Finite volume-Edge Finite Element scheme for a two-component two-compressible flow in nonhomogenous porous media

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Dubrovnik 29 september–03 october 2014

Dubrovnik, 29/09/2014

Outline

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4. FV-FE for two–compressible two–component flow
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    - Energy estimates
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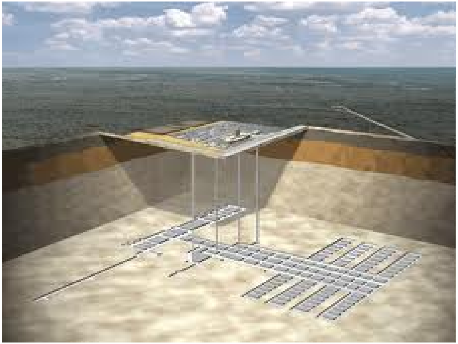
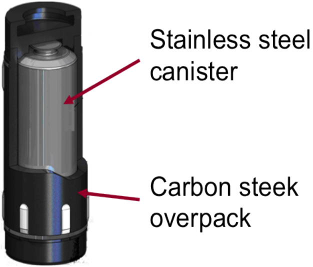
Hydrogen release in Nuclear waste management

In nuclear waste management, an important quantity of hydrogen can be produced by corrosion of the steel engineered barriers (carbon steel overpack and stainless steel envelope) of radioactive waste packages. Host rock safety function may be threatened by over pressurisation leading to opening fractures of the domain, inducing groundwater flow and transport of radionuclides.





Simulation of gas migration in deep geological repositories.
Compressible two-phase partially miscible flow

CO2 in liquid or gas form

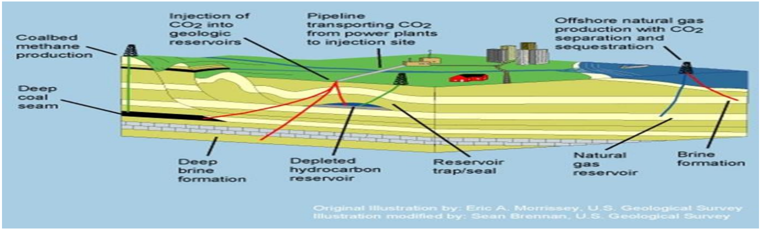
CO2 capture and storage.

The aim is to prevent the release of large quantities of CO2 into the atmosphere. The process consists of capturing waste CO2 and transporting it to a storage site.

Various forms have been conceived for storage CO2 into deep geological formations :

- CO2 is sometimes injected into declining oil fields to increase oil recovery.

This option is attractive because the geology of hydrocarbon reservoirs is generally well understood and storage costs may be partly offset by the sale of additional oil that is recovered.



Model 1 : Gas ≈ 90% CO2 $\Longrightarrow$ Oil–Gas model. two compressible flow

Model 2 : Dissolution of CO2 in water. Two compressible and partially miscible flow

CO2 in liquid or gas form

After the CO2 injection, several different trapping mechanisms lead to an entrapment of the CO2.

- Shortly after the injection, structural trapping through caprocks is the most important factor.
- Later solubility trapping, where CO2 is dissolved into water, and residual trapping get more important.
- After several thousand years, there could also occur mineral trapping caused by geochemical reactions

To simulate the process of dissolution of CO2, a multiphase flow equation with equilibrium phase exchange is used.

The CO2 storage can be modeled with two components (CO2 and water) in two phases (liquid and gas).

R. Neumann and P. Bastian and O. Ippisch, *Modeling and simulation of two-phase two-component flow with disappearing nonwetting phase*, Comput Geosci.,2013, 17, 139-149.

Two-phase two-component flow

We consider a porous medium saturated with a fluid composed of :

- two phases : liquid ($\alpha = l$) and gas ($\alpha = g$)
- two components in each phase : H_2 ($\beta = h$) and water ($\beta = w$)

The component H_2 is present in the two phases :

- In liquid form : dissolved H_2
- In gas form : H_2 in the gas phase

The component water exists only in liquid form (no vapor water).

Mathematical model

Mass conservation of water :

$$\Phi\partial_t\left(\rho_l^w s_l\right) + \mathrm{div}\left(\rho_l^w \mathbf{V}_l\right) = f_w \qquad (1)$$

Mass conservation of H_2 :

$$\Phi\partial_t\left(\rho_l^h(p_g)s_l + \rho_g^h(p_g)s_g\right) + \mathrm{div}\left(\rho_l^h(p_g)\mathbf{V}_l + \rho_g^h(p_g)\mathbf{V}_g\right) - \mathrm{div}\left(\phi\rho_l D_l^h(s_l)\nabla X_l^h\right) = f_g \qquad (2)$$

Φ = porosity
s_α = saturation of the α phase
p_α = pressure of the α phase
$\mathbf{V}_\alpha$ = velocity of the α phase
ρ_l^h : density of disolved hydrogen
ρ_g^h : density of H_2 in the gas phase

$X_l^h = \frac{\rho_l^h}{\rho_l}$: mass fraction of H_2 in the liquid
$D_l^h(s_l)$ diffusivity coefficient of the dissolved hydrogen
f_α= source term

Mathematical model

Mass conservation of water :

$$\Phi\partial_t \left(\rho_l^w s_l\right) + \mathrm{div}\left(\rho_l^w \mathbf{V}_l\right) = f_w \tag{1}$$

Mass conservation of H_2 :

$$\Phi\partial_t \left(\rho_l^h(p_g)s_l + \rho_g^h(p_g)s_g\right) + \mathrm{div}\left(\rho_l^h(p_g)\mathbf{V}_l + \rho_g^h(p_g)\mathbf{V}_g\right) - \mathrm{div}\left(\phi\rho_l D_l^h(s_l)\nabla X_l^h\right) = f_g \tag{2}$$

- Saturations :

$$s_l + s_g = 1 \tag{3}$$

- Capillary pressure :

$$p_c(s_l) = p_g - p_l \tag{4}$$

- Darcy law :

$$\mathbf{V}_\alpha = -\mathbf{\Lambda}(x)\frac{k_{r_\alpha}(s_\alpha)}{\mu_\alpha}\left(\nabla p_\alpha - \rho_\alpha(p_\alpha)\mathbf{g}\right),$$

Mathematical model : the densities

Ideal gas

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

Henri law

$$\rho_l^h = M^h H^h p_g$$

M^h: molar mass of hydrogen, M^h the henry constant for hydrogen.

$$\rho_g^h = \mathcal{C}_1 \rho_l^h \text{ where } \mathcal{C}_1 = \frac{1}{H_h RT} = 52,51.$$

Denote $m(s_l) = s_l + \mathcal{C}_1 s_g > 0$. The hydrogen equation is equivalent to

$$\partial_t \left(\Phi m(s_l) \rho_l^h(p_g) \right) + \operatorname{div} \left(\rho_l^h(p_g) \mathbf{V}_l + \mathcal{C}_1 \rho_l^h(p_g) \mathbf{V}_g \right) - \operatorname{div} \left(\mathcal{C}_2 X_l^w D_l^h(s_l) \nabla p_g \right) = f_g \quad (5)$$

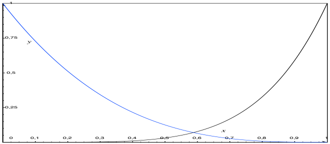
Primary variables : p_l, p_g.

Mathematical model

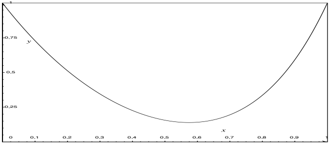
MIAN ASSUMPTIONS

- Degeneracy: The mobility of each phase vanishes in the region where the phase is missing

$$M_\alpha(s_\alpha = 0) = 0.$$



$M_l(s_l)$ mobility of liquid phase
$M_g(s_l)$ mobility of gas phase



Total mobility: $M = M_l + M_g \geq m_0$

- The density ρ_l^h is increasing and bounded :

$$0 < \rho_m \leq \rho_l^h(p_g) \leq \rho_M.$$

- The tensor of permeability is anisotropic and

$$\langle \Lambda(x)\xi, \xi \rangle \geq c_\Lambda |\xi|^2, \forall \xi \in \mathbb{R}^d.$$

- The diffusivity coefficient of the dissolved hydrogen D_l^h is positive.

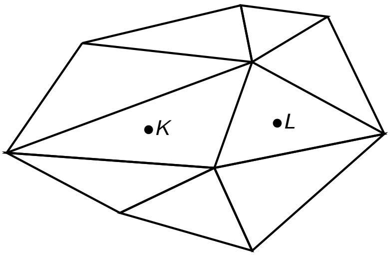
Motivation

Is there a convergent scheme (FV, FE, dG,...) for the partially miscible two–compressible two–component?

- B. Saad, M. Saad, Numerical analysis of a non equilibrium two-component two-compressible flow in porous media, DCDS-S, Volume **7**, Number **2**, April 2014, **pp. 317–346.**
- B. Saad, M. Saad. Study of full implicit petroleum engineering finite volume scheme for compressible two phase flow in porous media, SIAM J. Numer. Anal., 51(1), **pp. 716-741**, 2013.
- R. Eymard and V. Schleper, Study of a numerical scheme for miscible two-phase flow in porous media, hal-00741425, version 3, 2013.

Here, we present a combined FV–FE method of the degenerate problem, for anisotropic diffusion tensors and for general triangular meshes

Combined FV–Nonconforming FE: primal mesh



Primal mesh. Triangles $K, L \in \mathcal{T}_h$

Primal mesh. we perform a triangulation $\mathcal{T}_h$ of the domain Ω, such that $\overline{\Omega} = \cup_{K \in \mathcal{T}_h} K$.
We define

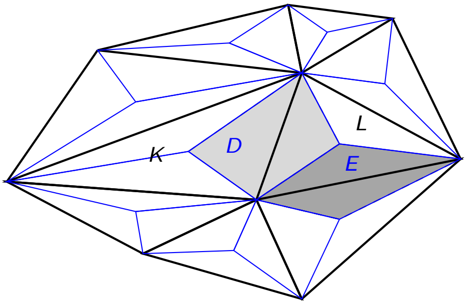
$$h := size(\mathcal{T}_h) = \max_{K \in \mathcal{T}_h} diam(K),$$

There exists a constant $\theta_{\mathcal{T}} > 0$

$$\max_{K \in \mathcal{T}_h} \frac{diam(K)}{\rho_K} \leq \theta_{\mathcal{T}}, \forall h > 0\,, (6)$$

where ρ_K is the diameter of the largest ball inscribed in K.

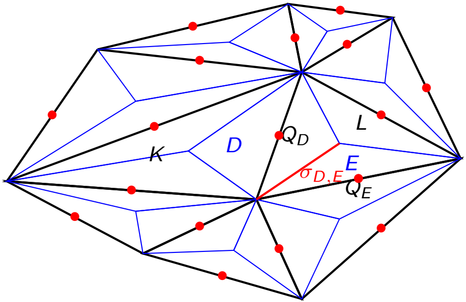
Combined FV–nonconforming FE: Dual mesh



Dual mesh $D, D \in D_h$, dual volumes associated with edges

Dual mesh.
We define a dual partition $\mathcal{D}_h$ s.t. $\bar{\Omega} = \cup_{D\in\mathcal{D}_h}\bar{D}$. There is one dual element D associated with each side $\sigma_D = \sigma_{K,L} \in \mathcal{E}_h$.
We construct it by connecting the barycenters of every $K \in \mathcal{T}_h$ that contains σ_D through the vertices of σ_D.

Combined FV–Nonconforming FE: Dual Mesh



•The unknown are on edges

We use the following notations:

- $|D| = meas(D)$ and $|\sigma| = meas(\sigma)$.
- Q_D the barycenter of the side σ_D.
- $\mathcal{N}(D)$ the set of neighbors of the volume D.
- $d_{D,E} := |Q_E - Q_D|$
- $\sigma_{D,E}$: interface between D and E
- $\eta_{D,E}$: the unit normal vector to $\sigma_{D,E}$ outward to D.
- $\mathcal{D}_h^{int}$ and $\mathcal{D}_h^{ext}$ are respectively the set of all interior and boundary dual volumes.

Combined FV–Nonconforming FE: Diffusion-Transport

We define the nonconforming finite-dimensional spaces:

$$X_h := \{\varphi_h \in L^2(\Omega); \varphi_h|_K \text{ is linear } \forall K \in \mathcal{T}_h, \varphi_h \text{ is continuous at } Q_D,\ D \in \mathcal{D}_h^{int}\},$$

$$X_h^0 := \{\varphi_h \in X_h; \varphi_h(Q_D) = 0,\ \forall D \in \mathcal{D}_h^{ext}\}.$$

$(\varphi_D)_{D\in\mathcal{D}_h}$ the basis of X_h s.t. $\varphi_D(Q_E) = \delta_{DE},\ E \in \mathcal{D}_h$.

Diffusion-transport equation

$$\underbrace{-\text{div}(\mathbf{\Lambda}\nabla u)}_{\text{Finite Element}} + \underbrace{\text{div}(\mathbf{c}u)}_{\text{Finite Volume}} = f$$

Combined scheme.

$$-\sum_{E\in\mathcal{N}(D)} \mathbf{\Lambda}_{D,E}(U_E - U_D) + \sum_{E\in\mathcal{N}(D)} G(U_D, U_E; \delta C_{D,E}) = 0$$

where the stiffness matrix is

$$\Lambda_{D,E} = -\sum_{K\in\mathcal{T}_h} \int_K \mathbf{\Lambda}(x)\nabla\varphi_E \cdot \nabla\varphi_D\, dx \quad \text{(nonconforming FE)}$$

and the numerical flux G is defined by

$$G(U_D, U_E; \delta C_{D,E}) = U_D(\delta C_{D,E})^+ + U_E(\delta C_{D,E})^- \quad \text{(upwind finite volume)}$$

where $\delta C_{D,E} = \int_{\sigma_{D,E}} \mathbf{c} \cdot \mathbf{n}_{D,E}\, d\sigma$.

Combined FV–Nonconforming FE: Diffusion-transport

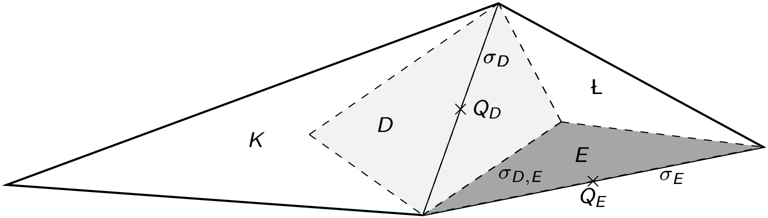
$$-\sum_{E\in\mathcal{N}(D)} \boldsymbol{\Lambda}_{D,E}(U_E - U_D) + \sum_{E\in\mathcal{N}(D)} G(U_D, U_E; \delta C_{D,E}) = 0$$

P. Angot, V. Dolejsi, M. Feistauer and J. Felcman,
Analysis of a combined barycentric finite volume-nonconforming finite element method for nonlinear convection-diffusion problems. Appl.Math.,43(4), p. 263-310, 1998.

R. Eymard, D. Hilhorst and M. Vohralik,
A combined finite volume-nonconforming/mixed hybrid finite element scheme for degenerate parabolic problems. Numer.Math., 105 : p. 73-131, 2006.

FV-FE for two–compressible two–component flow

Nonconforming FE/Implicit upwind scheme



We integrate the mass conversation law over the diamond D

$$\partial_t \left(\Phi m(s_l) \rho_l^h(p_g) \right) + \mathrm{div} \left(\rho_l^h(p_g) \mathbf{V}_l + \mathcal{C}_1 \rho_l^h(p_g) \mathbf{V}_g \right) - \mathrm{div} \left(\mathcal{C}_2 X_l^w D_l^h(s_l) \nabla p_g \right) = f_g$$

and we use :

- Fully implicit Euler scheme
- The mobility of each phase is decentred according to discrete gradient of the pressure on the interface $\sigma_{D,E}$
- Nonconforming FE for permeability tensor

The fully implicit combined finite combined FV–nonconforming FE scheme

$$|D|\,\phi_D \frac{s_{l,D}^n - s_{l,D}^{n-1}}{\delta t} - \sum_{E\in\mathcal{N}(D)} M_l(s_{l,D,E}^n)\,\Lambda_{D,E}\,\delta_{D,E}^n(p_l) = \frac{f_{w,D}^n}{\rho_l^w} \quad (water)$$

$$|D|\,\phi_D \frac{\rho_l^h(p_{g,D}^n)m(s_{l,D}^n) - \rho_l^h(p_{g,D}^{n-1})m(s_{l,D}^{n-1})}{\delta t}$$
$$- \sum_{E\in\mathcal{N}(D)} (\rho_l^h)_{D,E}^n\, M_l(s_{l,D,E}^n)\,\Lambda_{D,E}\,\delta_{D,E}^n(p_l) - \mathcal{C}_1 \sum_{E\in\mathcal{N}(D)} (\rho_l^h)_{D,E}^n\, M_g(s_{l,D,E}^n)\,\Lambda_{D,E}\,\delta_{D,E}^n(p_g)$$
$$- \mathcal{C}_2 \sum_{E\in\mathcal{N}(D)} \phi_D (X_l^w)_{D,E}^n\,(D_l^h)_{D,E}\,\delta_{D,E}^n(p_g) = f_{g,D}^n \quad (gas)$$

This system is completed by the capillary pressure

$$p_c(s_{l,D}^n) = p_{g,D}^n - p_{l,D}^n. \qquad (7)$$

The approximation of each term is important to handle with the energy estimates.

$$|D|\,\phi_D \frac{\rho_l^h(p_{g,D}^n)m(s_{l,D}^n) - \rho_l^h(p_{g,D}^{n-1})m(s_{l,D}^{n-1})}{\delta t}$$
$$- \sum_{E\in\mathcal{N}(D)} (\rho_l^h)_{D,E}^n \; M_l(s_{l,D,E}^n) \; \Lambda_{D,E} \; \delta_{D,E}^n(p_l) - \mathcal{C}_1 \sum_{E\in\mathcal{N}(D)} (\rho_l^h)_{D,E}^n \; M_g(s_{l,D,E}^n) \; \Lambda_{D,E} \; \delta_{D,E}^n(p_g)$$
$$- \mathcal{C}_2 \sum_{E\in\mathcal{N}(D)} \phi_D (X_l^w)_{D,E}^n \; (D_l^h)_{D,E} \; \delta_{D,E}^n(p_g) = f_{g,D}^n$$

- Discrete Gradient of pressure

$$\delta_{D,E}^n(p_\alpha) = p_{\alpha,E}^n - p_{\alpha,D}^n$$

$$|D|\,\phi_D \frac{\rho_l^h(p_{g,D}^n)m(s_{l,D}^n) - \rho_l^h(p_{g,D}^{n-1})m(s_{l,D}^{n-1})}{\delta t}$$

$$- \sum_{E\in\mathcal{N}(D)} (\rho_l^h)_{D,E}^n \, M_l(s_{l,D,E}^n) \, \Lambda_{D,E} \, \delta_{D,E}^n(p_l) - \mathcal{C}_1 \sum_{E\in\mathcal{N}(D)} (\rho_l^h)_{D,E}^n \, M_g(s_{l,D,E}^n) \, \Lambda_{D,E} \, \delta_{D,E}^n(p_g)$$

$$- \mathcal{C}_2 \sum_{E\in\mathcal{N}(D)} \phi_D (X_l^w)_{D,E}^n \, (D_l^h)_{D,E} \, \delta_{D,E}^n(p_g) = f_{g,D}^n$$

- Permeability on interfaces by FE

$$\Lambda_{D,E} = - \sum_{K\in\mathcal{T}_h} \int_K \mathbf{\Lambda}(x) \nabla\varphi_E \cdot \nabla\varphi_D \, dx$$

and

$$(D_l^h)_{D,E} = - \sum_{K\in\mathcal{T}_h} \int_K D_l^h \nabla\varphi_E \cdot \nabla\varphi_D \, dx$$

$$|D|\,\phi_D \frac{\rho_l^h(p_{g,D}^n)m(s_{l,D}^n) - \rho_l^h(p_{g,D}^{n-1})m(s_{l,D}^{n-1})}{\delta t}$$
$$- \sum_{E\in\mathcal{N}(D)} (\rho_l^h)_{D,E}^n \; M_l(s_{l,D,E}^n)\; \Lambda_{D,E}\; \delta_{D,E}^n(p_l) - \mathcal{C}_1 \sum_{E\in\mathcal{N}(D)} (\rho_l^h)_{D,E}^n \; M_g(s_{l,D,E}^n)\; \Lambda_{D,E}\; \delta_{D,E}^n(p_g)$$
$$- \mathcal{C}_2 \sum_{E\in\mathcal{N}(D)} \phi_D (X_l^w)_{D,E}^n \; (D_l^h)_{D,E}\; \delta_{D,E}^n(p_g) = f_{g,D}^n$$

- Upwind technics for the mobilities
  $M_\alpha(s_{\alpha,D,E}^n)$ denotes the upwind discretization of $M_\alpha(s_\alpha)$ on the interface $\sigma_{D,E}$ as

$$M_\alpha(s_{\alpha,D,E}^n) = \begin{cases} M_\alpha(s_{\alpha,D}^n) \text{ if } \Lambda_{D,E}\left(p_{\alpha,E}^n - p_{\alpha,D}^n\right) \le 0, \\ M_\alpha(s_{\alpha,E}^n) \text{ otherwise} \end{cases}$$

$$|D|\,\phi_D \frac{\rho_l^h(p_{g,D}^n)m(s_{l,D}^n) - \rho_l^h(p_{g,D}^{n-1})m(s_{l,D}^{n-1})}{\delta t}$$

$$- \sum_{E\in\mathcal{N}(D)} (\rho_l^h)_{D,E}^n \; M_l(s_{l,D,E}^n)\; \Lambda_{D,E}\; \delta_{D,E}^n(p_l) - \mathcal{C}_1 \sum_{E\in\mathcal{N}(D)} (\rho_l^h)_{D,E}^n \; M_g(s_{l,D,E}^n)\; \Lambda_{D,E}\; \delta_{D,E}^n(p_g)$$

$$- \mathcal{C}_2 \sum_{E\in\mathcal{N}(D)} \phi_D (X_l^w)_{D,E}^n \; (D_l^h)_{D,E}\; \delta_{D,E}^n(p_g) = f_{g,D}^n$$

Mean value of densities on interfaces

The mean value of the density of each phase on the interfaces is not classical since it is given as

$$\frac{1}{(\rho_l^h)_{D,E}^n} = \begin{cases} \frac{1}{p_{g,E}^n - p_{g,D}^n} \displaystyle\int_{p_{g,D}^n}^{p_{g,E}^n} \frac{1}{\rho_l^h(\zeta)}\, d\zeta & \text{if } p_{g,D}^n \neq p_{g,E}^n, \\ \frac{1}{(\rho_l^h)_D^n} & \text{otherwise.} \end{cases}$$

Proposition (Maximum principle)

Let $(s^0_{\alpha,D})_{D\in\mathcal{D}_h} \in [0,1]$. *Then, the saturation* $s^n_{l,D} \geq 0$ *for all* $D \in \mathcal{D}_h,\ n \in \{1,\dots,N\}$.

Proof by induction on n. Suppose $s^{n-1}_{l,D} \geq 0$ for all $D \in D_h$. Let $s^n_{l,D} = \min\left\{s^n_{l,E}\right\}_{E\in\mathcal{D}_h}$ and we seek that $s^n_{l,D} \geq 0$

Multiply the scheme by $-(s^n_{l,D})^-$, we obtain

$$-|D|\,\phi_D \frac{s^n_{l,D} - s^{n-1}_{l,D}}{\delta t}(s^n_{l,D})^- - \sum_{E\in\mathcal{N}(D)} \underbrace{G_l(s^n_{l,D}, s^n_{l,E}; \delta^n_{D,E}(p_l))(s^n_{l,D})^-}_{\leq\, 0,\ \text{since } G_l \text{ is monotone}} = -\underbrace{f^n_{l,D}(s^n_{l,D})^-}_{\leq 0}.$$

Then, we deduce that

$$|(s^n_{l,D})^-|^2 + s^{n-1}_{l,D}(s^n_{l,D})^- \leq 0,$$

and $s^n_{l,D} \geq 0$ for all $D \in D_h$.

Energy estimates : continuous case

Let us recall how to obtain the energy estimates in the continuous case. For that, consider

$$g(p_g) := \int_0^{p_g} \frac{1}{\rho_l^h(z)} \mathrm{d}z \text{ and } \mathcal{H}(p_g) := \rho_l^h(p_g) g(p_g) - p_g \geq 0.$$

Define the function

$$\mathcal{E} = m(s_l)\mathcal{H}_g(p_g) - \mathcal{C}_1 \int_0^{s_l} p_c(z)\mathrm{d}z.$$

By multiplying the hydrogen equation by $g(p_g)$ and water equation by $\mathcal{C}_1 p_l - p_g$, after integration and summation of equations, we deduce the estimate

$$\int_\Omega \Phi \partial_t \mathcal{E} \mathrm{d}x + c_\Lambda \underbrace{\int_\Omega M_l |\nabla p_l|^2 \mathrm{d}x + \int_\Omega M_g |\nabla p_g|^2 \mathrm{d}x}_{\text{bounded}} + \int_\Omega \mathcal{C}_2 X_l^w D_l^h \nabla p_g \cdot \nabla g_g(p_g) \mathrm{d}x \leq C.$$

Estimates on the velocities

$$\int_0^T \int_\Omega \left(M_l(s_l)|\nabla p_l|^2 + M_g(s_g)|\nabla p_g|^2 \right) \leq C$$

we cannot control the gradient of pressure since the mobility of each phase vanishes in the region where the phase is missing $M_\alpha(s_\alpha = 0) = 0$. So, we use the feature of global pressure to obtain uniform estimates on the gradient of the global pressure and on a function of the capillary term $\mathcal{B}$.

F. Caro, B. Saad, M. Saad, *Study of degenerate parabolic system modeling the hydrogen displacement in a nuclear waste repository*, DCDS-S, Vol. **7**, No **2**, April 2014, pp. 191–205.

Energy estimates.

Continuous case.

The global pressure p can be written as

$$p = p_l + \tilde{p}(s_l) = p_g + \bar{p}(s_l),$$

with the deviation pressures $\bar{p}$ and $\tilde{p}$:

$$\tilde{p}(s_l) = -\int_0^{s_l} \frac{M_g(z)}{M(z)} p_c'(z)\mathrm{d}z \text{ and } \overline{p}(s_l) = \int_0^{s_l} \frac{M_l(z)}{M(z)} p_c'(z)\mathrm{d}z.$$

Total mobility : $M(s_l) = M_l(s_l) + M_g(s_l) \geq m_0 > 0$.
From the definition of the global pressure we have :

$$M_l(s_l)|\nabla p_l|^2 + M_g(s_l)|\nabla p_g|^2 = M(s_l)|\nabla p|^2 + \underbrace{\frac{M_l(s_l)M_g(s_l)}{M(s_l)}|\nabla p_c(s_l)|^2}_{|\nabla \mathcal{B}(s_l)|^2}.$$

The control of velocities ensures the control of the gradient of the global pressure.

Discrete case.

In the discrete case, this relationship is not obtained in a straightforward way. This equality is replaced by four discrete inequalities.

A priori estimates : discrete case

We show the discrete version of $\int_0^T \int_\Omega \Lambda(x) M_\alpha \nabla p_\alpha \cdot \nabla p_\alpha \, dtdx \leq C$.

Proposition (Discrete velocities)

$$\sum_{n=0}^{N-1} \delta t \sum_{D\in\mathcal{D}_h} \sum_{E\in\mathcal{N}(D)} \Lambda_{D,E} M_\alpha(s^n_{\alpha,D|E}) \left| p^n_{\alpha,E} - p^n_{\alpha,D} \right|^2 \leq C. \tag{8}$$

Proof. The proof is based on the choice of the test functions

$$g(p_{g,D}) = \int_0^{p_{g,D}} \frac{1}{\rho_l^h(z)} dz, \text{ and } (\mathcal{C}_1 p^n_{l,D} - p^n_{g,D})$$

Term in time.

$$E_1 = \sum_{n,D} |D| \, \phi_D \Big((s^n_{l,D} - s^{n-1}_{l,D}) \, (\mathcal{C}_1 p^n_{l,D} - p^n_{g,D}) + (\rho_l^h(p^n_{g,D}) m(s^n_{l,D}) - \rho_l^h(p^{n-1}_{g,D}) m(s^{n-1}_{l,D})) \, g(p^n_{g,D}) \Big)$$

$$E_1 \geq \sum_{D\in\mathcal{D}_h} \phi_D \, |D| \left(\mathcal{H}(p^N_{g,D}) m(s^N_{l,D}) - \mathcal{H}(p^0_{g,D}) m(s^0_{l,D}) \right)$$
$$- \mathcal{C}_1 \sum_{D\in\mathcal{D}_h} \phi_D \, |D| \, \mathcal{P}_c(s^N_{l,D}) + \mathcal{C}_1 \sum_{D\in\mathcal{D}_h} \phi_D \, |D| \, \mathcal{P}_c(s^0_{l,D}). \tag{9}$$

A priori estimates : discrete case

We show the discrete version of $\int_0^T \int_\Omega \Lambda(x) M_\alpha \nabla p_\alpha \cdot \nabla p_\alpha \, dtdx \leq C$.

Proposition (Discrete velocities)

$$\sum_{n=0}^{N-1} \delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} \Lambda_{D,E} M_\alpha(s^n_{\alpha,D|E}) \left| p^n_{\alpha,E} - p^n_{\alpha,D} \right|^2 \leq C. \tag{8}$$

Proof. The proof is based on the choice of the test functions

$$g(p_{g,D}) = \int_0^{p_{g,D}} \frac{1}{\rho_l^h(z)} dz, \text{ and } (\mathcal{C}_1 p^n_{l,D} - p^n_{g,D})$$

Convective terms. After integration part by part

$$E_2 = \sum_{n,\sigma_{D,E}} \Lambda_{D,E} \, M_l(s^n_{l,D,E}) \delta^n_{D,E}(p_l) \Big(\mathcal{C}_1 \delta^n_{D,E}(p_l) - \delta^n_{D,E}(p_g) \Big)$$

$$+ \sum_{\mathbf{n},\sigma_{D,E}} \Lambda_{D,E} \, M_l(s^n_{l,D,E}) \delta^n_{D,E}(p_l) \underbrace{(\rho_l^h)^n_{D,E} \delta^n_{D,E}(g(p_g))}_{=\delta^n_{D,E}(p_g)}$$

$$+ \mathcal{C}_1 \sum_{n,\sigma_{D,E}} \Lambda_{D,E} \, M_g(s^n_{l,D,E}) \, \delta^n_{D,E}(p_g) \underbrace{(\rho_l^h)^n_{D,E} \delta^n_{D,E}(g(p_g))}_{=\delta^n_{D,E}(p_g)}$$

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Convective terms. After integration part by part

$$E_2 = \mathcal{C}_1 \sum_{n,\sigma_{D,E}} \Lambda_{D,E} \; M_l(s^n_{l,D,E}) \delta^n_{D,E}(p_l) \; \delta^n_{D,E}(p_l)$$

$$+ \mathcal{C}_1 \sum_{n,\sigma_{D,E}} \Lambda_{D,E} \; M_g(s^n_{l,D,E}) \delta^n_{D,E}(p_g) \delta^n_{D,E}(p_g).$$

Discrete lemma

Continuous case : $M(s_l)|\nabla p|^2 \leq M_l(s_l)|\nabla p_l|^2 + M_g(s_l)|\nabla p_g|^2$

Lemma (Total mobility and global pressure)

$$M^n_{l,D|E} + M^n_{g,D|E} \geq m_0, \ \forall (D,E) \in \mathcal{E}, \ \forall n \in [0,N],$$

$$m_0 \left(\delta^n_{D,E}(p)\right)^2 \leq M^n_{l,D|E}\left(\delta^n_{D,E}(p_l)\right)^2 + M^n_{g,D|E}\left(\delta^n_{D,E}(p_g)\right)^2.$$

Continuous case : $|\nabla \mathcal{B}(s_l)|^2 = \frac{M_l M_g}{M}|\nabla p_c|^2 \leq M_l(s_l)|\nabla p_l|^2 + M_g(s_g)|\nabla p_g|^2.$

Lemma (Capillary term)

$$(\delta^n_{D,E}(\mathcal{B}(s_l)))^2 \leq M^{n+1}_{g,D|E}\left(\delta^n_{D,E}(p_g)\right)^2 + M^{n+1}_{l,D|E}\left(\delta^n_{D,E}(p_l)\right)^2.$$

The proofs of these lemma depend only on the definition of the global pressure and the mesh.

Consequences

Corollary (Discrete Gradients)

Suppose $\Lambda_{D,E} \geq 0$, for all D, E.
From the preliminary lemmas, we have

$$\sum_{n=0}^{N-1} \delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} \delta_{D,E}^{n}(p)|^2 \leq C. \qquad \to p_{\mathcal{D}_h} \in L^2(0, T; H^1(\Omega))$$

$$\sum_{n=0}^{N-1} \delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} (\delta_{D,E}^{n}(\mathcal{B}(s_l)))^2 \leq C. \qquad \to \mathcal{B}(s_{l,\mathcal{D}_h}) \in L^2(0, T; H^1(\Omega))$$

Compactness : translates in space and time estimates

Define the discrete functions

$$U_{l,\mathcal{D}_h} = s_{l,\mathcal{D}_h} \; U_{g,\mathcal{D}_h} = m(s_{l,\mathcal{D}_h})\rho_l^h(p_{g,\mathcal{D}_h})$$

constant per cylinder $(t^n, t^{n+1}) \times K$. We derive estimates on translates in space and time of the functions $\bar{U}_{\alpha,\mathcal{D}_h}$ piecewise constant in t and constant in x for all $\mathcal{D}$.

Lemma (Translates in space and in time)

$$\iint_{\Omega' \times (0,T)} \left|\bar{U}_{\alpha,\mathcal{D}_h}(t,x+y) - \bar{U}_{\alpha,\mathcal{D}_h}(t,x)\right| \mathrm{d}x\mathrm{d}t \le \omega(|y|),$$

$$\iint_{\Omega\times(0,T-\tau)} \left|\bar{U}_{\alpha,\mathcal{D}_h}(t+\tau,x) - \bar{U}_{\alpha,\mathcal{D}_h}(t,x)\right|^2 dx\, dt \le \tilde{\omega}(\tau),$$

where $y \in \mathbb{R}^3$, $\tau \in (0,T)$, $\Omega' = \{x \in \Omega, \, [x, x+y] \subset \Omega\}$ *and* ω *satisfies* $\lim_{|y|\to 0} \omega(|y|) = 0$ *and* $\lim_{\tau\to 0} \tilde{\omega}(\tau) = 0$.

Strong convergence

The sequence $\bar{U}_{\alpha,\mathcal{D}_h}$ is relatively compact in $L^1(Q_T)$, $\alpha = l, g$.

Using Kolmogorov compactness theorem.

Theorem

The sequence $(p_{l,\mathcal{D}_h}, p_{g,\mathcal{D}_h})$ *converges to* (p_l, p_g) *satisfying*

$$p_\alpha \in L^2(Q_T)),\ s_l \geq 0,\ p,\ p_g \in L^2(0,T;H^1_{\Gamma_l}(\Omega)),\ \mathcal{B}(s_l) \in L^2(0,T;H^1_{\Gamma_l}(\Omega)) \quad (9)$$

in the sense that for all $\psi, \varphi \in C^1(0,T;H^1_{\Gamma_l}(\Omega))$ *with* $\psi(T,.) = \varphi(T,.) = 0$,

$$-\int_{Q_T} \Phi s_l \partial_t \psi \mathrm{d}x\mathrm{d}t - \int_\Omega \Phi s_l^0 \psi(0,x)\mathrm{d}x + \int_{Q_T} \mathbf{\Lambda}(M_l(s_l)\nabla p + \nabla\mathcal{B}(s_l)) \cdot \nabla\psi \mathrm{d}x\mathrm{d}t = \int_{Q_T} \frac{r_\omega}{\rho_l^w} \psi \mathrm{d}x\mathrm{d}t, \quad (10)$$

$$-\int_{Q_T} \Phi m(s_l)\rho_l^h(p_g)\partial_t\varphi \mathrm{d}x\mathrm{d}t - \int_\Omega \Phi m(s_l^0)\rho_l^h(p_g^0)\varphi(0,x)\mathrm{d}x + \int_{Q_T} \mathbf{\Lambda}\rho_l^h(p_g)(M_l(s_l)\nabla p + \nabla\mathcal{B}(s_l)) \cdot \nabla\varphi \mathrm{d}x\mathrm{d}t + \mathcal{C}_1 \int_{Q_T} \mathbf{\Lambda}\rho_l^h(p_g)M_g(s_l)\nabla p_g \cdot \nabla\varphi \mathrm{d}x\mathrm{d}t + \int_{Q_T} \mathcal{C}_2 X_l^w D_l^h \nabla p_g \cdot \nabla\varphi \mathrm{d}x\mathrm{d}t = \int_{Q_T} r_g \varphi \mathrm{d}x\mathrm{d}t. \quad (11)$$

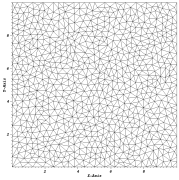
Numerical results

Parameter values for the porous medium and fluid characteristics

Porous medium		**Fluid characteristics**	
Parameter	*Value*	*Parameter*	*Value*
Φ [-]	0.15	D_l^h $[\mathrm{m}^2 \cdot \mathrm{s}^{-1}]$	3×10^{-9}
Λ $[\mathrm{m}^2]$	5.10^{-20}	μ_l $[\mathrm{Pa} \cdot \mathrm{s}]$	1×10^{-3}
p_r $[\mathrm{Pa}]$	2×10^6	μ_g $[\mathrm{Pa} \cdot \mathrm{s}]$	9×10^{-6}
n [-]	1.54	H^h $[\mathrm{mol.Pa}^{-1}.\mathrm{m}^{-3}]$	7.65×10^{-6}
s_{lr} [-]	0.4	M^h $[\mathrm{Kg} \cdot \mathrm{mol}^{-1}]$	2×10^{-3}
s_{gr} [-]	0	ρ_l^w $[\mathrm{Kg} \cdot \mathrm{mol}^{-3}]$	10^3

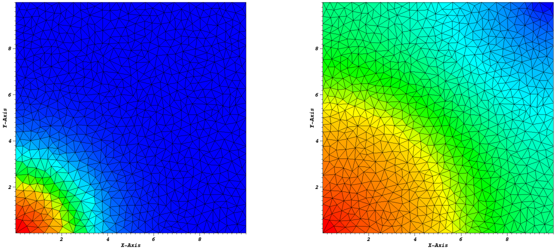
Initially $s_l(x,0) = 1.$ and $p_l(x,0) = 10.$bar in the whole domain.

- Inject hydrogen as a gas into the lower left corner with a flux of $f_g = 5.57\,10^{-4}\,kg.m^{-2}.s^{-1}$,
- liquid pressure is imposed at the top right corner ($p_l = 10$ bar).
- van Genuchten relative permeability,



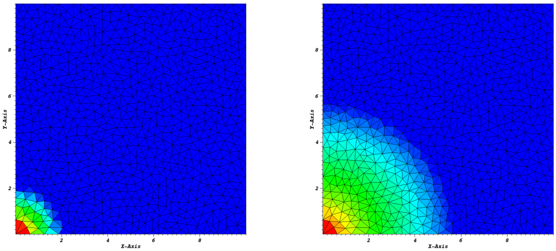
H_2 injection

variables : $(p_l,\ \rho_g^h)$



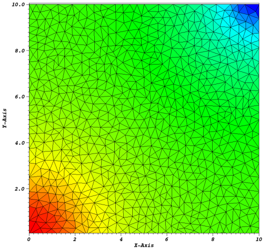
$$0 \leq \rho_g^h \leq 0.0235$$

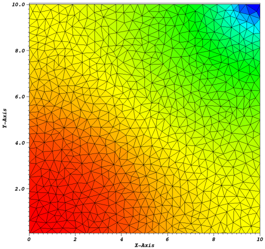
H_2 injection



$$0 \leq s_g \leq 0.0128$$

H_2 injection





$$10. \leq p_l \leq 11.5$$