numerical methods for flow and mechanic : spatial discretisation

➢ Limitations of previous formulation

- ✓ Poor quadrature rule induces lack of accuracy in stresses evaluations
- ✓ Instabilities appear when simulating gas injection problem

➢ CFV/DM (control finite volume/dual mesh)

- **Goal**
  - ✓ formulation VF compatible with architecture of EF software
- **Principle**
  - To use primal mesh for EF formulation of mechanical equations
  - To construct a finite volume cell surrounding each node of the primal mesh
  - To write mass balance on that polygonal cell



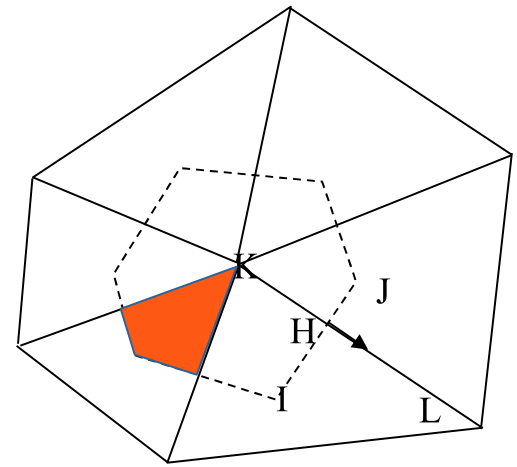
CFM/DM (control finite volume/dual mesh)

- **Model equation**

$$\frac{\partial m(u)}{\partial t} + \nabla . F(u) \;\; ; \;\; F = k(u) \nabla u$$

- **Mass balance:**

$$A_K \frac{m_K^{n+1} - m_K^{n+1}}{\Delta t} + \sum_L T_{KL} k\left(u_{KL}^{n+1}\right)\left(u_L^{n+1} - u_K^{n+1}\right) = 0$$



- **Up winding**

$$\text{si } u_L^{n+1} \text{¿} u_K^{n+1} u_{KL}^{n+1} = u_L^{n+1}$$

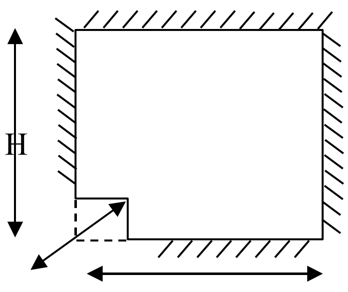
- **Loop over elements of primal mesh**

$$\sum_{e \in T_K} A_K^e \frac{m_{K,e}^{n+1} - m_{K,p,e}^n}{\Delta t} + \sum_e \sum_{L \in e \neq K} T_{KL}^e k\left(u_{KL}^{n+1}\right)\left(u_L^{n+1} - u_K^{n+1}\right) = 0$$

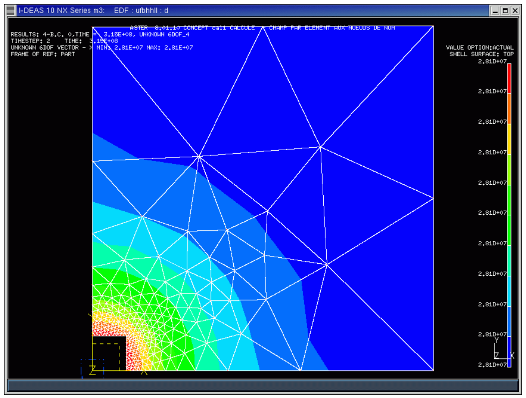
$$T_{KL}^e = \frac{d_{I,H}}{d_{K,L}} = -\int_e \nabla \lambda_K . \nabla \lambda_K$$

CFM/DM (control finite volume/dual mesh)

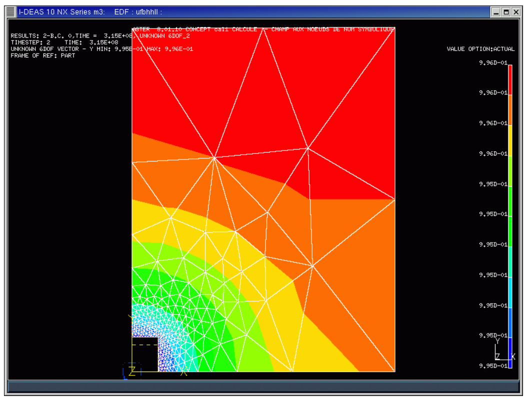
- **Theoretical predictions :**
  - ✓ stable, convergent and monotone for Delaunay meshes
- **Example**



Gas injection



Pg 10 years H/L=1

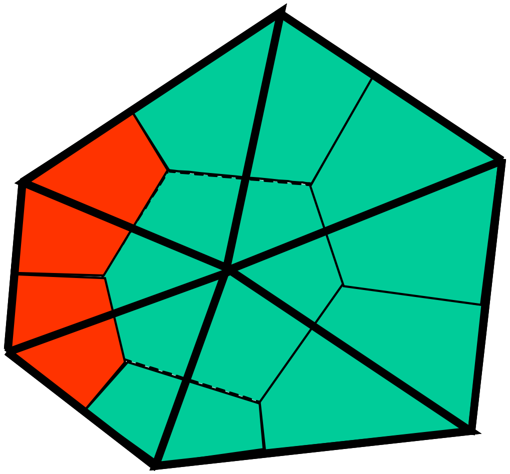


S 10 years H/L=4/3

- **For stretching H/L > 4/3 no convergence is achieved**

CFM/DM (control finite volume/dual mesh)

- **Remark about interfaces**
  - ✓ Differences between material properties can induce discontinuities.
  - ✓ It is better to ensure constant properties over the control cell



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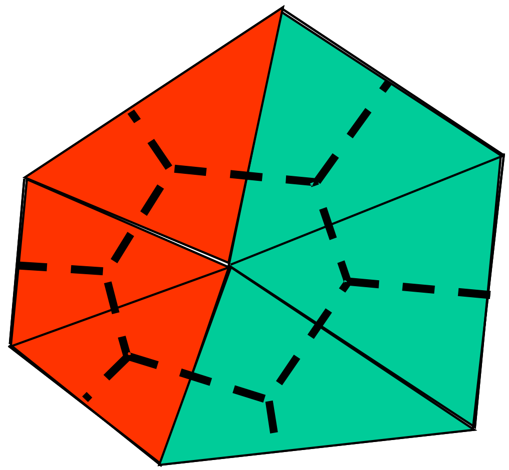


No OK

Numerical modelisation of brittle rocks

- Equilibrium equation

$$Div\,\sigma + f = 0$$

Mechanical law of behaviour

$$\sigma = F(\boldsymbol{\varepsilon}, \boldsymbol{\alpha})$$

$\dfrac{\partial \sigma}{\partial \varepsilon}$ is not positive

- Resulting weak formulation

$$\int_{OMEGA} \boldsymbol{\sigma} : \boldsymbol{\varepsilon}(u^{¿}) + \int_{OMEGA} f . u^{¿} = 0 \; \forall u^{¿}$$

- Lak of ellipticity
  - Possible bifurcations
  - Instabilities

Regularisation method

➢ Main idea :

✓ Introduce some term bounding gradients of strain

➢ Second gradient

$$\int_{OMEGA} \boldsymbol{\sigma}:\boldsymbol{\varepsilon}\left(u^{¿}\right)+\int_{OMEGA} D.\nabla \varepsilon : \nabla \varepsilon^{¿}+\int_{OMEGA} f.u^{¿}=0\ \forall u^{¿}$$

➢ Simplified second gradient : micro gradient dilation model

✓ For a dilatant material we can regularise only the volumic strain

$$\int_{OMEGA} \boldsymbol{\sigma}:\boldsymbol{\varepsilon}\left(u^{¿}\right)+\int_{OMEGA} D.\nabla Tr\left(\varepsilon\right).\nabla Tr\left(\varepsilon^{¿}\right)+\int_{OMEGA} f.u^{¿}=0\ \forall u^{¿}$$

$$\int_{OMEGA} D.\Delta u.\Delta u^{¿}$$

Mixed formulation of micro gradient dilation model

➢Weak formulation

$$\int_{OMEGA} \boldsymbol{\sigma}:\boldsymbol{\varepsilon}\left(u^{¿}\right)+\int_{OMEGA} D.\nabla\theta.\nabla\theta^{¿}-\int_{OMEGA}\lambda\left(\nabla.u^{¿}-\theta^{¿}\right)+\int_{OMEGA}\lambda^{¿}\left(\nabla.u-\theta\right)+\int_{OMEGA} f.u^{¿}=0\,\forall\left(u^{¿},\lambda^{¿}\right)$$

Approximation spaces	u	θ	λ
Quadrangles	Q2	Q1	P0
Triangles	P2	P1	P0

➢Possible free energy displacements modes w

$$\int_{OMEGA}\sigma\left(w\right):\boldsymbol{\varepsilon}\left(w\right)=0 \qquad \int_{e}\nabla.w=0\ \ \forall e$$

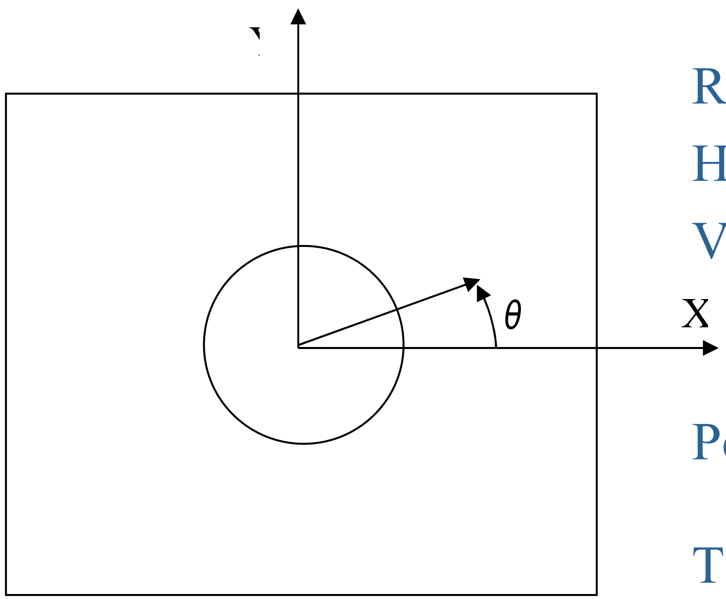
➢Two ways

- ✓ Enhancing degree of discretisation for λ
- ✓ Using penalisation

$$\int_{OMEGA} \boldsymbol{\sigma}:\boldsymbol{\varepsilon}\left(u^{¿}\right)+\int_{OMEGA} D.\nabla\theta.\nabla\theta^{¿}-\int_{OMEGA}\lambda\left(\nabla.u^{¿}-\theta^{¿}\right)+\int_{OMEGA}\lambda^{¿}\left(\nabla.u-\theta\right)+r\int_{OMEGA}\left(\nabla.u^{¿}-\theta^{¿}\right).\left(\nabla.u-\theta\right)+\int_{OMEGA} f.u^{¿}=0$$
$$\forall\left(u^{¿},\lambda^{¿}\right)$$

Benchmark Momas : Simulation of an Excavation under Brittle Hydro-mechanical behaviour

- Cylindrical cavity
- Excavation simulation
- Initial conditions : anisotropic state of stress (11.0MPa, -15.4MP) ; water pressure (4.7 Mpa)



Radius of cavity : 3 meters

Horizontal length for calculation domain : 60 meters

Vertical length for calculation domain : 60 meters

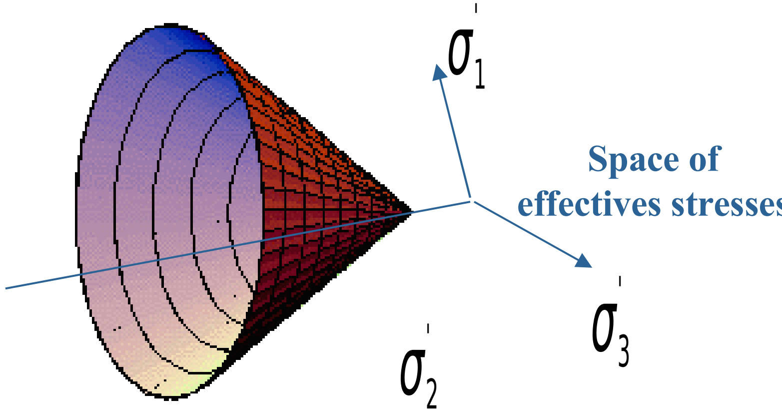
Permeability : $10^{-12} m.s^{-1}$

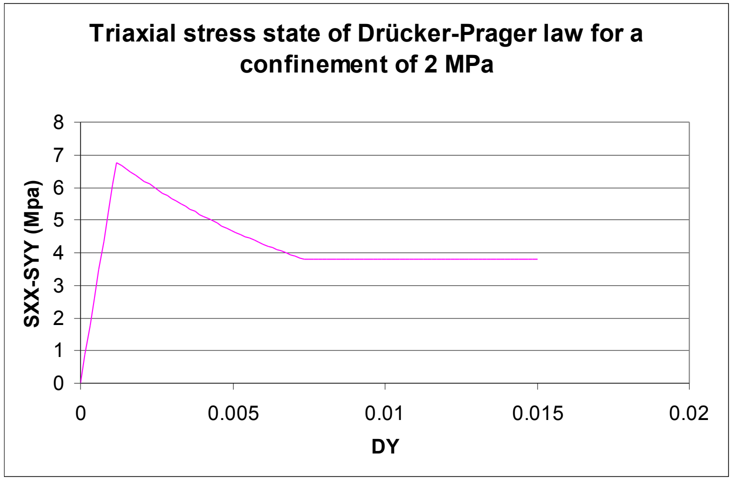
Time of simulation for excavation : 17 days

Time of simulation for consolidation : 10 years

Benchmark Momas : Simulation of an Excavation under Brittle Hydro-mechanical behaviour

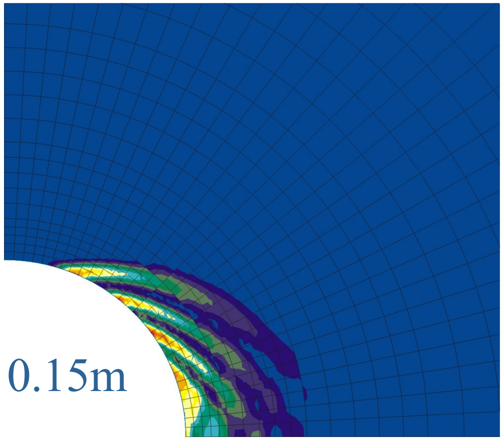
- Mechanical elasto-plastic formulation
- Drucker-Prager Yield Criterion
- Plastic rule : associated formulation
- Softening :
  decrease of cohesion / shear plastic deformation



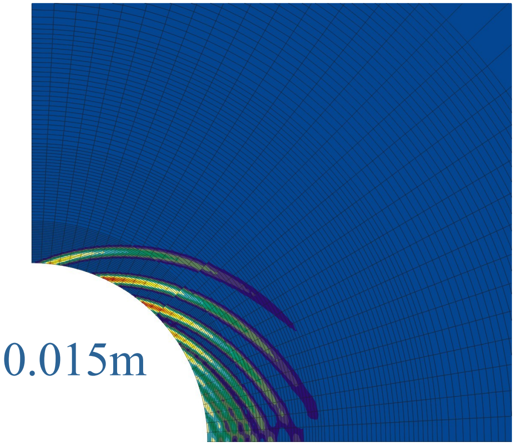


Benchmark Momas : Localisation Phenomenon

➢Coupled modelling – After 10 years – Shear bandings



Coupled modelling
Coarse mesh



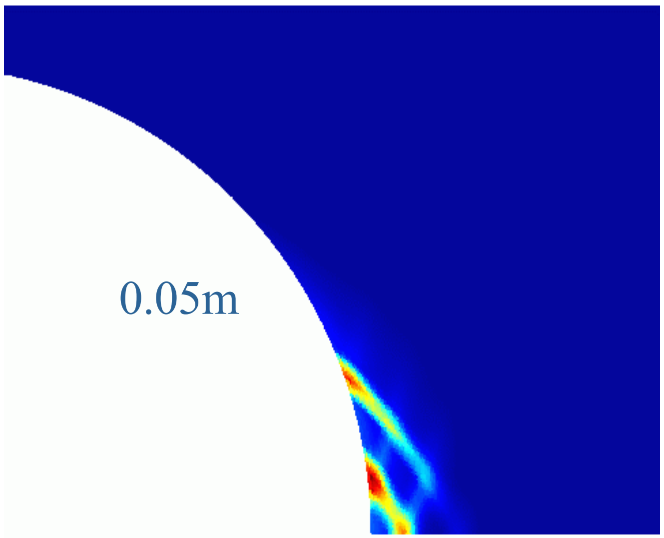
Coupled modelling
Refined mesh

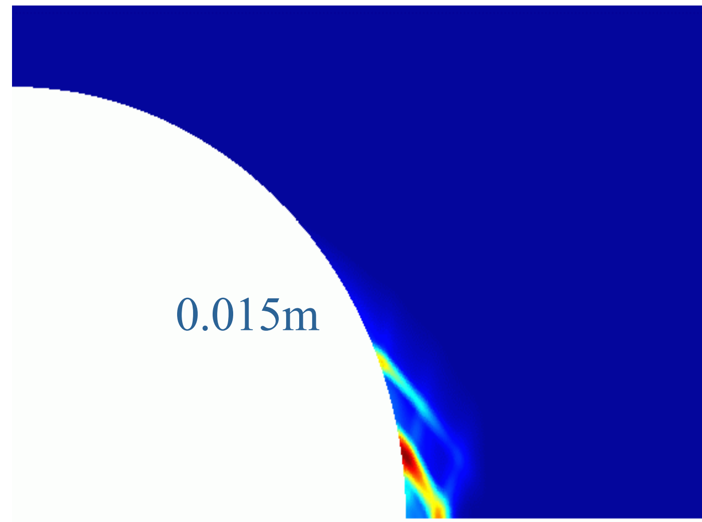
- ✓ Shear bands are related to softening model
- ✓ Localisation bands are influenced by the mesh
- ✓ Hydro-mechanical coupling provides no regularisation

Benchmark Momas :
simulation with Micro Gradient Dilation Model

Spatial discretisation with triangle elements

Visualisation of Shear bandings on Gauss Points during the excavation phasis





Band width is always greater than 2 elements

-> We can hope this result is independent of the spatial discretisation

Displacement / deconfinement

-> Regularisation gives results for higher deconfinement ratio

-> With a coarser mesh, simulation stops earlier

Conclusions

- Simulation of nuclear waste storage requires to solve non linear coupled equations in heterogeneous media
- Some simulations need to solve jointly difficulties relative to two phase flow and brittle mechanical behaviours
- Control finite volume/dual mesh is a reliable method for coupling darcean flows and mechanic
- Regularised brittle models seem to be useful in coupled (saturated) simulations
- Simplified second gradient (Micro Gradient Dilation) model gives reasonable results