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

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4 FV-FE for two–compressible two–component flow
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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.
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 $\approx 90\%$ CO2 $\Rightarrow$ 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).

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:

\[ \Phi \partial_t (\rho_w^l s_l) + \text{div} (\rho_w^l \mathbf{V}_l) = f_w \]  

(1)

Mass conservation of \( H_2 \):

\[ \Phi \partial_t \left( \rho_i^h (p_g) s_l + \rho_g^h (p_g) s_g \right) + \text{div} \left( \rho_i^h (p_g) \mathbf{V}_l + \rho_g^h (p_g) \mathbf{V}_g \right) \]

\[ - \text{div} \left( \phi \rho_i D_i^h (s_l) \nabla X_i^h \right) = f_g \]  

(2)

\[ \Phi = \text{porosity} \]
\[ s_\alpha = \text{saturation of the } \alpha \text{ phase} \]
\[ \rho_\alpha = \text{pressure of the } \alpha \text{ phase} \]
\[ \mathbf{V}_\alpha = \text{velocity of the } \alpha \text{ phase} \]
\[ \rho_i^h = \text{density of dissolved hydrogen} \]
\[ \rho_g^h = \text{density of } H_2 \text{ in the gas phase} \]
\[ X_i^h = \frac{\rho_i^h}{\rho_l} : \text{mass fraction of } H_2 \text{ in the liquid} \]
\[ D_i^h (s_l) \text{ diffusivity coefficient of the dissolved hydrogen} \]
\[ f_\alpha = \text{source term} \]
Mathematical model

Mass conservation of water:

\[ \Phi \partial_t (\rho_l^w s_l) + \text{div} (\rho_l^w \mathbf{V}_l) = f_w \]  \hspace{1cm} (1)

Mass conservation of \( H_2 \):

\[ \Phi \partial_t \left( \rho_l^h(p_g)s_l + \rho_g^h(p_g)s_g \right) + \text{div} \left( \rho_l^h(p_g)\mathbf{V}_l + \rho_g^h(p_g)\mathbf{V}_g \right) \\
- \text{div} \left( \phi \rho_l D_l^h(s_l) \nabla X^h_l \right) = f_g \]  \hspace{1cm} (2)

- Saturations:

\[ s_l + s_g = 1 \]  \hspace{1cm} (3)

- Capillary pressure:

\[ p_c(s_l) = p_g - p_l \]  \hspace{1cm} (4)

- Darcy law:

\[ \mathbf{V}_\alpha = -\Lambda(x) \frac{k_{r_\alpha}(s_\alpha)}{\mu_\alpha} \left( \nabla p_\alpha - \rho_\alpha(p_\alpha)g \right), \]
Mathematical model: the densities

Ideal gas

\[ \rho_g^h = \frac{M^h}{RT} \rho_g \]

Henri law

\[ \rho_l^h = M^h H^h \rho_g \]

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

\[ \rho_g^h = C_1 \rho_l^h \] where \( C_1 = \frac{1}{H^h RT} = 52.51 \).

Denote \( m(s_l) = s_l + C_1 s_g > 0 \). The hydrogen equation is equivalent to

\[
\partial_t \left( \Phi m(s_l) \rho_l^h(p_g) \right) + \text{div} \left( \rho_l^h(p_g) V_l + C_1 \rho_l^h(p_g) V_g \right) - \text{div} \left( C_2 X^w D_l^h(s_l) \nabla p_g \right) = f_g \tag{5}
\]

**Primary variables**: \( \rho_l, \rho_g \).
Mathematical model

MIAN ASSUMPTIONS

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

\[ M_\alpha(s_\alpha = 0) = 0. \]

- The density \( \rho^h_1 \) is increasing and bounded:

\[ 0 < \rho_m \leq \rho^h_1(p_g) \leq \rho_M. \]

- 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 \( D^h_1 \) is positive.
Motivation

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

- 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.
Primal mesh. we perform a triangulation on $\mathcal{T}_h$ of the domain $\Omega$, such that $\overline{\Omega} = \bigcup_{K \in \mathcal{T}_h} K$.

We define

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

There exists a constant $\theta_T > 0$

$$\max_{K \in \mathcal{T}_h} \frac{\text{diam}(K)}{\rho_K} \leq \theta_T, \forall h > 0,$$  \hspace{1cm} (6)

where $\rho_K$ is the diameter of the largest ball inscribed in $K$. 

Primal mesh. Triangles $K, L \in \mathcal{T}_h$
Combined FV–nonconforming FE: Dual mesh

**Dual mesh.**

We define a dual partition $\mathcal{D}_h$ s.t. $\bar{\Omega} = \bigcup_{D \in \mathcal{D}_h} \bar{D}$. 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 $\sigma_D$ through the vertices of $\sigma_D$.

Dual mesh $D,D \in D_h$, dual volumes associated with edges.
We use the following notations:

- $|D| = \text{meas}(D)$ and $|\sigma| = \text{meas}(\sigma)$.
- $Q_D$ the barycenter of the side $\sigma_D$.
- $\mathcal{N}(D)$ 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 $D$.
- $\mathcal{D}_h^{\text{int}}$ and $\mathcal{D}_h^{\text{ext}}$ are respectively the set of all interior and boundary dual volumes.
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

\[
-\text{div}(\Lambda \nabla u) + \text{div}(cu) = f
\]

Combined scheme.

\[
- \sum_{E \in \mathcal{N}(D)} \Lambda_{D,E}(U_E - U_D) + \sum_{E \in \mathcal{N}(D)} G(U_D, U_E; \delta C_{D,E}) = 0
\]

where the stiffness matrix is

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

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 \(\delta C_{D,E} = \int_{\sigma_{D,E}} c \cdot n_{D,E} \, d\sigma\).
Combined FV–Nonconforming FE: Diffusion-transport

\[- \sum_{E \in \mathcal{N}(D)} \Lambda_{D,E}(U_E - U_D) + \sum_{E \in \mathcal{N}(D)} G(U_D, U_E; \delta C_{D,E}) = 0\]

P. Angot, V. Dolejsi, M. Feistauer and J. Felcman,

R. Eymard, D. Hilhorst and M. Vohralik,
Nonconforming FE/Implicit upwind scheme

We integrate the mass conservation law over the diamond $D$

$$\partial_t \left( \Phi m(s_l) \rho_l^h(p_g) \right) + \text{div} \left( \rho_l^h(p_g) \mathbf{V}_l + C_1 \rho_l^h(p_g) \mathbf{V}_g \right) - \text{div} \left( C_2 X_l^w D_l^h(s_l) \nabla p_g \right) = f_g$$

and we use:

- Fully implicit Euler scheme
- The mobility of each phase is centered 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

$$\left| D \right| \phi_D \frac{s^n_{l,D} - s^{n-1}_{l,D}}{\delta t} - \sum_{E \in \mathcal{N}(D)} M_I(s^n_{l,D,E}) \Lambda_{D,E} \delta^n_{D,E}(p_I) = \frac{f^n_{w,D}}{\rho^n_w} \quad (\text{water})$$

$$\left| D \right| \phi_D \frac{\rho^n_h(p^n_{g,D})m(s^n_{l,D}) - \rho^n_h(p^n_{g,D}^{-1})m(s^{n-1}_{l,D})}{\delta t} - \sum_{E \in \mathcal{N}(D)} (\rho^n_I)_{D,E} M_I(s^n_{l,D,E}) \Lambda_{D,E} \delta^n_{D,E}(p_I) - C_1 \sum_{E \in \mathcal{N}(D)} (\rho^n_h)_{D,E} M_g(s^n_{l,D,E}) \Lambda_{D,E} \delta^n_{D,E}(p_g) - C_2 \sum_{E \in \mathcal{N}(D)} \phi_D(X^n_w)_{D,E} (D^n_h)_{D,E} \delta^n_{D,E}(p_g) = f^n_{g,D} \quad (\text{gas})$$

This system is completed by the capillary pressure

$$p_c(s^n_{l,D}) = p^n_{g,D} - p^n_{l,D}. \quad (7)$$

The approximation of each term is important to handle with the energy estimates.
\[
\begin{align*}
|D| \phi_D \frac{\rho^h_l(p^n_{g,D}) m(s^n_{l,D}) - \rho^h_l(p^{n-1}_{g,D}) m(s^{n-1}_{l,D})}{\delta t} \\
- \sum_{E \in \mathcal{N}(D)} \left( \rho^h_l \right)_{D,E}^n M_l(s^n_{l,D,E}) \Lambda_{D,E} \delta^n_{D,E}(p_l) - C_1 \sum_{E \in \mathcal{N}(D)} \left( \rho^h_l \right)_{D,E}^n M_g(s^n_{l,D,E}) \Lambda_{D,E} \delta^n_{D,E}(p_g) \\
- C_2 \sum_{E \in \mathcal{N}(D)} \phi_D \left( X^{w}_l \right)_{D,E}^n (D^h_l)_{D,E} \delta^n_{D,E}(p_g) = f^n_{g,D}
\end{align*}
\]

- **Discrete Gradient of pressure**

\[
\delta^n_{D,E}(p_\alpha) = p^n_{\alpha,E} - p^n_{\alpha,D}
\]
\[ |D| \phi_D \frac{\rho^h_I(p^n_{g,D}) m(s^n_{l,D}) - \rho^h_I(p^{n-1}_{g,D}) m(s^{n-1}_{l,D})}{\delta t} \]

\[ - \sum_{E \in \mathcal{N}(D)} (\rho^h_I)^n_{D,E} M_I(s^n_{l,D,E}) \Lambda_{D,E} \delta^n_{D,E}(\rho_I) - C_1 \sum_{E \in \mathcal{N}(D)} (\rho^h_I)^n_{D,E} M_g(s^n_{l,D,E}) \Lambda_{D,E} \delta^n_{D,E}(p_g) \]

\[ - C_2 \sum_{E \in \mathcal{N}(D)} \phi_D(X^n_{l,E})(D^h_I)_{D,E} \delta^n_{D,E}(p_g) = f^n_{g,D} \]

- **Permeability on interfaces by FE**

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

and

\[ (D^h_I)_{D,E} = - \sum_{K \in \mathcal{T}_h} \int_K D^h_i \nabla \varphi_E \cdot \nabla \varphi_D \, dx \]
\[ |D| \frac{\phi_D}{\delta t} \left( \rho_I^h(p_{g,D}^n)m(s_{l,D}^n) - \rho_I^h(p_{g,D}^{n-1})m(s_{l,D}^{n-1}) \right) \]

\[ - \sum_{E \in \mathcal{D}(D)} (\rho_I^h)_{D,E}^n M_I(s_{l,D,E}^n) \Lambda_{D,E} \delta_{D,E}^n(p_I) - C_1 \sum_{E \in \mathcal{D}(D)} (\rho_I^h)_{D,E}^n M_g(s_{l,D,E}^n) \Lambda_{D,E} \delta_{D,E}^n(p_g) \]

\[ - C_2 \sum_{E \in \mathcal{D}(D)} \phi_D(X_{l,w}^n)_{D,E} \left( D_{l,D}^h \right)_{D,E} \delta_{D,E}^n(p_g) = f_{g,D}^n \]

- **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

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

\[
\frac{1}{(\rho^h)_{D,E}^n} = \begin{cases} 
\frac{1}{p^n_{g,D_D}\int_{p^n_{g,D}}}^{p^n_{g,E}} \int_{p^n_{g,D}}}^{p^n_{g,E}} \frac{1}{\rho^h_I(\zeta)} d\zeta & \text{if } p^n_{g,D} \neq p^n_{g,E}, \\
\frac{1}{(\rho^h)_{D}^n} & \text{otherwise.}
\end{cases}
\]
Proposition (Maximum principle)

Let \((s_{\alpha,D}^0)_{D \in D_h} \in [0,1]\). Then, the saturation \(s_{l,D}^n \geq 0\) for all \(D \in D_h, n \in \{1, \ldots, N\}\).

Proof by induction on \(n\). Suppose \(s_{l,D}^{n-1} \geq 0\) for all \(D \in D_h\). Let \(s_{l,D}^n = \min \{s_{l,E}^n\}_{E \in D_h}\) and we seek that \(s_{l,D}^n \geq 0\).

Multiply the scheme by \(-(s_{l,D}^n)^-\), we obtain

\[-|D| \phi_D \frac{s_{l,D}^n - s_{l,D}^{n-1}}{\delta t} (s_{l,D}^n)^- - \sum_{E \in N(D)} G_{l}(s_{l,D}^n, s_{l,E}^n; \delta^n_{D,E}(p_l))(s_{l,D}^n)^- = -f_{l,D}^n (s_{l,D}^n)^- \leq 0,\]

since \(G_l\) is monotone.

Then, we deduce that

\[|(s_{l,D}^n)^-|^2 + s_{l,D}^{n-1}(s_{l,D}^n)^- \leq 0,\]

and \(s_{l,D}^n \geq 0\) 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

\[ g(p_g) := \int_0^{p_g} \frac{1}{\rho_i^h(z)} \, dz \quad \text{and} \quad \mathcal{H}(p_g) := \rho_i^h(p_g)g(p_g) - p_g \geq 0. \]

Define the function

\[ E = m(s_l)\mathcal{H}_g(p_g) - C_1 \int_0^{s_l} p_c(z) \, dz. \]

By multiplying the hydrogen equation by \( g(p_g) \) and water equation by \( C_1 p_l - p_g \), after integration and summation of equations, we deduce the estimate

\[
\int_\Omega \Phi \partial_t E \, dx + c_\Lambda \left[ \int_\Omega M_l |\nabla p_l|^2 \, dx + \int_\Omega M_g |\nabla p_g|^2 \, dx + \int_\Omega C_2 X^w D_h \nabla g \cdot \nabla g(p_g) \, dx \right] \leq C.
\]

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 \( B \).

Energy estimates.

Continuous case.
The global pressure $p$ can be written as

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

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

$$ \bar{p}(s_l) = -\int_0^{s_l} \frac{M_g(z)}{M(z)} p_c'(z)dz \quad \text{and} \quad \bar{p}(s_l) = \int_0^{s_l} \frac{M_l(z)}{M(z)} p_c'(z)dz. $$

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:

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

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

**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

\[
g(p_{g,D}) = \int_0^{p_{g,D}} \frac{1}{\rho^h_i(z)} \, dz, \text{ and } (C_1 p^n_{l,D} - p^n_{g,D})
\]

**Term in time.**

\[E_1 = \sum_{n,D} \phi_D \left( (s^n_{l,D}-s^{n-1}_{l,D}) (C_1 p^n_{l,D} - p^n_{g,D}) + \rho^h_i(p^n_{g,D}) m(s^n_{l,D}) - \rho^h_i(p^{n-1}_{g,D}) m(s^{n-1}_{l,D}) \right) g(p^n_{g,D}) \]

\[E_1 \geq \sum_{D \in \mathcal{D}_h} \phi_D |D| \left( \mathcal{H}(p^N_{g,D}) m(s^N_{l,D}) - \mathcal{H}(p^0_{g,D}) m(s^0_{l,D}) \right) \]

\[- C_1 \sum_{D \in \mathcal{D}_h} \phi_D |D| \mathcal{P}_c(s^N_{l,D}) + C_1 \sum_{D \in \mathcal{D}_h} \phi_D |D| \mathcal{P}_c(s^0_{l,D}). \tag{9}\]
A priori estimates: discrete case

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

**Proposition (Discrete velocities)**

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

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

$$g(p_g,D) = \int_0^{p_g,D} \frac{1}{\rho^h(z)} \, dz, \text{ and } (C_1 p^n_{l,D} - p^n_{g,D})$$

**Convective terms.** After integration part by part

$$E_2 = \sum_{n, \sigma_{D,E}} \Lambda_{D,E} M_l(s^n_{l,D,E}) \delta^n_{D,E}(p_l) \left( C_1 \delta^n_{D,E}(p_l) - \delta^n_{D,E}(p_g) \right)$$

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

$$+ C_1 \sum_{n, \sigma_{D,E}} \Lambda_{D,E} M_g(s^n_{l,D,E}) \delta^n_{D,E}(p_g) (\rho^n_{l,D} \delta^n_{D,E}(g(p_g)) = \delta^n_{D,E}(p_g)$$
A priori estimates: discrete case

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

**Proposition (Discrete velocities)**

\[
\sum_{n=0}^{N-1} \delta t \sum_{D \in D_h} \sum_{E \in \mathcal{N}(D)} \Lambda_{D,E} M_\alpha(s_{\alpha,D|E}^n) \left| p_{\alpha,E}^n - p_{\alpha,D}^n \right|^2 \leq C. \tag{8}
\]

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

\[
g(p_g,D) = \int_0^{p_g,D} \frac{1}{\rho^h_l(z)} \, dz, \text{ and } (C_1 p_{l,D}^n - p_{g,D}^n)
\]

**Convective terms.** After integration part by part

\[
E_2 = C_1 \sum_{n,\sigma_{D,E}} \Lambda_{D,E} M_l(s_{l,D,E}^n) \delta_{D,E}^n(p_l) \delta_{D,E}^n(p_l)
\]

\[
+ C_1 \sum_{n,\sigma_{D,E}} \Lambda_{D,E} M_g(s_{l,D,E}^n) \delta_{D,E}^n(p_g) \delta_{D,E}^n(p_g).
\]
Discrete lemma

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

Lemma (Total mobility and global pressure)

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

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

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

Lemma (Capillary term)

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

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* \[ \sum_{n=0}^{N-1} \delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} \left| \delta_{D,E}^n(p) \right|^2 \leq C. \rightarrow p_{D_h} \in L^2(0, T; H^1(\Omega)) \]

\[ \sum_{n=0}^{N-1} \delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} (\delta_{D,E}^n(B(s_l)))^2 \leq C. \rightarrow B(s_{l,D_h}) \in L^2(0, T; H^1(\Omega)) \]
Compactness: translates in space and time estimates

Define the discrete functions

\[ U_l, D_h = s_l, D_h, \quad U_g, D_h = m(s_l, D_h) \rho^l_h(p_g, D_h) \]

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

**Lemma (Translates in space and in time)**

\[
\begin{align*}
\int \int_{\Omega' \times (0, T)} |\bar{U}_\alpha, D_h(t, x+y) - \bar{U}_\alpha, D_h(t, x)| \, dx \, dt & \leq \omega(|y|), \\
\int \int_{\Omega \times (0, T-\tau)} |\bar{U}_\alpha, D_h(t+\tau, x) - \bar{U}_\alpha, D_h(t, x)|^2 \, dx \, dt & \leq \tilde{\omega}(\tau),
\end{align*}
\]

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

**Strong convergence**

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

Using Kolmogorov compactness theorem.
The sequence \((p_l, D_h, p_g, D_h)\) converges to \((p_l, p_g)\) satisfying

\[ p_\alpha \in L^2(Q_T), \quad s_l \geq 0, \quad p, \quad p_g \in L^2(0, T; H^1_\Gamma(\Omega)), \quad B(s_l) \in L^2(0, T; H^1_\Gamma(\Omega)) \] (9)

in the sense that for all \(\psi, \varphi \in C^1(0, T; H^1_\Gamma(\Omega))\) with \(\psi(T, \cdot) = \varphi(T, \cdot) = 0\),

\[
- \int_{Q_T} \Phi s_l \partial_t \psi \, dx \, dt - \int_{\Omega} \Phi s^0_l \psi(0, x) \, dx + \int_{Q_T} \Lambda (M_l(s_l) \nabla p + \nabla B(s_l)) \cdot \nabla \psi \, dx \, dt = \int_{Q_T} \frac{r_\omega}{\rho^w_l} \psi \, dx \, dt, \tag{10}
\]

\[
- \int_{Q_T} \Phi m(s_l) \rho^h_l(p_g) \partial_t \varphi \, dx \, dt - \int_{\Omega} \Phi m(s^0_l) \rho^h_l(p^0_g) \varphi(0, x) \, dx + \int_{Q_T} \Lambda \rho^h_l(p_g) (M_l(s_l) \nabla p + \nabla B(s_l)) \cdot \nabla \varphi \, dx \, dt + C_1 \int_{Q_T} \Lambda \rho^h_l(p_g) M_g(s_l) \nabla p_g \cdot \nabla \varphi \, dx \, dt + \int_{Q_T} C_2 X^w_l \nabla p_g \cdot \nabla \varphi \, dx \, dt = \int_{Q_T} r_g \varphi \, dx \, dt. \tag{11}
\]
Parameter values for the porous medium and fluid characteristics

<table>
<thead>
<tr>
<th>Porous medium</th>
<th>Value</th>
<th>Fluid characteristics</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Phi$ [-]</td>
<td>0.15</td>
<td>$D^h_l$ $[m^2 \cdot s^{-1}]$</td>
<td>$3 \times 10^{-9}$</td>
</tr>
<tr>
<td>$\Lambda$ $[m^2]$</td>
<td>$5.10^{-20}$</td>
<td>$\mu_l$ $[Pa \cdot s]$</td>
<td>$1 \times 10^{-3}$</td>
</tr>
<tr>
<td>$p_r$ $[Pa]$</td>
<td>$2 \times 10^6$</td>
<td>$\mu_g$ $[Pa \cdot s]$</td>
<td>$9 \times 10^{-6}$</td>
</tr>
<tr>
<td>$n$ [-]</td>
<td>1.54</td>
<td>$H^h$ $[mol.Pa^{-1}m^{-3}]$</td>
<td>$7.65 \times 10^{-6}$</td>
</tr>
<tr>
<td>$s_{lr}$ [-]</td>
<td>0.4</td>
<td>$M^h$ $[Kg \cdot mol^{-1}]$</td>
<td>$2 \times 10^{-3}$</td>
</tr>
<tr>
<td>$s_{gr}$ [-]</td>
<td>0</td>
<td>$\rho^w_l$ $[Kg \cdot mol^{-3}]$</td>
<td>$10^3$</td>
</tr>
</tbody>
</table>

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 $f_g = 5.57 \times 10^{-4} kg.m^{-2}.s^{-1}$,
- 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. $\leq p_l \leq 11.5$