

Convergence analysis of a FV-FE scheme for partially miscible two-phase flow in anisotropic porous media

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Abstract We study the convergence of a combined finite volume nonconforming finite element scheme on general meshes for a partially miscible two-phase flow model in anisotropic porous media. This model includes capillary effects and exchange between the phase. The diffusion term, which can be anisotropic and heterogeneous, is discretized by piecewise linear nonconforming triangular finite elements. The other terms are discretized by means of a cell-centered finite volume scheme on a dual mesh. The relative permeability of each phase is decentred according the sign of the velocity at the dual interface. The convergence of the scheme is proved thanks to an estimate on the two pressures which allows to show estimates on the discrete time and compactness results in the case of degenerate relative permeabilities. A key point in the scheme is to use particular averaging formula for the dissolution function arising in the diffusion term. We show also a simulation of CO_2 injection in a water saturated reservoir and nuclear waste management. Numerical results are obtained by in-house numerical code.

1 Introduction

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. A direct consequence of this production is the growth of hydrogen pressure around alveolus which can affect all the

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functions allocated to the canisters, waste forms, backfill, host rock. Host rock safety function may be threatened by over pressurisation leading to opening fractures of the domain, inducing groundwater flow and transport of radionuclides.

In this work, we address the construction and convergence analysis of a combined finite volume nonconforming finite element scheme, based on a two pressures formulation, for two-phase two-component flow in porous media where the dissolution of the non-wetting phase can occur in different engineering application (e.g. nuclear storage and CO2 storage). The convergence analysis is done in the degenerate case and for the general model including capillarity and gravity effects.

2 Mathematical formulation of the continuous problem

We consider herein a porous medium saturated with a fluid composed of two phases (liquid and gas) and a mixture of two components (water and hydrogen). The water is supposed only present in the liquid phase (no vapor of water due to evaporation). Let $T > 0$, let be Ω a bounded open subset of \mathbb{R}^d ($d \geq 1$) and we set $Q_T = (0, T) \times \Omega$. We write the *mass conservation* of each component

$$\Phi \partial_t (\rho_l^w s_l) + \operatorname{div} (\rho_l^w \mathbf{V}_l) = f_w, \quad (1)$$

$$\begin{aligned} \Phi \partial_t (\rho_l^h(p_g) s_l + \rho_g^h(p_g) s_g) + \operatorname{div} (\rho_l^h(p_g) \mathbf{V}_l + \rho_g^h(p_g) \mathbf{V}_g) \\ - \operatorname{div} (\phi s_l \rho_l D_l^h \nabla X_l^h) = f_g, \end{aligned} \quad (2)$$

where $\Phi(x)$, $s_\alpha(t, x)$ ($s_l + s_g = 1$), $p_\alpha(t, x)$, $\rho_l^h(p_g)$, $\rho_g^h(p_g)$, $\rho_\alpha = \rho_\alpha^h + \rho_\alpha^w$, $X_l^h = \rho_l^h / \rho_l$ ($X_l^h + X_l^w = 1$) and D_l^h represent respectively the (given) porosity of the medium, the saturation of the α phase ($\alpha = l, g$), the pressure of the α phase, the density of dissolved hydrogen, the density of the hydrogen in the gas phase, the density of the α phase, the mass fraction of the hydrogen in the liquid phase, the diffusivity coefficient of the dissolved gas phase in the liquid phase. The velocity of each fluid \mathbf{V}_α is given by the Darcy law

$$\mathbf{V}_\alpha = -\mathbf{K} \frac{k_{r\alpha}(s_\alpha)}{\mu_\alpha} (\nabla p_\alpha - \rho_\alpha(p_\alpha) \mathbf{g}),$$

where $\mathbf{K}(x)$ is the intrinsic (given) permeability tensor of the porous medium, $k_{r\alpha}$ the relative permeability of the α phase, μ_α the constant α -phase's viscosity, p_α the α -phase's pressure and \mathbf{g} the gravity. For detailed presentation of the model we refer to the presentation of the benchmark Couplex-Gaz [4].

To define the hydrogen densities, we use the ideal gas law and the Henry law $\rho_g^h = \frac{M^h}{RT} p_g$, $\rho_l^h = M^h H^h p_g$, where the quantities M^h , H^h , R and T represent respectively the molar mass of hydrogen, the Henry constant for hydrogen, the universal constant of perfect gases and T the temperature. To close the system, we introduce

the capillary pressure law which links the jump of pressure of the two phases to the saturation

$$p_c(s_l) = p_g - p_l, \quad (3)$$

the application $s_l \mapsto p_c(s_l)$ is decreasing. This model also corresponding to the application of CO₂ storage when hydrogen is replaced by CO₂.

Let $T > 0$ be the final time fixed, let be Ω a bounded open subset of \mathbb{R}^d ($d \geq 1$) where $\partial\Omega$ is \mathcal{C}^1 . We set $\Sigma_T = (0, T) \times \partial\Omega$ and we note Γ_l the part of the boundary of Ω where the liquid saturation is imposed to one and $\Gamma_n = \Gamma \setminus \Gamma_l$. The chosen mixed boundary conditions on the pressures are

$$\begin{cases} p_g(t, x) = p_l(t, x) = 0 \text{ on } (0, T) \times \Gamma_l, \\ \mathbf{V}_l \cdot \mathbf{n} = \mathbf{V}_g \cdot \mathbf{n} = \phi_{s_l} \rho_l D_l^h \nabla X_l^h \cdot \mathbf{n} = 0 \text{ on } (0, T) \times \Gamma_n, \end{cases}$$

where \mathbf{n} is the outward normal to Γ_n . The initial conditions are defined on pressures

$$p_\alpha(t=0) = p_\alpha^0 \text{ in } \Omega, \text{ for } \alpha = l, g. \quad (4)$$

Next we introduce a classically physically relevant assumptions on the coefficients of the system.

(H1) **Degeneracy.** The functions $M_l = \frac{k_{rl}}{\mu_l}$ and $M_g = \frac{k_{rg}}{\mu_g} \in \mathcal{C}^0([0, 1], \mathbb{R}^+)$, $M_\alpha(s_\alpha = 0) = 0$ and there is a positive constant $m_0 > 0$ such that for all $s_l \in [0, 1]$,

$$M_l(s_l) + M_g(s_g) \geq m_0.$$

(H2) **Density Bounded.** The density ρ_l^h is in $\mathcal{C}^1(\mathbb{R})$, increasing and there exists two positive constants $\rho_m > 0$ and $\rho_M > 0$ such that $0 < \rho_m \leq \rho_l^h(p_g) \leq \rho_M$.

(H3) The capillary pressure function $p_c \in \mathcal{C}^1([0, 1]; \mathbb{R}^+)$ and there exists $\underline{p}_c > 0$ such that $\frac{dp_c}{ds_l} \leq -\underline{p}_c < 0$.

(H4) The functions $f_w, f_g \in L^2(Q_T)$ and $f_w, f_g \geq 0$ a.e. for all $(t, x) \in Q_T$.

(H5) D_l^h is a possibly null positive constant.

This problem renews the mathematical and numerical interest in the equation describing multiphase multicomponent flows through porous media. Existence of weak solutions for the two compressible, partially miscible flow in porous media, under various assumptions on physical data, we refer to [1]. In [2] and [7] the authors study respectively the convergence of a combined FV-FE scheme of the Keller-Segel model and of a immiscible compressible two phase flows un porous media. Study of the convergence of a finite volume scheme for a model of miscible two-phase flow in porous media under non-degeneracy and regularization of the physical situation on the relative permeability of each phase which physically vanishes when its saturation goes to zero, we refer to [3].

3 Combined finite volume–nonconforming finite element scheme

3.1 Primal and dual meshes

We perform a triangulation \mathcal{T}_h of the domain Ω such that $\overline{\Omega} = \cup_{K \in \mathcal{T}_h} K$. We denote by \mathcal{E}_h the set of all sides, by $\mathcal{E}_h^{\text{int}}$ the set of all interior sides, by $\mathcal{E}_h^{\text{ext}}$ the set of all exterior sides, and by \mathcal{E}_K the set of all the sides of an element $K \in \mathcal{T}_h$. We define $h := \max\{\text{diam}(K), K \in \mathcal{T}_h\}$. We assume the following shape regularity : there exists a positive constant κ_T such that

$$\min_{K \in \mathcal{T}_h} \frac{|K|}{\text{diam}(K)^d} \geq \kappa_T. \quad (5)$$

We also use a dual partition \mathcal{D}_h of Ω such that $\overline{\Omega} = \cup_{D \in \mathcal{D}_h} D$. There is one dual

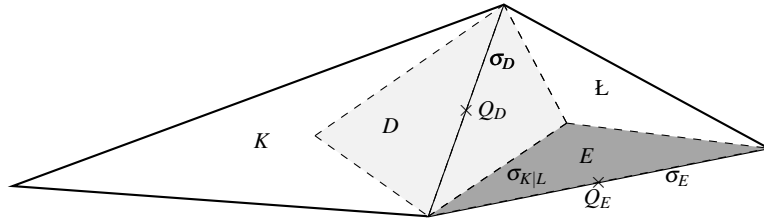


Fig. 1 Triangles $K, L \in \mathcal{T}_h$ and dual volumes $D, E \in \mathcal{D}_h$ associated with edges $\sigma_D, \sigma_E \in \mathcal{E}_h$

element D associated with each side $\sigma_D \in \mathcal{E}_h$. We construct it by connecting the barycenters of every $K \in \mathcal{T}_h$ that contains σ_D through the vertices of σ_D . We denote by Q_D the barycenter of the side σ_D . As for the primal mesh, we set $\mathfrak{F}_h, \mathfrak{F}_h^{\text{int}}, \mathfrak{F}_h^{\text{ext}}$ and \mathfrak{F}_D for the dual mesh sides. We denote by $\mathcal{D}_h^{\text{int}}$ the set of all interior and by $\mathcal{D}_h^{\text{ext}}$ the set of all boundary dual volumes. We finally denote by $\mathcal{N}(D)$ the set of all adjacent volumes to the volume D , $\mathcal{N}(D) := \{E \in \mathcal{D}_h; \exists \sigma \in \mathfrak{F}_h^{\text{int}} \text{ such that } \sigma = \partial D \cap \partial E\}$. For $E \in \mathcal{N}(D)$, we also set $d_{K|L} := |Q_E - Q_D|$, $\sigma_{K|L} := \partial D \cap \partial E$ and $K_{D|E}$ the element of \mathcal{T}_h such that $\sigma_{K|L} \subset K_{D|E}$.

We consider a uniform step time δt , and define $t^n = n\delta t$ for $n \in [0, N]$. We define the following finite-dimensional spaces:

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

we equip X_h with the seminorm $\|u_h\|_{X_h}^2 := \sum_{K \in \mathcal{T}_h} \int_K |\nabla u_h|^2 dx$.

3.2 The combined scheme

For clarity and simplicity, we restrict the theoretical demonstration to a horizontal field, i.e. we neglect the gravity effect. The Henry law combined to the ideal gas law, to obtain that the density of hydrogen gas is proportional to the density of hydrogen dissolved $\rho_g^h = \mathcal{C}_1 \rho_l^h$ where $\mathcal{C}_1 = \frac{1}{H_h RT}$. Remark that the density of water ρ_l^w in the liquid phase is constant and from the Henry law, we can write $\rho_l \nabla X_l^h = X_l^w \nabla p_g$, where \mathcal{C}_2 is a constant equal to $H^h M^h$.

Definition 1. (Combined scheme) The fully implicit combined finite volume-nonconforming finite element scheme for the problem (1)–(2) reads: find the values $p_{\alpha,D}^n$, $D \in \mathcal{D}_h$, $n \in \{1, \dots, N\}$, such that

$$p_{\alpha,D}^0 = \frac{1}{|D|} \int_D p_{\alpha}^0(x) dx, \quad s_{\alpha,D}^0 = \frac{1}{|D|} \int_D s_{\alpha}^0(x) dx, \quad \text{for all } D \in \mathcal{D}_h^{\text{int}}, \quad (6)$$

$$|D| \phi_D \frac{s_{l,D}^n - s_{l,D}^{n-1}}{\delta t} - \sum_{E \in \mathcal{N}(D)} M_l(s_{l,D|E}^n) \Lambda_{D,E} \delta_{D|E}^n(p_l) = \frac{f_{w,D}^n}{\rho_l^w}, \quad (7)$$

$$\begin{aligned} |D| \phi_D \frac{\rho_l^h(p_{g,D}^n) m(s_{l,D}^n) - \rho_l^h(p_{g,D}^{n-1}) m(s_{l,D}^{n-1})}{\delta t} \\ - \sum_{E \in \mathcal{N}(D)} (\rho_l^h)_{D|E}^n M_l(s_{l,D|E}^n) \Lambda_{D,E} \delta_{D|E}^n(p_l) \\ - \mathcal{C}_1 \sum_{E \in \mathcal{N}(D)} (\rho_l^h)_{D|E}^n M_g(s_{l,D|E}^n) \Lambda_{D,E} \delta_{D|E}^n(p_g) \\ - \mathcal{C}_2 \sum_{E \in \mathcal{N}(D)} \phi_D s_{l,D|E}^n (X_l^w)_{D|E}^n D_l^h \delta_{D|E}^n(p_g) = f_{g,D}^n, \quad (8) \end{aligned}$$

$$p_c(s_{l,D}^n) = p_{g,D}^n - p_{l,D}^n. \quad (9)$$

Where $m(s_l) = s_l + \mathcal{C}_1 s_g$. We refer to the matrix Λ of elements $\Lambda_{D,E}$, $D, E \in \mathcal{D}_h^{\text{int}}$, as the diffusion matrix. The stiffness matrix of the nonconforming finite element method, is defined as follow

$$\Lambda_{D,E} := - \sum_{K \in \mathcal{T}_h} (\Lambda(x) \nabla \varphi_E, \nabla \varphi_D)_{0,K} \quad D, E \in \mathcal{D}_h. \quad (10)$$

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

$$\frac{1}{(\rho_l^h(p_g))_{D|E}^n} = \begin{cases} \frac{1}{p_{g,E}^n - p_{g,D}^n} \int_{p_{g,D}^n}^{p_{g,E}^n} \frac{1}{\rho_l^h(\zeta)} d\zeta & \text{if } p_{g,D}^n \neq p_{g,E}^n, \\ \frac{1}{\rho_l^h(p_{g,D}^n)} & \text{otherwise,} \end{cases} \quad (11)$$

this choice is crucial to obtain estimates on discrete pressures.

This scheme consists in a finite volume method together with a phase-by-phase upstream scheme. The implicit finite volume scheme satisfies industrial constraints of robustness and stability. In comparison with incompressible fluid, compressible fluids requires more powerful techniques. We show that the proposed scheme satisfy, a discrete energy estimate on the pressures and a function of the saturation that denote capillary terms, that allow us to derive the convergence of a subsequence to a weak solution of the continuous equations as the size of the discretization tends to zero. The treatment of the degeneracy needs the introduction of powerful technics to link the velocities to the global pressure and the capillary pressure on the discrete form [6].

3.3 A priori estimates and convergence

We summarize the main estimates :

Proposition 1. 1. (Maximum principle). Let $(s_{\alpha,D}^0)_{D \in \mathcal{T}} \in [0, 1]$. Then, the saturation $(s_{l,D}^n)_{D \in \mathcal{T}, n \in \{0, \dots, N\}}$ is positive.

2. Assume that all transmissibilities are non-negative, i.e. $\Lambda_{D,E} \geq 0 \quad \forall D \in \mathcal{D}_h^{int}, E \in \mathcal{N}(D)$. Then, the solution of the combined scheme satisfies

$$\sum_{n=1}^N \delta t \sum_{D \in \mathcal{D}_h} \sum_{E \in \mathcal{N}(D)} \Lambda_{D,E} M_{\alpha} (s_{\alpha,D|E}^n) |p_{\alpha,E}^n - p_{\alpha,D}^n|^2 \leq C, \quad (12)$$

3. The discrete global pressure satisfies

$$\sum_{n=1}^N \delta t \|p_h\|_{X_h}^2 \leq C, \quad (13)$$

where $p = p_g + \tilde{p}(s_l)$, and $\tilde{p}(s_l) = - \int_0^{s_l} \frac{M_l(z)}{M(z)} p_c'(z) dz$.

To prove the estimate (12), we multiply (7) by $\mathcal{C}_1 p_{l,D}^n - p_{g,D}^n$ and (8) by the nonlinear function $g_g(p_{g,D}^n) = \int_0^{p_g} \frac{1}{\rho^g(z)} dz$, then summing the resulting equation over $D \in \mathcal{D}_h$ and $n \in \{1, \dots, N\}$ to deduce the estimates on velocities. The estimates (13) is a consequence of the proof done in [6], the authors prove this property on primal mesh satisfying the orthogonal condition. This proof use only two neighbors elements and it is based only on the definition of the global pressure. Thus, the estimate (13) remains valid on the dual mesh, that allow us, based on the use of the Kolmogorov relative compactness theorem, to derive the convergence of these approximation to a weak solution of the continuous problem in this paper provided the mesh size and the time step tend to zero.

The main result of this paper is the following theorem.

Theorem 1. There exists an approximate solutions $(p_{\alpha,D}^n)_{n,D}$ corresponding to the system (7)-(8), which converges in $L^2(Q_T)$ (up to a subsequence) to a weak solution p_{α} of the system (1)–(2).

4 Numerical results: Gas phase (dis)appearance (quasi-1D)

In this section, we evaluate numerically the finite volume-nonconforming finite element method derived in the above section on a test case dedicated to gas-phase (dis)appearance(see the Couplex-Gas benchmark [4] for more details). The method has been implemented into in-house Fortran code.

The porous medium and fluid characteristics are presented in [4] and summarized in 1.

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

Table 1 Parameter values for the porous medium and fluid characteristics used in test case 1

Initial conditions are $p_l(t=0) = 10^6$ Pa and $p_g(t=0) = 0$ Pa. For boundary conditions on the left, the hydrogen flow rate is given $q_h = 5.57 \times 10^{-6} \chi_{[0, T_{\text{inj}}]}(t) \text{ kg/m}^2/\text{year}$, where $\chi_{[0, T_{\text{inj}}]}$ denote the characteristic function of the set $[0, T_{\text{inj}}]$ and we impose a zero water flow rate $q_w = 0$. The Dirichlet boundary conditions for the outflow boundary are the same as the initial conditions.

A structured grid with 200×20 cells was used for the computations and we used a constant time step of 10 years. Figure 2 show the phase pressures, with respect to time (years) during and after injection. For $0 < t < 14 \times 10^3$ years, the gas saturation is zero and the liquid pressure stay constant; the whole domain is saturated with water. For $14 \times 10^3 \leq t \leq 1.6 \times 10^5$ years, the gas phase appears. For $t > 5 \times 10^5$ years, the gas saturation decreases and after a while, the gas phase disappears. At the end of the simulation the system reaches a stationary state and the liquid pressure gradient goes to zero.

5 CO2 injection in a fully water saturated domaine

The figure 3 shows the CO2 phase saturation at different time. CO2 is injected into the lower left part of a rectangular geometry ($200 \times 50 \text{ m}$) with a flux of $4.10^{-2} \text{ kg} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$. Densities, viscosities and all other parameters are chosen as suggested in [5]. In this example, we used the Brooks-Corey model for the soil water characteristic and relative permeabilities. The CO2 migrates upwards until it reaches the top of the domain with the nonflux conditions and is then driven to the right by advective forces.

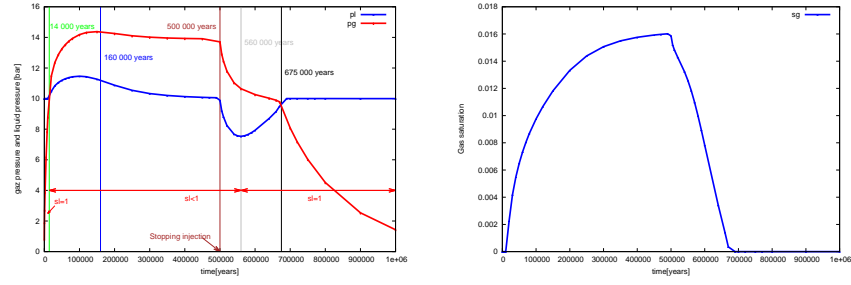


Fig. 2 Liquid and gas pressures p_l (left) and p_g (right) at the $(0, 10)$ with respect to time (years).

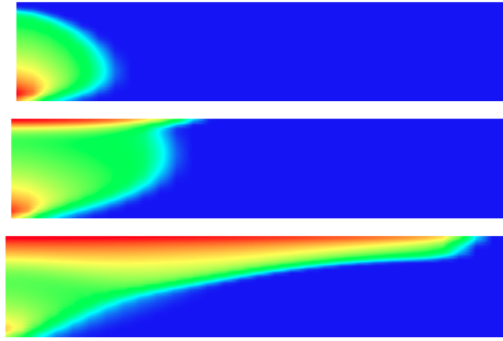


Fig. 3 CO2 phase saturation, color scale ranges from $s_\ell = 0$ (blue) to $s_\ell = \max(s_\ell)$ (red)

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