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Convergence of a finite volume scheme for immiscible compressible two-phase flow in porous media by the concept of the global pressure

Brahim Amaziane*, Mladen Jurak†, Ivana Radišić ‡

June 13, 2021

Abstract

This paper deals with development and analysis of a finite volume (FV) method for the coupled system describing immiscible compressible two-phase flow, such as water-gas, in porous media, capillary and gravity effects being taken into account. We investigate a fully coupled fully implicit cell-centred “phase-by-phase” FV scheme for the discretization of such system. The main goal is to incorporate some of the most recent improvements in the scheme and the convergence of the numerical approximation to the weak solution of such models. The spatial discretization uses a TPFA scheme and a new strategy for handling the upwinding. Based on a priori estimates and compactness arguments, we prove the convergence of the numerical approximation to the weak solution. [The particular feature in this convergence analysis of the classical engineering scheme based on the “phase-by-phase” upwinding on an orthogonal mesh relies on the global pressure–saturation fractional flow formulation as was defined relatively recently for immiscible compressible flow in porous media.](#) We have developed and implemented this scheme in a new module in the context of the open source platform DuMu^X. Two numerical experiments are presented to demonstrate the [efficiency](#) of this scheme. The first test addresses the evolution in 2D of gas migration through engineered and geological barriers for a deep repository for radioactive waste. The second test case is chosen to test the ability of the method to approximate solutions for 3D problems modeling scenarios of CO₂ injection in a fully water-saturated domain.

Keywords: Compressible two–phase flow; Porous media; Finite volume; Nonlinear degenerate system; DuMu^X; Water-gas.

AMS Subject Classification: 35K65; 35Q35; 65N12; 76S05; 76T10; 76M12.

1 Introduction

Modeling of two-phase flow through the subsurface is important for many practical applications, from groundwater modeling and oil and gas recovery to CO₂ sequestration or management of nuclear waste repositories. In this work we focus on CO₂ sequestration and nuclear waste underground storage.

The modeling and simulation of the injection and the spreading of carbon dioxide in the underground is essential for the proper understanding of the physical and chemical processes at different length and time scales, to ascertain migration and trapping of CO₂ in the porous formations, and in assessing the capacity as well as the safety (possible leakage) of the reservoir, see for instance [57].

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The long-term safety of the disposal of nuclear waste is an important issue in all countries with a significant nuclear program. Repositories for the disposal of high-level and long-lived radioactive waste generally rely on a multi-barrier system to isolate the waste from the biosphere. The multi-barrier system typically comprises the natural geological barrier provided by the repository host rock and its surroundings and an engineered barrier system, i.e. engineered materials placed within a repository, including the waste form, waste canisters, buffer materials, backfill and seals. One of the major issues in the safety of a deep geological repository for radioactive waste is the migration of hydrogen resulting mainly from anaerobic metal corrosion and from water and waste radiolysis, see for instance [64].

The mathematical analysis of the system describing the flow of two incompressible immiscible fluids in porous media is quite understood. Existence, uniqueness of weak solutions to these equations, and their regularity has been shown under various assumptions on physical data; see for instance [2, 12, 14, 21, 25, 26, 27, 41, 53] and the references therein. However, as reported in [9], the situation is quite different for immiscible compressible two-phase flow in porous media, where, only recently few results have been obtained. In the case of immiscible two-phase flows with one (or more) compressible fluids without any exchange between the phases, some approximate models were studied in [42, 43, 44]. Namely, in [42] certain terms related to the compressibility are neglected, and in [43, 44] the mass densities are assumed not to depend on the physical pressure, but on Chavent's global pressure. In the articles [23, 45, 50, 51], a more general immiscible compressible two-phase flow model in porous media is considered for fields with a single rock type and [9] treated the case with several types of rocks. Lastly, a compressible two-phase **two-component** flow in porous media in low solubility regime was studied in [49].

The numerical modeling and analysis of two-phase flow in porous media has been a problem of interest for many years and many methods have been developed. There is an extensive literature on this subject. We will not attempt a literature review here, but merely mention a few references. We refer to the books [15, 25, 28, 48] and the references therein. For a recent review, we refer for instance to [30, 31]. For simplicity of exposition, our focus here is on the cell-centred finite volume method, following [37].

Finite volume methods have long been popular in reservoir engineering owing to their numerous advantages: they meet the industrial constraints of robustness and low computational cost, they satisfy local conservation, are simple to code, and can be used on a large variety of meshes. The classical cell-centred Two-Point Flux Approximation (TPFA) is the most widely used technique for discretizing Darcy's law in commercial reservoir simulators. The prevalence of that method within the oil-and-gas industry mostly stems from its simple implementation, intuitive understanding, high execution speed, and robustness but its consistency requires strong orthogonality conditions on the mesh. Multi-Point Flux Approximations (MPFA) extend TPFA to consistent discretizations on general meshes with anisotropic heterogeneous media [1, 32].

Concerning the convergence study of the numerical approximation of the solution of the flow of two incompressible immiscible fluids in porous media, it has been the object of several studies during the past decades. We refer for instance to [20, 22, 34, 35, 36, 38, 55, 63] and the references therein. Later the convergence study to compressible flow of the "phase-by-phase" upstream weighting scheme was extended in [16, 60] in the case of a homogeneous domain. Then similar works have been done in [39, 61, 62] for a partially miscible compressible two-phase two component flow model. Lastly, the convergence of combined finite volume-finite element schemes for compressible two-phase flows in homogeneous and anisotropic porous media were studied in [46, 47, 59]. Closer to the present problem, a convergence of a combined mixed finite element and vertex centred finite volume method for immiscible compressible flow in heterogeneous porous media was obtained in [33].

The model of two-phase flow in porous media consists of the usual equations derived from the mass conservation of both fluids along with the Darcy-Muskat and the capillary pressure laws. There have been two main approaches to modeling such problem for immiscible incompressible two-phase flow. The first one, the problem is written in terms of the phase formulation, i.e. the saturation of one phase and the pressure of the second phase are primary unknowns. The second one, it has been shown that these equations can be written in a fractional flow formulation, i.e., in terms of a global pressure and saturation [12, 25]. All the aforementioned works concerning the convergence study for immiscible incompressible two-phase flow used the phase formulation and the fractional flow formulation. For the compressible model, the phase formulation is used and the notion of the global pressure as defined for the incompressible model is used as a tool in the convergence proof.

The global pressure for compressible two-phase flow is quite different from the case of incompressible one. Indeed, in the incompressible case the global pressure is defined from the phase pressures and the saturation of a phase by a simple algebraic relation, while in the compressible case it requires a solution of an ordinary differential equation (ODE). The fractional flow formulation for compressible two-phase flow employs the saturation of one of the phases and the global pressure as independent variables. This formulation, derived in [3, 4] without any simplifying assumptions, is fully equivalent to the original phase equations formulation. The fractional flow approach treats the two-phase flow problem as a total fluid flow of a single mixed fluid, and then describes the individual phases as fractions of the total flow. This approach leads to a less strong coupling between the two coupled equations: the global pressure equation and the saturation equation. The fractional flow formulation leads to a coupled system which consists of a nonlinear parabolic equation (the global pressure equation) and a nonlinear diffusion–convection one (the saturation equation). Further, it has been proven that this fractional flow approach is suitable for mathematical and numerical simulation; for more details, see [5, 6, 7]. Let us also mention that a fully equivalent global pressure formulation for three-phase compressible flows was established in [24] and validated by numerical results in [29].

In this article, we focus our attention on the study of immiscible, compressible two-phase flow in porous media taking into account gravity, capillary effects, and heterogeneity using the classical engineering model that is used in many petroleum engineering simulators. The fractional flow formulation described above has the central role in the convergence proof since it is essential for the basic energy estimate derivation. The results obtained earlier in [38] for the incompressible case and in [60] for the compressible case are revisited. The main goal is to incorporate some of the most recent improvements in the scheme and the convergence of the numerical approximation to the weak solution of such models. Let us mention that the main difficulties related to the mathematical analysis of such equations are the degeneracy caused by the fact that the phase mobility and time derivative vanish when the corresponding phase is missing. The common approach for solving this type of degeneracy is the transition to the fractional flow formulation which introduces new types of degeneracy, the degeneracy of the diffusion term in the saturation equation, and the degeneracy of the temporal term in the global pressure equation. Despite this degeneracy, the fractional flow formulation is suitable for energy estimate derivation, unlike the formulation based on the phase pressures.

The present paper has several objectives. First, we will outline a new strategy for handling the upwinding in the classical cell-centred TPFA “phase-by-phase” upstream weighting scheme. The second objective of this paper is to present a new proof of the convergence of this scheme based on the concept of the global pressure as defined in [3, 4] for immiscible compressible flow in heterogeneous porous media. Lastly, we have developed and implemented this scheme in a new module in the context of the parallel open source platform DuMu^X [52]. The overall objective of this part is the development of a new-generation framework and reservoir simulator suitable for

massively parallel processors.

The rest of the paper is organized as follows. Section 2 is devoted to the statement of the problem. Namely, in this section we introduce the system of equations describing immiscible compressible two-phase flow in porous media on a reservoir scale. Then we introduce the notion of the global pressure for compressible two-phase flow. Then we formulate the main assumptions on the data. Finally, we give the definition of a weak solution to our problem. In Section 3 we recall the general FV framework and formulate the fully coupled fully implicit cell-centered FV scheme that will be studied. Several auxiliary results including the discrete maximum principle, that will be used in the energy estimates for the scheme, are proven in Section 4. In Section 5, we first establish some energy estimates followed by the existence of discrete solutions to the FV scheme and we recall a compactness result which will be used for the convergence of the numerical scheme. Finally, in Section 6 we pass to the limit in the discrete equations, as discretization parameters go to zero, and we find the weak solution to the continuous two-phase flow model, which completes the convergence proof. [Let us note that to shorten the proof, some technical parts are omitted in this paper. However, detailed convergence analysis can be found in \[58\].](#) In Section 7, a description of the implementation of our strategy in DuMu^X is given. Then, to validate our approach, we consider two test cases, for which numerical results are exhibited by comparison with published results. The first test case is a 2D benchmark exercise [10], named Couplex-Gaz launched by the French Agency for the Management of Radioactive Waste (ANDRA), for modeling waste-generated gas flow systems. The second test case from [56] concerns the injection of CO₂ in a 3D homogeneous porous domain fully saturated with water. Finally, some concluding remarks and perspectives are presented in Section 8.

2 Statement of the problem

In this section we formulate the studied problem. First, in subsection 2.1 we introduce the system of equations that describes isothermal immiscible compressible two-phase flow in a porous medium. Then in subsection 2.2 we define the so-called global pressure for compressible flow. Subsection 2.3 provides the main assumptions on the data. Finally, in subsection 2.4 we give the definition of a weak solution to our problem.

2.1 Governing equations

We consider the flow of two immiscible compressible fluids in a porous reservoir Ω subset of \mathbb{R}^l , $l = 2$, or 3 . [We set \$Q_T = \Omega \times \(0, T\)\$ where \$T > 0\$ is a fixed time and we assume that \$\Omega\$ is a polyhedral domain. Its Lipschitz continuous boundary \$\partial\Omega\$ is divided in two parts \$\partial\Omega = \Gamma_N \cup \Gamma_D\$.](#) Standard flow models consist of equations for mass conservation and the multiphase extension of Darcy's law for fluid flow in porous media (see, e.g., [48]):

$$\Phi \partial_t(\rho_n(p_n)S_n) - \operatorname{div}(\lambda_n(S_w)\rho_n(p_n)\mathbb{K}(\nabla p_n - \rho_n(p_n)\mathbf{g})) = F_n, \quad (1)$$

$$\Phi \partial_t(\rho_w(p_w)S_w) - \operatorname{div}(\lambda_w(S_w)\rho_w(p_w)\mathbb{K}(\nabla p_w - \rho_w(p_w)\mathbf{g})) = F_w, \quad (2)$$

where Φ is the porosity and \mathbb{K} is the absolute permeability of the porous medium, \mathbf{g} being the gravity vector, and S_α , p_α , ρ_α , λ_α , and F_α are respectively saturation, pressure, density, mobility, and source term of the phase $\alpha = w$ (wetting phase), n (nonwetting phase).

The system is completed by no void space assumption, $S_w + S_n = 1$, and by the capillary pressure law $p_c(S_w) = p_n - p_w$.

The boundary conditions are imposed as follows. On Γ_N the fluxes satisfy a homogeneous Neumann boundary condition:

$$\begin{aligned} \lambda_n(S_w)\rho_n(p_n)\mathbb{K}(\nabla p_n - \rho_n(p_n)\mathbf{g}) \cdot \mathbf{n} &= 0, \\ \lambda_w(S_w)\rho_w(p_w)\mathbb{K}(\nabla p_w - \rho_w(p_w)\mathbf{g}) \cdot \mathbf{n} &= 0, \end{aligned} \quad \text{on } \Gamma_N \times (0, T), \quad (3)$$

while on Γ_D the pressures satisfy a homogeneous Dirichlet boundary condition:

$$p_n(x, t) = 0, \quad p_w(x, t) = 0, \quad \text{on } \Gamma_D \times (0, T). \quad (4)$$

The sources and sinks in the model, F_w and F_n , are taken in the following simple form:

$$F_w = \rho_w(p_w)(S_w^I F_I - S_w F_P), \quad F_n = \rho_n(p_n)(S_n^I F_I - S_n F_P), \quad (5)$$

where $F_I \geq 0$ is the injection rate and $F_P \geq 0$ is the production rate. Note that the injection values of phase saturation S_w^I and S_n^I , $S_w^I + S_n^I = 1$, are known but the pressures are given by the reservoir pressures.

Finally, the initial conditions are given by

$$p_n(0, x) = p_n^0(x), \quad p_w(0, x) = p_w^0(x), \quad x \in \Omega. \quad (6)$$

2.2 Global pressure and useful relations

In this article we rely on the global pressure variable p which is introduced in [3, 4] and it is related to the wetting phase pressure p_w by the following integral equation

$$p_w(S_w, p) = p - \int_1^{S_w} \hat{f}_n(s, p) p'_c(s) ds, \quad p_n(S_w, p) = p_w(S_w, p) + p_c(S_w). \quad (7)$$

The fractional flow function f_n of the nonwetting phase is defined as usual by

$$f_n(S_w, p_n) = \rho_n(p_n)\lambda_n(S_w)/\lambda(S_w, p_n), \quad \lambda(S_w, p_n) = \rho_w(p_w)\lambda_w(S_w) + \rho_n(p_n)\lambda_n(S_w), \quad (8)$$

and $\hat{f}_n(S_w, p) = f_n(S_w, p_n(S_w, p))$. The fractional flow function f_w of the wetting phase is given by $f_w = 1 - f_n$ and $\hat{f}_w(S_w, p) = f_w(S_w, p_n(S_w, p))$. The integral equation in (7) corresponds to a Cauchy problem for the ODE in which the global pressure p is just a parameter giving the value at $S_w = 1$. Under assumptions (A.3)-(A.5) this problem defines a unique function $p_w(S_w, p)$, see [3, 4].

Between the gradients of the phase pressures and the gradient of the global pressure, the following relation holds

$$\nabla p_n = \omega(S_w, p)\nabla p + \hat{f}_w(S_w, p)\nabla p_c(S_w), \quad (9)$$

$$\nabla p_w = \omega(S_w, p)\nabla p - \hat{f}_n(S_w, p)\nabla p_c(S_w), \quad (10)$$

where the function $\omega(S_w, p)$ is given by

$$\omega(S_w, p) = \frac{\partial p_n(S_w, p)}{\partial p} = \frac{\partial p_w(S_w, p)}{\partial p}. \quad (11)$$

It should be noted that [this formulation](#) for compressible flows requires to solve a family of ODE which could numerically be done by using standard libraries existing in the literature, for more details see [3, 4].

Let us mention that for incompressible flows, the global pressure introduced in [12, 25] is defined as follows:

$$p = p_w + \int_1^{S_w} \frac{\lambda_n(s)}{\lambda_w(s) + \lambda_n(s)} p'_c(s) ds,$$

which is an algebraic equation while the global pressure in the compressible case is defined by an ODE (7).

The degeneracy of the two-phase flow system leads us to replace the saturation S_w with suitably defined saturation potential $\beta(S_w)$,

$$\beta(S_w) = \int_0^{S_w} \lambda_w(s) \lambda_n(s) p'_c(s) ds, \quad (12)$$

which leads to the following relation between the gradients of the phase pressures and the gradient of the global pressure (9), (10)

$$\lambda_n(S_w) \rho_n(p_n) \nabla p_n = \lambda_n(S_w) \rho_n(p_n) \omega(S_w, p) \nabla p + \tilde{\alpha}(S_w, p) \nabla \beta(S_w), \quad (13)$$

$$\lambda_w(S_w) \rho_w(p_w) \nabla p_w = \lambda_w(S_w) \rho_w(p_w) \omega(S_w, p) \nabla p - \tilde{\alpha}(S_w, p) \nabla \beta(S_w), \quad (14)$$

where we define the function $\tilde{\alpha}(S_w, p)$ by

$$\tilde{\alpha}(S_w, p) = \frac{\rho_n(p_n(S_w, p)) \rho_w(p_w(S_w, p))}{\lambda(S_w, p)}. \quad (15)$$

2.3 Main assumptions

The main assumptions on the data are as follows:

- (A.1) The porosity Φ belongs to $L^\infty(\Omega)$, and there exist constants $\Phi_M \geq \Phi_m > 0$, such that $\Phi_m \leq \Phi(x) \leq \Phi_M$ a.e. in Ω a polyhedral domain of \mathbb{R}^l , $l = 2$, or 3 .
- (A.2) The absolute permeability $\mathbb{K} = k(x)\mathbb{I}$, $k \in L^\infty(\Omega)$, is a piecewise continuous function with finitely many surfaces of discontinuity of finite $(l - 1)$ dimensional measure (see also Definition 3.1, item vi). Moreover, there exist constants $k_M \geq k_m > 0$ such that $k_m \leq k(x) \leq k_M$ a.e. in Ω .
- (A.3) The relative mobilities λ_w, λ_n are Lipschitz continuous functions from $[0, 1]$ to \mathbb{R}^+ , $\lambda_w(S_w = 0) = 0$ and $\lambda_n(S_n = 0) = 0$; λ_α is a nondecreasing function of S_α for $\alpha = w, n$. Moreover, there exist constants $\lambda_M \geq \lambda_m > 0$ such that for all $s \in [0, 1]$

$$0 < \lambda_m \leq \lambda_w(s) + \lambda_n(s) \leq \lambda_M. \quad (16)$$

- (A.4) The capillary pressure function $p_c \in C^1([0, 1])$ is a monotone decreasing function.
- (A.5) ρ_n and ρ_w are $C^1(\mathbb{R})$ increasing functions, and there are constants $\rho_m, \rho_M, \rho_M^d > 0$ such that for all $p \in \mathbb{R}$ it holds $\rho_m \leq \rho_\alpha(p) \leq \rho_M$, $\rho'_\alpha(p) \leq \rho_M^d$, $\alpha = w, n$.
- (A.6) $F_P, F_I \in L^2(Q_T)$, $p_w^0, S_w^0 \in L^2(\Omega)$ with $0 \leq S_w^0 \leq 1$ and $p_n^0 = p_w^0 + p_c(S_w^0)$.
- (A.7) The inverse of the function $\beta(S_w)$ is a Hölder continuous function of order $\tau \in (1/2, 1)$, which can be written as (for some positive constant $C \geq 0$)

$$C \left| \int_{S_1}^{S_2} \lambda_w(s) \lambda_n(s) p'_c(s) ds \right|^\tau \geq |S_1 - S_2|. \quad (17)$$

The assumptions (A.1)–(A.7) are classical and physically meaningful for two-phase flow in porous media. They are similar to the assumptions made in [5, 42] that dealt with the existence of a weak solution.

Remark 2.1. In [4] it has been shown that due to the assumptions (A.4) and (A.5) there exist constants ω_m, ω_M such that for all $S \in [0, 1]$ and $p \in \mathbb{R}$, it holds $0 < \omega_m \leq \omega(S, p) \leq \omega_M < +\infty$.

Remark 2.2. From (7) and (A.4) it easily follows that there is a constant $M > 0$ such that $p - M \leq p_w \leq p$, $p \leq p_n \leq p + M$.

2.4 Definition of a weak solution

In order to define a weak solution to our problem, we introduce the following Sobolev space:

$$V = \{u \in H^1(\Omega); u = 0 \text{ on } \Gamma_D\}.$$

We give below a definition of a weak solution to our problem, see for instance [51].

Definition 2.3. Let (A.1)–(A.7) hold true and assume $(p_n^0, p_w^0) \in L^2(\Omega) \times L^2(\Omega)$, $0 \leq S_w^0 \leq 1$ a.e. $\in \Omega$. Then the pair (p_n, p_w) is a weak solution to problem (1), (2), (3), (4) and (6) satisfying

$$\begin{aligned} p_\alpha &\in L^2(0, T; L^2(\Omega)), \quad \sqrt{\lambda_\alpha(S_w)} \nabla p_\alpha \in \left(L^2(0, T; L^2(\Omega))\right)^l, \quad p \in L^2(0, T; V), \\ 0 \leq S_w &\leq 1 \text{ a.e. in } Q_T, \quad \Phi \partial_t(\rho_n S_n), \Phi \partial_t(\rho_w S_w) \in L^2(0, T; V'), \\ \beta(S_w) - \beta(1) &\in L^2(0, T; V), \end{aligned}$$

such that: for all $\varphi \in C^1([0, T]; V)$ with $\varphi(T, \cdot) = 0$,

$$\begin{aligned} & - \int_0^T \Phi \rho_w(p_w) S_w \partial_t \varphi \, dx \, dt - \int_\Omega \Phi(x) \rho_w(p_w^0(x)) S_w^0(x) \varphi(0, x) \, dx \\ & + \int_{Q_T} [\lambda_w(S_w) \rho_w(p_w) \mathbb{K} \nabla p_w - \lambda_w(S_w) \rho_w^2(p_w) \mathbb{K} \mathbf{g}] \cdot \nabla \varphi \, dx \, dt \\ & + \int_{Q_T} \rho_w(p_w) S_w F_P \varphi \, dx \, dt = \int_{Q_T} \rho_w(p_w) S_w^I F_P \varphi \, dx \, dt; \end{aligned} \tag{18}$$

for all $\psi \in C^1([0, T]; V)$ with $\psi(T, \cdot) = 0$,

$$\begin{aligned} & - \int_0^T \Phi \rho_n(p_n) S_n \partial_t \psi \, dx \, dt - \int_\Omega \Phi(x) \rho_n(p_n^0(x)) (1 - S_w^0(x)) \psi(0, x) \, dx \\ & + \int_{Q_T} [\lambda_n(S_w) \rho_n(p_n) \mathbb{K} \nabla p_n - \lambda_n(S_w) \rho_n^2(p_n) \mathbb{K} \mathbf{g}] \cdot \nabla \psi \, dx \, dt \\ & + \int_{Q_T} \rho_n(p_n) S_n F_P \psi \, dx \, dt = \int_{Q_T} \rho_n(p_n) S_n^I F_P \psi \, dx \, dt. \end{aligned} \tag{19}$$

According to [51], this problem has at least one solution.

3 Finite volume discretization

We now introduce our notation and the general form of the FV approximations that will be considered in the rest of the paper. We formulate a fully coupled fully implicit cell-centered FV scheme for the spatial discretization and a first-order (backward Euler) scheme for the integration

in time. We consider the classical two-point flux discretization with “phase-by-phase” upwinding on an orthogonal mesh which is often used in the petroleum engineering simulators. The only difference between the scheme considered in this article and the classical petroleum engineering scheme is in the treatment of the gravity flux which we consider separately from the viscose flux and we use stabilization by upwinding with respect to the gravity. This modification behaves similarly to the classical scheme in practice and simplifies the convergence proof.

3.1 Mesh and discrete operators

In this subsection, we recall the definition of a FV mesh on $\Omega \times (0, T)$ according to the framework of [37].

Definition 3.1. (*Admissible mesh of Ω*) Let Ω be an open bounded connected polyhedral subset of \mathbb{R}^l , $l = 2$, or 3. An admissible FV mesh of Ω , denoted by \mathcal{T} , is given by a family of "control volumes", which are open polyhedral convex subsets of Ω , a family of subsets of $\overline{\Omega}$ contained in hyperplanes of \mathbb{R}^l , denoted by \mathcal{E} (these are edges (two-dimensional) or sides (three-dimensional) of the control volumes), with strictly positive $(l - 1)$ -dimensional measure, and a family of points $(x_K)_{K \in \mathcal{T}}$ satisfying the properties (i)–(v) from Definition 9.1 from [37].

We assume also the following property:

- vi) For any $L \in \mathcal{T}$, the absolute permeability $k|_L$ is a continuous function on L . The surfaces of discontinuity of $k(x)$ are, therefore, exactly represented in the mesh \mathcal{T} and they will be denoted by $\mathcal{E}_{\text{disc}} \subset \mathcal{E}_I = \{\sigma \in \mathcal{E}; \sigma \not\subseteq \partial\Omega\}$.

The mesh size is defined as $\text{size}(\mathcal{T}) = \sup\{\text{diam}(K), K \in \mathcal{T}\}$. We denote by $N(K)$ the set of neighboring volumes of K and with \mathcal{E}_K set of faces of K . For any $K \in \mathcal{T}$ and $\sigma \in \mathcal{E}$, $|K|$ is the l -dimensional Lebesgue measure of K , and $|\sigma|$ is the $(l - 1)$ -dimensional measure of σ . If the K and L are two control volumes we denote by $d_{K|L}$ distance between x_K and x_L ; for $\sigma \in \mathcal{E}_K$ by $d_{K,\sigma}$ we denote distance between x_K and σ . For shorter notation we use the transmissibility $\tau_{K|L} = |\sigma_{K|L}|/d_{K|L}$ and $\tau_{K,\sigma} = |\sigma|/d_{K,\sigma}$.

In the set of edges $\sigma \in \mathcal{E}$ included in the boundary $\partial\Omega$ we distinguish subsets \mathcal{E}_D and \mathcal{E}_N , such that $\Gamma_D = \cup_{\sigma \in \mathcal{E}_D} \sigma$ and $\Gamma_N = \cup_{\sigma \in \mathcal{E}_N} \sigma$. In order to simplify the treatment of the Dirichlet boundary conditions we will use the notation of the ghost volume attached to the Dirichlet side $\sigma \in \mathcal{E}_D$. The ghost volume has the Dirichlet values of the phase pressures attached to it, that is for the ghost volume L we set $p_{w,L} = p_{n,L} = 0$. By $N_D(K) \supseteq N(K)$ we denote the set of all neighboring volumes of K , including possible ghost volumes.

For the mesh we also assume the following regularity

$$\begin{aligned} \exists \gamma > 0 \quad \forall h \quad \forall K \in \mathcal{T} \quad \forall L \in N(K) \quad \text{diam}(K) + \text{diam}(L) &\leq \gamma d_{K|L}, \\ \exists \zeta > 0 \quad \forall K \in \mathcal{T}, \forall \sigma \in \mathcal{E}_K \quad d_{K,\sigma} &\geq \zeta d_\sigma, \end{aligned} \tag{20}$$

where

$$d_\sigma = \begin{cases} d_{K|L} & \text{if } \sigma \not\subseteq \partial\Omega \\ d_{K,\sigma} & \text{if } \sigma \subseteq \partial\Omega \end{cases}.$$

3.2 Approximation spaces

In this subsection, we focus on the following discrete function spaces that will be used. We denote by $H_h(\Omega)$ the space of functions from $L^2(\Omega)$ which are piecewise constants on each $K \in \mathcal{T}$, and for

function $u_h \in H_h(\Omega)$ we denote the constant value of u_h on K by u_K . For $(u_h, v_h) \in (H_h(\Omega))^2$, the inner product is defined in the following way (see for instance [60])

$$\langle u_h, v_h \rangle_{H_h} = \frac{l}{2} \sum_{K \in \mathcal{T}} \sum_{L \in N(K)} \tau_{K|L} (u_L - u_K)(v_L - v_K) + l \sum_{K \in \mathcal{T}} \sum_{\sigma \in \partial K \cap \Gamma_D} \tau_{K,\sigma} u_K v_K.$$

The norm in $H_h(\Omega)$ is defined by $\|u_h\|_{H_h(\Omega)} = (\langle u_h, u_h \rangle_{H_h})^{1/2}$.

We denote by $L_h(\Omega)$ the space of functions from $L^2(\Omega)$ which are piecewise constants on each $K \in \mathcal{T}$, with the inner product and the norm

$$(u_h, v_h)_{L_h} = \sum_{K \in \mathcal{T}} |K| u_K v_K, \quad \|u_h\|_{L_h(\Omega)}^2 = \sum_{K \in \mathcal{T}} |K| |u_K|^2. \quad (21)$$

The discrete gradient $\nabla_h u_h$ of a function u_h is defined on the dual mesh (see [11]) in which the control volumes are attached to the sides $\sigma \in \mathcal{E}$. To the interface $\sigma_{K|L}$ we associate the volume $T_{K|L}$ constructed as a diamond upon $\sigma_{K|L}$ with x_K and x_L as vertices; to $\sigma \in \mathcal{E}_K$, $\sigma \subset \partial\Omega$, we associate the volume $T_{K,\sigma}$ constructed as a diamond upon σ with x_K as a vertex. The l -dimensional measure of $T_{K|L}$ and $T_{K,\sigma}$ is respectively equal to $|T_{K|L}| = |\sigma_{K|L}| d_{K|L} / l$ and $|T_{K,\sigma}| = |\sigma| d_{K,\sigma} / l$.

The discrete gradient $\nabla_h u_h$ is defined as a function constant by dual volumes, in the following way:

$$\nabla_h u_h(x) = \begin{cases} l \frac{u_L - u_K}{d_{K|L}} \eta_{K|L} & \text{if } x \in T_{K|L}, \\ l \frac{u_\sigma - u_K}{d_{K,\sigma}} \eta_{K|\sigma} & \text{if } x \in T_{K,\sigma}, \sigma \subset \Gamma_D, \\ 0 & \text{if } x \in T_{K,\sigma}, \sigma \subset \Gamma_N, \end{cases} \quad (22)$$

where $\eta_{K|\sigma}$ and $\eta_{K|L}$ are unit normals to σ and $\sigma_{K|L}$ respectively, directed outside of the volume K . It is easy to show that $\|\nabla_h u_h\|_{L^2(\Omega)} = \|u_h\|_{H_h(\Omega)}$. In order to make the notation more uniform, for the ghost cell L connected to the volume K by the side σ we will denote the distance $d_{K,\sigma}$ by $d_{K|L}$. With this convention we can write

$$\nabla_{K|L} u_h := (\nabla_h u_h)|_{T_{K|L}} = l \frac{u_L - u_K}{d_{K|L}} \eta_{K|L},$$

which is valid for interior and the Dirichlet sides.

In sequel, we will use a discrete Poincaré inequality, see e.g. [17, 37]:

Lemma 3.2. (*Discrete Poincaré inequality*) *Let Ω be an open bounded polyhedral subset of \mathbb{R}^l , $l = 2$, or 3 , \mathcal{T} an admissible FV mesh in the sense of Definition 3.1, satisfying (20), and $u \in H_h(\Omega)$. Then*

$$\|u\|_{L^2(\Omega)} \leq C(\Omega) \|u\|_{H_h(\Omega)},$$

where the constant $C(\Omega)$ depends only on Ω .

Remark 3.3. *The first constraint on the family of meshes $(\mathcal{T}_h)_h$ in (20) is used in the compactness proof (see [11]) in order to estimate the discrete gradient of the piecewise constant function $u_h = (u_K)_{K \in \mathcal{T}_h}$ with $u_K = \frac{1}{|K|} \int_K u(x) dx$ for $u \in W^{1,\infty}(\Omega)$ by*

$$\|\nabla_h u_h\|_{L^2(\Omega)} \leq C \|\nabla u\|_{L^\infty(\Omega)}.$$

The second constraint on the family of meshes $(\mathcal{T}_h)_h$ is used in the proof of the discrete Poincaré inequality (see [17, 37]).

A time discretization on the interval $(0, T)$ is given by an integer N , the time step $\delta t = T/N$ and a sequence of time points $t^i = i\delta t$, $i \in \{0, 1, \dots, N\}$, with $t^N = T$. The FV discretization of $\Omega \times (0, T)$, denoted by D , consists of an admissible mesh \mathcal{T} of Ω and a time discretization on interval $(0, T)$, $D = D(\mathcal{T}, N, \delta t, \{t^i\}_{i=0}^N)$. We define $\text{size}(D) = \max(\text{size}(\mathcal{T}), \delta t)$, and we will write $D = D_h$, where $h = \text{size}(D)$.

We denote by $X(\mathcal{T}, \delta t)$ the set of functions u from $\Omega \times (0, T)$ to \mathbb{R} such that there exists a family of values $\{u_K^i, K \in \mathcal{T}, i = 0, 1, \dots, N\}$ satisfying

$$u(x, t) = u_K^{i+1} \text{ for } x \in K \text{ and } t \in (i\delta t, (i+1)\delta t].$$

For a function $u \in X(\mathcal{T}, \delta t)$ we define the discrete $L^2(0, T; V)$ norm as follows

$$\|u\|_{L^2(0, T; H_h(\Omega))}^2 = \sum_{i=0}^{N-1} \delta t \left(\frac{l}{2} \sum_{K \in \mathcal{T}} \sum_{L \in N(K)} \tau_{K|L} |u_L^{i+1} - u_K^{i+1}|^2 + l \sum_{K \in \mathcal{T}} \sum_{\sigma \in \partial K \cap \Gamma_D} \tau_{K, \sigma} |u_K^{i+1}|^2 \right).$$

The following lemma gives the discrete integration by parts formula.

Lemma 3.4. *Let $\varphi \in (C^1(\overline{Q}_T))^l$ be a function equal to zero on the Neumann boundary Γ_N . Then there exists a constant C depending only on φ and Ω such that for all $p_h \in L^2(0, T; H_h(\Omega))$ it holds,*

$$E_h = \left| \int_0^T \int_{\Omega} \nabla_h p_h \cdot \varphi \, dx dt + \int_0^T \int_{\Omega} p_h \, \text{div} \varphi \, dx dt \right| \leq Ch \left(\|p_h\|_{L^2(0, T; H_h(\Omega))}^2 + 1 \right). \quad (23)$$

The proof is similar to the one in Proposition 6.1. in [16], therefore it is omitted here.

Remark 3.5. *In order to simplify notation when applying gathering by the edges we introduce the following notation. Let $F_{K|L} \in \mathbb{R}$ for $K \in \mathcal{T}$, $L \in N_D(K)$ has the property $F_{K|L} = -F_{L|K}$ if $L \in N(K)$ and let φ be a piecewise constant function on Ω , precisely $\varphi(x) = \varphi_K$, $x \in K$. We also assume that $\varphi_L = 0$ for ghost elements L . Then we have*

$$\sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} |\sigma_{K|L}| F_{K|L} \varphi_K = \frac{1}{2} \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} |\tilde{\sigma}_{K|L}| F_{K|L} (\varphi_K - \varphi_L).$$

where

$$|\tilde{\sigma}_{K|L}| = \begin{cases} |\sigma_{K|L}| & \text{if } L \in N(K) \\ 2|\sigma| & \text{if } \sigma \in \partial K \cap \Gamma_D. \end{cases}$$

Using this definition we also introduce $\tilde{\tau}_{K|L} = |\tilde{\sigma}_{K|L}|/d_{K|L}$ and $|\tilde{T}_{K|L}| = |\tilde{\sigma}_{K|L}|d_{K|L}/l$ to simplify the norm in $H_h(\Omega)$.

3.3 Fully implicit finite volume scheme

In this subsection, we provide a description of the fully coupled fully implicit FV scheme for the system modeling immiscible compressible two-phase flow in heterogeneous porous media. It is based on the ‘‘phase-by-phase’’ upwind discretization of the two-phase flow equations. We refer for instance to [13, 19, 40, 54] and the references therein.

The system (1)–(2) is discretized by the two-point cell-centered FV scheme with implicit Euler’s time discretization. The phase mobilities λ_α on the interface $\sigma_{K|L}$ are approximated by an upwind scheme with respect to the corresponding phase pressure:

$$\lambda_{\alpha, K|L}^{up, i} = \begin{cases} \lambda_\alpha(S_{w, K}^i) & \text{if } p_{\alpha, K}^i - p_{\alpha, L}^i \geq 0 \\ \lambda_\alpha(S_{w, L}^i) & \text{if } p_{\alpha, K}^i - p_{\alpha, L}^i < 0 \end{cases} \quad \alpha = w, n. \quad (24)$$

The gradients ∇p_α on the edge $\sigma_{K|L}$ are approximated by the two-point approximation, and the phase mass densities are also approximated by the upwind approximation with respect to the corresponding phase pressure:

$$\rho_{\alpha,K|L}^{up,i} = \begin{cases} \rho_\alpha(p_{\alpha,K}^i) & \text{if } p_{\alpha,K}^i - p_{\alpha,L}^i \geq 0 \\ \rho_\alpha(p_{\alpha,L}^i) & \text{if } p_{\alpha,K}^i - p_{\alpha,L}^i < 0 \end{cases} \quad \alpha = w, n. \quad (25)$$

For the energy estimates presented in Section 5 we will also need the harmonic mean approximation used in [60], and given by

$$\rho_{\alpha,K|L}^i = \begin{cases} (p_{\alpha,K}^i - p_{\alpha,L}^i) / \int_{p_{\alpha,L}^i}^{p_{\alpha,K}^i} \frac{d\sigma}{\rho_n(\sigma)} & \text{if } p_{\alpha,K}^i \neq p_{\alpha,L}^i \\ \rho_\alpha(p_{\alpha,K}^i) & \text{if } p_{\alpha,K}^i = p_{\alpha,L}^i \end{cases} \quad \alpha = w, n. \quad (26)$$

For the discretization of the mass density in the gravity term we will use weighted arithmetic mean:

$$\rho_{\alpha,K|L}^{G,i} = \frac{\rho_\alpha(p_{\alpha,K}^i)d_{K,\sigma} + \rho_\alpha(p_{\alpha,L}^i)d_{L,\sigma}}{d_{K|L}}, \quad g_{K|L} = \mathbf{g} \cdot \eta_{K|L}, \quad (27)$$

where $\eta_{K|L}$ is the K -outer unit normal vector to the edge $\sigma_{K|L}$. The phase mobilities in the gravity term are approximated by an upwind value with respect to the gravity:

$$\lambda_{\alpha,K|L}^{G,i} = \begin{cases} \lambda_\alpha(S_{w,K}^i) & \text{if } g_{K|L} \geq 0 \\ \lambda_\alpha(S_{w,L}^i) & \text{if } g_{K|L} < 0. \end{cases} \quad (28)$$

The absolute permeability is approximated by a function k_h that is defined on the dual mesh as in [37]. More precisely, on the dual volume $T_{K|L}$ the function k_h is equal to the weighted harmonic mean

$$k_{K|L} = \frac{d_{K|L}}{d_{K,\sigma}/k_K + d_{L,\sigma}/k_L}, \quad (29)$$

where the values k_K and k_L are defined as the mean values over the elements K and L respectively,

$$k_K = \frac{1}{|K|} \int_K k(x) dx.$$

The corresponding function from $L_h(\Omega)$ is denoted by k^h .

Remark 3.6. *In a standard way, one can prove $\|k - k^h\|_{L^2(\Omega)} \rightarrow 0$ as $h \rightarrow 0$. By using simple calculation we obtain*

$$\|k_h - k^h\|_{L^2(\Omega)}^2 \leq \|k\|_{L^\infty(\Omega)}^2 \sum_{K|L \in \mathcal{E}_{\text{disc}}} |T_{K|L}| + \sum_{K|L \notin \mathcal{E}_{\text{disc}}} |k_K - k_L|^2 |T_{K|L}|.$$

The first term on the right-hand side tends to zero as $h \rightarrow 0$ due to the finite measure of $\mathcal{E}_{\text{disc}}$, and the second term goes to zero due to the continuity of k outside of $\mathcal{E}_{\text{disc}}$. It follows that $\|k - k_h\|_{L^2(\Omega)} \rightarrow 0$ as $h \rightarrow 0$.

The FV scheme for the discretization of equations (1)–(2) with boundary conditions (3), (4), and initial conditions (6) is given by the following set of equations with the unknowns $(p_{w,K}^{i+1})_{K \in \mathcal{T}}$, $(p_{n,K}^{i+1})_{K \in \mathcal{T}}$, $(S_{n,K}^{i+1})_{K \in \mathcal{T}}$, and $(S_{w,K}^{i+1})_{K \in \mathcal{T}}$, $i \in \{0, 1, \dots, N-1\}$:

$$p_{n,K}^{i+1} - p_{w,K}^{i+1} = p_c(S_{w,K}^{i+1}), \quad S_{w,K}^{i+1} + S_{n,K}^{i+1} = 1, \quad (30)$$

$$\begin{aligned} |K|\Phi_K \frac{\rho_{n,K}^{i+1} S_{n,K}^{i+1} - \rho_{n,K}^i S_{n,K}^i}{\delta t} + \sum_{L \in N_D(K)} \tau_{K|L} k_{K|L} \lambda_{n,K|L}^{up,i+1} \rho_{n,K|L}^{up,i+1} (p_{n,K}^{i+1} - p_{n,L}^{i+1}) \\ + \sum_{L \in N_D(K)} |\sigma_{K|L}| k_{K|L} \lambda_{n,K|L}^{G,i+1} \left(\rho_{n,K|L}^{G,i+1} \right)^2 g_{K|L} = |K|F_{n,K}^{i+1}, \end{aligned} \quad (31)$$

$$\begin{aligned} |K|\Phi_K \frac{\rho_{w,K}^{i+1} S_{w,K}^{i+1} - \rho_{w,K}^i S_{w,K}^i}{\delta t} + \sum_{L \in N_D(K)} \tau_{K|L} k_{K|L} \lambda_{w,K|L}^{up,i+1} \rho_{w,K|L}^{up,i+1} (p_{w,K}^{i+1} - p_{w,L}^{i+1}) \\ + \sum_{L \in N_D(K)} |\sigma_{K|L}| k_{K|L} \lambda_{w,K|L}^{G,i+1} \left(\rho_{w,K|L}^{G,i+1} \right)^2 g_{K|L} = |K|F_{w,K}^{i+1}. \end{aligned} \quad (32)$$

For $\sigma_{K|L} \in \Gamma_N$ the Neumann boundary conditions are given by:

$$\lambda_{w,K|L}^{up,i+1} \rho_{w,K|L}^{up,i+1} (p_{w,K}^{i+1} - p_{w,L}^{i+1}) + \lambda_{w,K|L}^{G,i+1} \left(\rho_{w,K|L}^{G,i+1} \right)^2 g_{K|L} = 0, \quad (33)$$

$$\lambda_{n,K|L}^{up,i+1} \rho_{n,K|L}^{up,i+1} (p_{n,K}^{i+1} - p_{n,L}^{i+1}) + \lambda_{n,K|L}^{G,i+1} \left(\rho_{n,K|L}^{G,i+1} \right)^2 g_{K|L} = 0. \quad (34)$$

For $\sigma_{K|L} \in \Gamma_D$ the Dirichlet boundary condition is implemented by setting

$$p_{n,L}^{i+1} = 0, \quad p_{w,L}^{i+1} = 0 \quad (35)$$

in the ghost cell L . The initial conditions are given by

$$p_{w,K}^0 = \frac{1}{|K|} \int_K p_w^0(x) dx, \quad p_{n,K}^0 = \frac{1}{|K|} \int_K p_n^0(x) dx, \quad S_{w,K}^0 = p_c^{-1}(p_{n,K}^0 - p_{w,K}^0). \quad (36)$$

4 Preliminary results

In this section, we present a set of preliminary results, related to the global pressure, which are needed for the analysis of the scheme and the discrete maximum principle for the saturation.

As mentioned before, our approach to proof the convergence of the scheme (30)–(36) use the global pressure p defined in (7). For this we need to discretize the relations (9) and (10). In order to simplify notation we will denote S_w by S in this section.

The function ω is given by (11) and its approximation $\omega_{K|L}^i$ on edge $\sigma_{K|L}$ is given by

$$\omega_{K|L}^i = \begin{cases} \frac{p_w(S_{K|L}^i, p_K^i) - p_w(S_{K|L}^i, p_L^i)}{p_K^i - p_L^i} & \text{if } p_K^i \neq p_L^i \\ \frac{\partial p_w}{\partial p}(S_{K|L}^i, p_K^i) & \text{if } p_K^i = p_L^i. \end{cases} \quad (37)$$

In (37) we have denoted $\bar{S}_{K|L}^i = \frac{S_K^i + S_L^i}{2}$ and $S_{K|L}^i$ will be defined as $S_{K|L}^{gup,i}$ later in (40).

We want the equations that relate the global pressure gradient to the phase pressure gradients (9) and (10), to be valid in the discrete case too. Therefore we will use (9) and (10) to determine suitable approximation for the fractional flow functions f_n and f_w .

From (7) the wetting phase pressure p_w is defined for any S^i as

$$p_w(S^i, p_K^i) = p_K^i - \int_1^{S^i} \hat{f}_n(s, p_K^i) p_c'(s) ds. \quad (38)$$

Assuming the discrete version of equation (10) written as

$$p_{w,K}^i - p_{w,L}^i = \omega_{K|L}^i (p_K^i - p_L^i) - f_{n,K|L}^i (p_c(S_K^i) - p_c(S_L^i)),$$

we get the following expression for $f_{n,K|L}^i$:

$$f_{n,K|L}^i = \frac{1}{u_K^i - u_L^i} \left(\int_{S_{K|L}^i}^{S_K^i} \hat{f}_n(s, p_K^i) p_c'(s) ds - \int_{S_{K|L}^i}^{S_L^i} \hat{f}_n(s, p_L^i) p_c'(s) ds \right), \quad (39)$$

where we have denoted $u_K^i = p_c(S_K^i)$ and $u_L^i = p_c(S_L^i)$. Let us define the upwind value $S_{K|L}^{sup,i}$ with respect to the global pressure

$$S_{K|L}^{sup,i} = \begin{cases} S_K^i & \text{if } p_K^i - p_L^i \geq 0 \\ S_L^i & \text{if } p_K^i - p_L^i < 0, \end{cases} \quad (40)$$

and the corresponding upwind mobility as $\lambda_{\alpha,K|L}^{sup,i} = \lambda_\alpha(S_{K|L}^{sup,i})$ for $\alpha = w, n$. We set $S_{K|L}^i = S_{K|L}^{sup,i}$ in (39) and we get

$$f_{n,K|L}^i = \frac{1}{u_K^i - u_L^i} \int_{S_L^i}^{S_K^i} \hat{f}_n(s, p_{K|L}^i) p_c'(s) ds, \quad p_{K|L}^i = \min\{p_K^i, p_L^i\}. \quad (41)$$

In the limit $S_K^i = S_L^i = S$ we have $f_{n,K|L}^i = \hat{f}_n(S, p_{K|L}^i)$. By setting $f_{w,K|L}^i = 1 - f_{n,K|L}^i$, meaning

$$f_{w,K|L}^i = \frac{1}{u_K^i - u_L^i} \int_{S_L^i}^{S_K^i} \hat{f}_w(s, p_{K|L}^i) p_c'(s) ds, \quad p_{K|L}^i = \min\{p_K^i, p_L^i\}, \quad (42)$$

we obtain on the interface $\sigma_{K|L}$

$$p_{n,K}^i - p_{n,L}^i = \omega_{K|L}^i (p_K^i - p_L^i) + f_{w,K|L}^i (u_K^i - u_L^i). \quad (43)$$

We have proved the following result.

Proposition 4.1. *Assume that p_K^i and p_L^i are two given values of the global pressure, $u_K^i = p_c(S_K^i)$ and $u_L^i = p_c(S_L^i)$ are two given values of the capillary pressure. We denote by $p_{n,K}^i$, $p_{n,L}^i$, $p_{w,K}^i$, and $p_{w,L}^i$ the corresponding values of the nonwetting and the wetting phase pressures defined by (7). Then we have*

$$p_{n,K}^i - p_{n,L}^i = \omega_{K|L}^i (p_K^i - p_L^i) + f_{w,K|L}^i (u_K^i - u_L^i), \quad (44)$$

$$p_{w,K}^i - p_{w,L}^i = \omega_{K|L}^i (p_K^i - p_L^i) - f_{n,K|L}^i (u_K^i - u_L^i), \quad (45)$$

where $\omega_{K|L}^i$ is defined by (37) with $S_{K|L}^i = S_{K|L}^{sup,i}$ (see (40)); $f_{n,K|L}^i$ is given by (41), and $f_{w,K|L}^i = 1 - f_{n,K|L}^i$ (see (42)).

Next we present four auxiliary lemmas. The first one is an easy consequence of the monotonicity of the function ρ_α .

Lemma 4.2. For $\alpha \in \{w, n\}$ it holds $\rho_{\alpha, K|L}^{up, i} \geq \rho_{\alpha, K|L}^i$, where $\rho_{\alpha, K|L}^{up, i}$ is defined by (25) and $\rho_{\alpha, K|L}^i$ is defined by (26).

Lemma 4.3. With the same notation as in Proposition 4.1, we have the following estimates:

$$f_{w, K|L}^i(u_K^i - u_L^i)(p_K^i - p_L^i) \geq \hat{f}_w(S_{K|L}^{gup, i}, p_{K|L}^i)(u_K^i - u_L^i)(p_K^i - p_L^i), \quad (46)$$

$$f_{n, K|L}^i(u_K^i - u_L^i)(p_K^i - p_L^i) \leq \hat{f}_n(S_{K|L}^{gup, i}, p_{K|L}^i)(u_K^i - u_L^i)(p_K^i - p_L^i). \quad (47)$$

Proof. From the fact that the capillary pressure p_c is a nonincreasing function of s , f_w is a nondecreasing function of s , and f_n is a nonincreasing function of s it is easy to show that for all $p \in \mathbb{R}$, $S_K, S_L \in [0, 1]$ and $\alpha \in \{w, n\}$ it holds:

$$\hat{f}_\alpha(S_K, p)(u_K - u_L) \leq \int_{S_L}^{S_K} \hat{f}_\alpha(s, p) p'_c(s) ds \leq \hat{f}_\alpha(S_L, p)(u_K - u_L). \quad (48)$$

Using (42), (48), (40), and the monotonicity of the function $S \mapsto \hat{f}_w(S, p_{K|L}^i)$, we get

$$\begin{aligned} f_{w, K|L}^i(u_K^i - u_L^i)(p_K^i - p_L^i) &= \int_{S_L^i}^{S_K^i} \hat{f}_w(s, p_{K|L}^i) p'_c(s) ds (p_K^i - p_L^i) \\ &\geq \hat{f}_w(S_{K|L}^{gup, i}, p_{K|L}^i)(u_K^i - u_L^i)(p_K^i - p_L^i). \end{aligned}$$

The inequality (47) is proved in the same way. \square

The following lemma compares the ‘‘phase-by-phase’’ upwinding to the global pressure upwinding.

Lemma 4.4. For $\alpha \in \{w, n\}$ it holds $\lambda_{\alpha, K|L}^{up, i} \geq \lambda_{\alpha, K|L}^{gup, i}$.

Proof. Assume that $p_K^i - p_L^i \geq 0$ holds, which implies $\lambda_{\alpha, K|L}^{gup, i} = \lambda_\alpha(S_K^i)$, $\alpha = w, n$. Then it is not possible to have at the same time $p_{n, K}^i - p_{n, L}^i < 0$ and $p_{w, K}^i - p_{w, L}^i < 0$. Indeed, this follows from the equations (45) and (44) and the fact that $\omega_{K|L}^i(p_K^i - p_L^i) \geq 0$, $f_{n, K|L}^i \geq 0$, and $f_{w, K|L}^i \geq 0$. Therefore, we have three possibilities:

- i) $p_{w, K}^i - p_{w, L}^i \geq 0$ and $p_{n, K}^i - p_{n, L}^i \geq 0$. In this case all the upwind values are the same.
- ii) $p_{w, K}^i - p_{w, L}^i \geq 0$ and $p_{n, K}^i - p_{n, L}^i < 0$. In this case we have $\lambda_{n, K|L}^{up, i} = \lambda_n(S_L^i)$ and $\lambda_{w, K|L}^{up, i} = \lambda_w(S_K^i)$, and also $f_{w, K|L}^i(p_c(S_K^i) - p_c(S_L^i)) < 0$, and consequently using (A.4) we get $S_K^i > S_L^i$. Due to the monotonicity of the function λ_n one has

$$\lambda_{n, K|L}^{up, i} = \lambda_n(S_L^i) \geq \lambda_n(S_K^i) = \lambda_{n, K|L}^{gup, i}.$$

- iii) $p_{w, K}^i - p_{w, L}^i < 0$ and $p_{n, K}^i - p_{n, L}^i \geq 0$. In this case we have $\lambda_{n, K|L}^{up, i} = \lambda_n(S_K^i)$ and $\lambda_{w, K|L}^{up, i} = \lambda_w(S_L^i)$, and also $f_{n, K|L}^i(p_c(S_K^i) - p_c(S_L^i)) > 0$, and consequently using (A.4) we get $S_K^i < S_L^i$. Due to the monotonicity of λ_w one has

$$\lambda_{w, K|L}^{up, i} = \lambda_w(S_L^i) \geq \lambda_w(S_K^i) = \lambda_{w, K|L}^{gup, i}.$$

This proves the statement in the case $p_K^i - p_L^i \geq 0$. In the similar way one proves the statement in the case $p_K^i - p_L^i < 0$. \square

Lemma 4.5. *Let D_h be a FV discretization of $\Omega \times (0, T)$ and let assumptions (A.1)–(A.7) hold. Then the following inequality holds:*

$$\begin{aligned} & \lambda_{w,K|L}^{gup,i} \bar{\rho}_{w,K|L}^i (p_{w,K}^i - p_{w,L}^i)^2 + \lambda_{n,K|L}^{gup,i} \bar{\rho}_{n,K|L}^i (p_{n,K}^i - p_{n,L}^i)^2 \\ & \geq \rho_m \lambda_m \omega_m^2 (p_K^i - p_L^i)^2 + C_\beta (\beta(S_K^i) - \beta(S_L^i))^2, \end{aligned} \quad (49)$$

for all $K \in \mathcal{T}$, $L \in N(K)$, and $i \in \{1, \dots, N\}$, where we have denoted $\bar{\rho}_{\alpha,K|L}^i = \rho_\alpha(p_\alpha(S_{K|L}^{gup,i}, p_{K|L}^i))$, $\alpha \in \{w, n\}$. The constant C_β is given by $1/C_\beta = \frac{\rho_M^2 \lambda_M^2}{\rho_m^3} \max \left\{ \frac{1}{\mu_w}, \frac{1}{\mu_n} \right\}$.

Proof. After introducing (45) and (44) in the left side of (49) we obtain

$$\begin{aligned} & \lambda_{w,K|L}^{gup,i} \bar{\rho}_{w,K|L}^i (p_{w,K}^i - p_{w,L}^i)^2 + \lambda_{n,K|L}^{gup,i} \bar{\rho}_{n,K|L}^i (p_{n,K}^i - p_{n,L}^i)^2 \\ & = (\lambda_{n,K|L}^{gup,i} \bar{\rho}_{n,K|L}^i + \lambda_{w,K|L}^{gup,i} \bar{\rho}_{w,K|L}^i) (\omega_{K|L}^i)^2 (p_K^i - p_L^i)^2 \\ & + 2\omega_{K|L}^i \left(\lambda_{n,K|L}^{gup,i} \bar{\rho}_{n,K|L}^i f_{w,K|L}^i - \lambda_{w,K|L}^{gup,i} \bar{\rho}_{w,K|L}^i f_{g,K|L}^i \right) (p_K^i - p_L^i) (u_K^i - u_L^i) \\ & + \left(\lambda_{w,K|L}^{gup,i} \bar{\rho}_{w,K|L}^i (f_{n,K|L}^i)^2 + \lambda_{n,K|L}^{gup,i} \bar{\rho}_{n,K|L}^i (f_{w,K|L}^i)^2 \right) (u_K^i - u_L^i)^2. \end{aligned}$$

The first term on the right-hand side is straightforward to estimate. The second term can be neglected since from Lemma 4.3 we get

$$\begin{aligned} & 2\omega_{K|L}^i \left(\lambda_{n,K|L}^{gup,i} \bar{\rho}_{n,K|L}^i f_{w,K|L}^i - \lambda_{w,K|L}^{gup,i} \bar{\rho}_{w,K|L}^i f_{n,K|L}^i \right) (p_K^i - p_L^i) (u_K^i - u_L^i) \\ & \geq 2\omega_{K|L}^i \left(\lambda_{n,K|L}^{gup,i} \bar{\rho}_{n,K|L}^i \hat{f}_w(S_{K|L}^{gup,i}, p_{K|L}^i) - \lambda_{w,K|L}^{gup,i} \bar{\rho}_{w,K|L}^i \hat{f}_n(S_{K|L}^{gup,i}, p_{K|L}^i) \right) (p_K^i - p_L^i) (u_K^i - u_L^i) = 0. \end{aligned}$$

The third term is estimated as follows. From the monotonicity of the mobilities and using $S_{K|L}^{gup,i} \in \{S_K^i, S_L^i\}$ we get

$$\begin{aligned} (\beta(S_K^i) - \beta(S_L^i))^2 & \leq \lambda_w^2(S_{K|L}^{gup,i}) \left(\int_{S_L^i}^{S_K^i} \lambda_n(s) p'_c(s) ds \right)^2 + \lambda_n^2(S_{K|L}^{gup,i}) \left(\int_{S_L^i}^{S_K^i} \lambda_w(s) p'_c(s) ds \right)^2 \\ & \leq \frac{\lambda_w(S_{K|L}^{gup,i})}{\mu_w} \left(\int_{S_L^i}^{S_K^i} \lambda_n(s) p'_c(s) ds \right)^2 + \frac{\lambda_n(S_{K|L}^{gup,i})}{\mu_n} \left(\int_{S_L^i}^{S_K^i} \lambda_w(s) p'_c(s) ds \right)^2, \end{aligned}$$

and the estimate

$$\begin{aligned} (\beta(S_K^i) - \beta(S_L^i))^2 & \leq (1/C_\beta) \left\{ \bar{\rho}_{w,K|L}^i \lambda_w(S_{K|L}^{gup,i}) \left(\int_{S_L^i}^{S_K^i} \hat{f}_n(s, p_{K|L}^i) p'_c(s) ds \right)^2 \right. \\ & \quad \left. + \bar{\rho}_{n,K|L}^i \lambda_n(S_{K|L}^{gup,i}) \left(\int_{S_L^i}^{S_K^i} \hat{f}_w(s, p_{K|L}^i) p'_c(s) ds \right)^2 \right\}. \end{aligned}$$

This proves (49). \square

The discrete maximum principle for the saturation can be proved as in [60] and therefore we omit this part of the proof.

Lemma 4.6. (Maximum principle) *Let D_h be a FV discretization of $\Omega \times (0, T)$ and let $(p_{n,h}, p_{w,h})$ be a solution to the FV scheme (30)–(36). Assume that $(S_{w,K}^0)_{K \in \mathcal{T}} \in [0, 1]$. Then we have*

$$0 \leq S_{w,K}^i \leq 1, \quad \forall K \in \mathcal{T}, \quad \forall i \in \{0, \dots, N\}.$$

5 Energy estimates and compactness result

In this section we first present some energy estimates followed by the existence of discrete solutions to the FV scheme and a compactness result which will be used for the convergence of the numerical scheme. Similar works have already been done, for example, in [60] in the case of a homogeneous domain. Therefore, in the following proofs, we only insist on the new elements which appear in our study, mainly related to the use of [the formulation obtained by the global pressure for compressible flow concept](#).

The first main result of the section reads.

Theorem 5.1. *Let D_h be a FV discretization of $\Omega \times (0, T)$ and let $(p_{n,h}, p_{w,h})$ be a solution to the FV scheme (30)–(36). Then, there exists a constant $C > 0$, depending only on $\Omega, T, p_{w,h}^0, p_{n,h}^0, S_w^I, S_n^I, F_P, F_I$, such that the following estimates hold:*

$$\begin{aligned} & \sum_{K \in \mathcal{T}} |K| \Phi_K \mathcal{H}(p_{n,K}^N, p_{w,K}^N) - \sum_{K \in \mathcal{T}} |K| \Phi_K \mathcal{H}(p_{n,K}^0, p_{w,K}^0) \\ & + \frac{\lambda_m}{\rho_M} \frac{\rho_m \omega_m^2 k_m}{4} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} |p_K^{i+1} - p_L^{i+1}|^2 \\ & + \frac{C_\beta k_m}{4\rho_M} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} |\beta(S_K^{i+1}) - \beta(S_L^{i+1})|^2 \leq C, \end{aligned} \quad (50)$$

and

$$\begin{aligned} & \sum_{K \in \mathcal{T}} |K| \Phi_K \mathcal{H}(p_{n,K}^N, p_{w,K}^N) - \sum_{K \in \mathcal{T}} |K| \Phi_K \mathcal{H}(p_{n,K}^0, p_{w,K}^0) \\ & + \frac{\rho_m k_m}{4\rho_M} \sum_{\alpha \in \{w,n\}} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} \lambda_{\alpha,K|L}^{up,i+1} (p_{\alpha,K}^{i+1} - p_{\alpha,L}^{i+1})^2 \leq C, \end{aligned} \quad (51)$$

where we have denoted

$$\mathcal{H}(p_n, p_w) = S_w(\rho_w(p_w)g_w(p_w) - p_w) + S_n(\rho_n(p_n)g_n(p_n) - p_n) - \int_0^{S_w} p_c(s) ds \quad (52)$$

with C_β given in Lemma 4.5. The functions $g_w(p_w)$ and $g_n(p_n)$ are given by

$$g_w(p_w) = \int_0^{p_w} \frac{d\sigma}{\rho_w(\sigma)} \quad \text{and} \quad g_n(p_n) = \int_0^{p_n} \frac{d\sigma}{\rho_n(\sigma)}.$$

Proof. We use the functions $g_w(p_w)$ and $g_n(p_n)$ as the test functions in (31) and (32). By summing those two equations, multiplying by δt , and summing over all elements and all time levels we get

$$\begin{aligned} & \sum_{\alpha \in \{w,n\}} \sum_{i=0}^{N-1} \sum_{K \in \mathcal{T}} |K| \Phi_K (\rho_{\alpha,K}^{i+1} S_{\alpha,K}^{i+1} - \rho_{\alpha,K}^i S_{\alpha,K}^i) g_\alpha(p_{\alpha,K}^{i+1}) \\ & + \sum_{\alpha \in \{w,n\}} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} \tau_{K|L} k_{K|L} \lambda_{\alpha,K|L}^{up,i+1} \rho_{\alpha,K|L}^{up,i+1} (p_{\alpha,K}^{i+1} - p_{\alpha,L}^{i+1}) g_\alpha(p_{\alpha,K}^{i+1}) \\ & = - \sum_{\alpha \in \{w,n\}} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} |\sigma_{K|L}| k_{K|L} \lambda_{\alpha,K|L}^{G,i+1} (\rho_{\alpha,K|L}^{G,i+1})^2 g_{K|L} g_\alpha(p_{\alpha,K}^{i+1}) \end{aligned} \quad (53)$$

$$\begin{aligned}
& + \sum_{\alpha \in \{w,n\}} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{J}} |K| \rho_{\alpha}(p_{\alpha,K}^{i+1}) S_{\alpha,K}^{I,i+1} F_{I,K}^{i+1} g_{\alpha}(p_{\alpha,K}^{i+1}) \\
& - \sum_{\alpha \in \{w,n\}} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{J}} |K| \rho_{\alpha}(p_{\alpha,K}^{i+1}) S_{\alpha,K}^{i+1} F_{P,K}^{i+1} g_{\alpha}(p_{\alpha,K}^{i+1}).
\end{aligned}$$

In order to simplify notation we will write equation (53) as

$$A^1 + A^2 = A^3 + A^4 + A^5$$

where A^i are the successive terms in equation (53).

1. The accumulation term A^1 can be estimated from below in a standard way as in [60] to obtain

$$A^1 \geq \sum_{i=0}^{N-1} \sum_{K \in \mathcal{J}} |K| \Phi_K \left(\mathcal{H}(p_{n,K}^{i+1}, p_{w,K}^{i+1}) - \mathcal{H}(p_{n,K}^i, p_{w,K}^i) \right). \quad (54)$$

2. Gradient estimate. The term A^2 can be written as sums over all interior and Dirichlet's sides:

$$A^2 = \frac{1}{2} \sum_{\alpha \in \{w,n\}} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{J}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} \lambda_{\alpha,K|L}^{up,i+1} \rho_{\alpha,K|L}^{up,i+1} k_{K|L} \left(p_{\alpha,K}^{i+1} - p_{\alpha,L}^{i+1} \right) \left(g_{\alpha}(p_{\alpha,K}^{i+1}) - g_{\alpha}(p_{\alpha,L}^{i+1}) \right).$$

Due to the Lemma 4.2 and monotonicity of the functions g_{α} we can replace $\rho_{\alpha,K|L}^{up,i+1}$ by $\rho_{\alpha,K|L}^{i+1}$, for $\alpha \in \{w,n\}$ in A^2 . Then, from the definition of the mass densities on the interface (26) for $\alpha \in \{w,n\}$ we have

$$\rho_{\alpha,K|L}^{i+1} (g_{\alpha}(p_{\alpha,K}^{i+1}) - g_{\alpha}(p_{\alpha,L}^{i+1})) = p_{\alpha,K}^{i+1} - p_{\alpha,L}^{i+1},$$

which leads to

$$A^2 \geq \frac{1}{2} \sum_{\alpha \in \{w,n\}} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{J}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} k_{K|L} \lambda_{\alpha,K|L}^{up,i+1} (p_{\alpha,K}^{i+1} - p_{\alpha,L}^{i+1})^2. \quad (55)$$

By Lemma 4.4 we can replace the phase upwind mobilities $\lambda_{\alpha,K|L}^{up,i+1}$ by the global upwind mobilities $\lambda_{\alpha,K|L}^{gup,i+1}$. By introducing the factors $\bar{\rho}_{\alpha,K|L}^{i+1}/\rho_M \leq 1$ in terms of A^2 , from Lemma 4.5 it follows

$$\begin{aligned}
A^2 & \geq \frac{\rho_m \lambda_m \omega_m^2 k_m}{2\rho_M} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{J}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} (p_K^{i+1} - p_L^{i+1})^2 \\
& + \frac{C_{\beta} k_m}{2\rho_M} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{J}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} (\beta(S_{w,K}^{i+1}) - \beta(S_{w,L}^{i+1}))^2.
\end{aligned} \quad (56)$$

3. Note that $A^3 = A_w^3 + A_n^3$. Using Remark 3.5 and Proposition 4.1 for summand $\alpha = w$ we get

$$\begin{aligned}
A_w^3 & = \frac{1}{2} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{J}} \sum_{L \in N_D(K)} |\tilde{\sigma}_{K|L}| k_{K|L} \lambda_{w,K|L}^{G,i+1} \left(\rho_{w,K|L}^{G,i+1} \right)^2 g_{K|L} G_{w,K|L}^{i+1} \omega_{K|L} (p_L^{i+1} - p_K^{i+1}) \\
& - \frac{1}{2} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{J}} \sum_{L \in N_D(K)} |\tilde{\sigma}_{K|L}| k_{K|L} \lambda_{w,K|L}^{G,i+1} \left(\rho_{w,K|L}^{G,i+1} \right)^2 g_{K|L} G_{w,K|L}^{i+1} f_{n,K|L}^{i+1} (u_L^{i+1} - u_K^{i+1})
\end{aligned}$$

$$= A_I^3 + A_{II}^3,$$

where

$$G_{w,K|L}^{i+1} = \frac{g_w(p_{w,L}^{i+1}) - g_w(p_{w,K}^{i+1})}{p_{w,L}^{i+1} - p_{w,K}^{i+1}}, \quad 0 < \frac{1}{\rho_M} \leq G_{w,K|L}^{i+1} \leq \frac{1}{\rho_m}.$$

In order to estimate the term A_I^3 we use $|\tilde{\sigma}_{K|L}| = \sqrt{d_{K|L}|\tilde{\sigma}_{K|L}|} \frac{\sqrt{|\tilde{\sigma}_{K|L}|}}{\sqrt{d_{K|L}}}$ and the Cauchy-Schwarz inequality to obtain

$$A_I^3 \leq CT|\Omega| + \frac{\varepsilon}{2} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} |p_L^{i+1} - p_K^{i+1}|^2,$$

where $C = C(\lambda_M, \rho_M, \rho_m, |g|, \omega_M, k_M, \varepsilon)$, and ε is an arbitrary small parameter. After introducing the definition of $f_{n,K|L}^{i+1}$ into the term A_{II}^3 we obtain

$$A_{II}^3 = \frac{1}{2} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} |\tilde{\sigma}_{K|L}| k_{K|L} \lambda_{w,K|L}^{G,i+1} (\rho_{w,K|L}^{G,i+1})^2 g_{K|L} G_{w,K|L}^{i+1} \int_{S_{w,L}^{i+1}}^{S_{w,K}^{i+1}} \hat{f}_n(s, p_{K|L}^{i+1}) p'_c(s) ds.$$

In the case $g_{K|L} \geq 0$ we have $\lambda_{w,K|L}^{G,i+1} = \lambda_w(S_{w,K}^{i+1})$. If $S_{w,K}^{i+1} \geq S_{w,L}^{i+1}$ the term A_{II}^3 is nonpositive, so it can be neglected. If we have $S_{w,K}^{i+1} < S_{w,L}^{i+1}$, due to the monotonicity of the wetting phase mobility, we can estimate

$$\begin{aligned} A_{II}^3 &\leq \frac{1}{2} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} |\tilde{\sigma}_{K|L}| k_{K|L} (\rho_{w,K|L}^{G,i+1})^2 g_{K|L} G_{w,K|L}^{i+1} \int_{S_{w,L}^{i+1}}^{S_{w,K}^{i+1}} \lambda_w(s) \hat{f}_n(s, p_{K|L}^{i+1}) p'_c(s) ds \\ &\leq \frac{\rho_M^3 |g| k_M}{2 \lambda_m \rho_m^2} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} |\tilde{\sigma}_{K|L}| \left| \int_{S_{w,L}^{i+1}}^{S_{w,K}^{i+1}} \lambda_w(s) \lambda_n(s) p'_c(s) ds \right|. \end{aligned}$$

In the case $g_{K|L} < 0$ we come to the same conclusion which then leads to the estimate

$$A_{II}^3 \leq CT|\Omega| + \frac{\tilde{\varepsilon}}{2} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} |\beta(S_{w,L}^{i+1}) - \beta(S_{w,K}^{i+1})|^2,$$

with $C = C(\rho_M, \rho_m, \lambda_m, k_M, |g|, \tilde{\varepsilon})$, for any $\tilde{\varepsilon} > 0$. The same estimates can be applied to A_n^3 which leads to the following estimate:

$$\begin{aligned} A^3 &\leq CT|\Omega| + \varepsilon \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} |p_L^{i+1} - p_K^{i+1}|^2 \\ &\quad + \tilde{\varepsilon} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} |\beta(S_{w,L}^{i+1}) - \beta(S_{w,K}^{i+1})|^2. \end{aligned} \tag{57}$$

4. Using the estimates $|\rho_\alpha(p_\alpha) g_\alpha(p_\alpha)| \leq \frac{\rho_M}{\rho_m} |p_\alpha|$, $\alpha \in \{w, n\}$, we get

$$A^5 \leq C \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} |K| |F_{P,K}^{i+1}| (|S_{w,K}^{i+1} p_{w,K}^{i+1}| + |S_{n,K}^{i+1} p_{n,K}^{i+1}|).$$

By Remark 2.2 and the fact that $F_P \in L^2(Q_T)$ we get

$$A^5 \leq C \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} |K| |F_{P,K}^{i+1}| (|p_K^{i+1}| + M) \leq C_1 + \frac{\varepsilon_1}{2} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} |K| |p_K^{i+1}|^2,$$

where $C_1 = C_1(|\Omega|, T, \rho_M, \rho_m, \|F_P\|_{L^2(Q_T)}, M, \varepsilon_1)$. Using the discrete Poincaré's inequality we obtain

$$A^5 \leq C_1 + \frac{\varepsilon_1 C_\Omega}{2} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} |p_K^{i+1} - p_L^{i+1}|^2. \quad (58)$$

We note first that the wetting phase term in A^4 is nonpositive for $p_{w,K}^{i+1} \leq 0$ and then it can be neglected. From the definition of the global pressure (7) we have $p_w \leq p \leq |p|$. This fact, combined with $g_w(p_w) \leq \frac{1}{\rho_m} p_w$ and $|g_n(p_n)| \leq \frac{1}{\rho_m} |p_n|$, leads to

$$A^4 \leq \frac{\rho_M}{\rho_m} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} |K| |F_{I,K}^{i+1}| (|p_K^{i+1}| + M) \leq C_2 + \frac{\varepsilon_1}{2} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} |K| |p_K^{i+1}|^2,$$

where $C_2 = C_2(\Omega, T, \rho_M, \rho_m, \|F_I\|_{L^2(Q_T)}, M, \varepsilon_1)$. Again by using the discrete Poincaré inequality we have

$$A^4 \leq C_2 + \frac{\varepsilon_1 C_\Omega}{2} \sum_{i=0}^{N-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} |p_K^{i+1} - p_L^{i+1}|^2. \quad (59)$$

By taking $\varepsilon = \varepsilon_1 C_\Omega = \frac{\rho_m \lambda_m \omega_m^2 k_m}{8 \rho_M}$ and $\tilde{\varepsilon} = \frac{C_{\beta k m}}{4 \rho_M}$ we obtain (50). The estimate (51) is obtained from (54), (55), (57), (58), (59), and an application of the estimate (50). \square

Remark 5.2. *From the monotonicity of the phase pressures, Lemma 4.6, and the assumption (A.4) we conclude that there is a constant $C > 0$ such that*

$$\mathcal{H}(p_n, p_w) \geq - \int_0^{S_w} p_c(s) ds \geq -C. \quad (60)$$

Let us note that Theorem 5.1 and (60) prove the following corollary.

Corollary 5.3. *Let D_h be a FV discretization of $\Omega \times (0, T)$ and let $(p_{n,h}, p_{w,h})$ be a solution to the FV scheme (30)–(36). Then, there exists a constant $C > 0$, independent of h , such that the following estimates hold:*

$$\|p_h\|_{L^2(0,T;H_h(\Omega))} \leq C, \quad \|\beta(S_h)\|_{L^2(0,T;H_h(\Omega))} \leq C.$$

The existence of a solution of the FV scheme (30)–(36) can be proved as in [60]. We have the following result.

Proposition 5.4. *The FV scheme (30)–(36) admits at least one solution $(p_{n,K}^{i+1}, p_{w,K}^{i+1})_{K \in \mathcal{T}}$, $i \in \{0, \dots, N-1\}$.*

The strong convergence of the FV approximation can be proved by applying the compactness theorem of Kolmogorov, Riesz and Fréchet (see [11, 37, 60]). For this, we introduce the functions

$$U_h = \rho_w(p_{w,h}) S_{w,h}, \quad V_h = \rho_n(p_{n,h}) S_{n,h}. \quad (61)$$

and by following [60] (see also [11]) the estimates on space and time translates of the functions U_h and V_h , and its corresponding piecewise linear in time representations, can be obtained. Then by using Kolmogorov's compactness theorem and the fact that the mapping $(u, v) = G(S_w, p)$ given by

$$u = \rho_w(p_w(S_w, p))S_w, \quad v = \rho_n(p_n(S_w, p))(1 - S_w)$$

is a diffeomorphism, then the following result is proved (see [60]).

Theorem 5.5. *Let $(D_h)_h$ be a sequence of FV discretizations of $\Omega \times (0, T)$ such that $\lim_{h \rightarrow 0} \text{size}(D_h) = 0$. Then there exist subsequences $(p_{\alpha, h})_h$, $\alpha \in \{w, n\}$, $(S_{w, h})_h$, and $(p_h)_h$ such that*

$$U_h \rightarrow U \quad \text{strongly in } L^p(Q_T), \quad 1 \leq p < \infty, \quad \text{and a.e. in } Q_T, \quad (62)$$

$$V_h \rightarrow V \quad \text{strongly in } L^p(Q_T), \quad 1 \leq p < \infty, \quad \text{and a.e. in } Q_T, \quad (63)$$

$$S_{w, h} \rightarrow S_w \quad \text{a.e. in } Q_T, \quad 0 \leq S_w \leq 1, \quad (64)$$

$$p_h \rightarrow p \quad \text{a.e. in } Q_T, \quad (65)$$

and $U = \rho_w(p_w(S_w, p))S_w$, $V = \rho_n(p_n(S_w, p))(1 - S_w)$.

From the priori estimates (50), the Poincaré inequality, and Lemma 3.2 it is easy to prove the following weak convergences.

Lemma 5.6. *Let $(D_h)_h$ be a sequence of FV discretizations of $\Omega \times (0, T)$ such that $\lim_{h \rightarrow 0} \text{size}(D_h) = 0$. Then there exist subsequences $(S_{w, h})_h$ and $(p_h)_h$ such that*

$$p, \beta(S_w) - \beta(1) \in L^2(0, T; V), \quad (66)$$

$$\nabla_h \beta(S_{w, h}) \rightarrow \nabla \beta(S_w) \quad \text{weakly in } (L^2(Q_T))^l, \quad (67)$$

$$\nabla_h p_h \rightarrow \nabla p \quad \text{weakly in } (L^2(Q_T))^l, \quad (68)$$

where p and S_w are the limits from Theorem 5.5.

6 Convergence results

In this section, we present some convergence results based on the estimates established in the last sections. Our goal is to prove the following theorem.

Theorem 6.1. *Assume hypothesis (A.1)–(A.7) hold. Let $(D_h)_h$ be a sequence of discretization of $\Omega \times (0, T)$ such that $h \rightarrow 0$. Then there exists a subsequence of solutions to the discrete problem (30)–(36), which converges to a weak solution of the problem (1), (2), (3), (4), (6) in the sense of Definition 2.3.*

In order to prove Theorem 6.1, we first prove some auxiliary lemmas. From (A.3), (A.4), and (A.5) we have the following results.

Lemma 6.2. *The functions $\rho_\alpha(p_\alpha(S_\alpha, p))$ and $\rho_\alpha(p_\alpha(S_w, p))/\lambda(S_w, p)$ are Lipschitz continuous for $\alpha \in \{w, n\}$.*

Lemma 6.3. *Let $S_{w, h}$ and p_h be convergent subsequences from Theorem 5.5, and define the functions \bar{S}_h , \underline{S}_h , \bar{p}_h , and \underline{p}_h on the dual mesh composed of elements $T_{K|L}$, $K \in \mathcal{T}_h$, $L \in N_D(K)$, by*

$$\bar{S}_h|_{\langle t^i, t^{i+1} \rangle \times T_{K|L}} := \max\{S_{w, K}^{i+1}, S_{w, L}^{i+1}\}, \quad \underline{S}_h|_{\langle t^i, t^{i+1} \rangle \times T_{K|L}} := \min\{S_{w, K}^{i+1}, S_{w, L}^{i+1}\},$$

$$\bar{p}_h|_{\langle t^i, t^{i+1} \rangle \times T_{K|L}} := \max\{p_K^{i+1}, p_L^{i+1}\}, \quad \underline{p}_h|_{\langle t^i, t^{i+1} \rangle \times T_{K|L}} := \min\{p_K^{i+1}, p_L^{i+1}\}.$$

Then there is a constant C independent of discretization such that

$$\|\beta(\bar{S}_h) - \beta(\underline{S}_h)\|_{L^2(Q_T)} \leq C \text{size}(\mathcal{T}), \quad \|\bar{p}_h - \underline{p}_h\|_{L^2(Q_T)} \leq C \text{size}(\mathcal{T}). \quad (69)$$

If \tilde{S}_h and \tilde{p}_h are any other dual mesh functions satisfying $\underline{S}_h \leq \tilde{S}_h \leq \bar{S}_h$, $\underline{p}_h \leq \tilde{p}_h \leq \bar{p}_h$ then for any continuous function $\mathcal{A}: [0, 1] \times \mathbb{R} \rightarrow \mathbb{R}$ we have

$$\mathcal{A}(\tilde{S}_h, \tilde{p}_h) \rightarrow \mathcal{A}(S_w, p) \text{ a.e. in } Q_T, \quad (70)$$

where S_w and p are given limits in Theorem 5.5.

Proof. The estimates (69) are proven in [60] and (70) follows from the continuity of \mathcal{A} . \square

Lemma 6.4. Let $\tilde{\alpha}(S_w, p)$ be given by (15). Then the following equality holds

$$\lambda_{n,K|L}^{up,i+1} \rho_{n,K|L}^{up,i+1} f_{w,K|L}^{i+1} (u_K^{i+1} - u_L^{i+1}) = \tilde{\alpha}(\underline{S}_{w,K|L}^{i+1}, \underline{p}_{K|L}^{i+1}) (\beta(S_{w,K}^{i+1}) - \beta(S_{w,L}^{i+1})) + \Delta_{K|L}^{i+1}$$

where

$$\begin{aligned} |\Delta_{K|L}^{i+1}| &\leq C \left| \beta(S_{w,K}^{i+1}) - \beta(S_{w,L}^{i+1}) \right|^{2\tau} \\ &\quad + C \left(\left| \bar{S}_{w,K|L}^{i+1} - \underline{S}_{w,K|L}^{i+1} \right| + \left| \bar{p}_{K|L}^{i+1} - \underline{p}_{K|L}^{i+1} \right| \right) \left| \beta(S_{w,K}^{i+1}) - \beta(S_{w,L}^{i+1}) \right|, \end{aligned} \quad (71)$$

with the constant C independent of the discretization parameters.

Proof. For simplicity of notation we will denote S_w by S and we will omit the time level index $i+1$ since all the quantities are given on the same time level.

From the definition of $f_{w,K|L}$ we conclude that there exists $\bar{a} \in [\underline{S}_{K|L}, \bar{S}_{K|L}]$ such that

$$\lambda_{n,K|L}^{up} \rho_{n,K|L}^{up} f_{w,K|L} (u_K - u_L) = \lambda_n(S_{K|L}) \rho_n(p_{n,K|L}^{up}) \frac{\rho_w(p_w(\bar{a}, p_{K|L})) \lambda_w(\bar{a})}{\lambda(\bar{a}, p_{K|L})} (u_K - u_L),$$

and therefore, we can estimate

$$\begin{aligned} |\Delta_{K|L}| &\leq \frac{\rho_n(p_{n,K|L}^{up}) \rho_w(p_w(\bar{a}, p_{K|L}))}{\lambda(\bar{a}, p_{K|L})} \left| \lambda_n(S_{K|L}) \lambda_w(\bar{a}) (u_K - u_L) - (\beta(S_K) - \beta(S_L)) \right| \\ &\quad + \left| \frac{\rho_n(p_{n,K|L}^{up}) \rho_w(p_w(\bar{a}, p_{K|L}))}{\lambda(\bar{a}, p_{K|L})} - \tilde{\alpha}(\underline{S}_{K|L}, \underline{p}_{K|L}) \right| |\beta(S_K) - \beta(S_L)| := c_1 + c_2. \end{aligned}$$

The term c_1 can be estimated as

$$c_1 \leq \frac{\rho_M^2}{\lambda_m \rho_m} \left| \lambda_n(S_{K|L}) \lambda_w(\bar{a}) - \lambda_n(a_1) \lambda_w(a_1) \right| |u_K - u_L|,$$

for some $a_1 \in [\underline{S}_{K|L}, \bar{S}_{K|L}]$. By applying (A.3), (A.4), and (A.7) we get

$$c_1 \leq C |S_K - S_L| |\beta(S_K) - \beta(S_L)|^\tau \leq C |\beta(S_K) - \beta(S_L)|^{2\tau}.$$

Using Lemma 6.2, (A.3), and (A.5) it is easy to show that

$$\left| \frac{\rho_n(p_{n,K|L}^{up})\rho_w(p_w(\bar{a}, p_{K|L}))}{\lambda(\bar{a}, p_{K|L})} - \tilde{\alpha}(\underline{S}_{K|L}, \underline{p}_{K|L}) \right| \leq C \left(|\bar{S}_{K|L} - \underline{S}_{K|L}| + |\bar{p}_{K|L} - \underline{p}_{K|L}| \right),$$

leading to

$$c_2 \leq C \left(|\bar{S}_{K|L} - \underline{S}_{K|L}| + |\bar{p}_{K|L} - \underline{p}_{K|L}| \right) |\beta(S_K) - \beta(S_L)|.$$

This concludes the proof. \square

We now pass to the proof of Theorem 6.1. Let $\varphi \in D([0, T] \times \bar{\Omega})$ and set $\varphi_K^i := \varphi(x_K, t^i)$ for all $K \in \mathcal{T}_h$ and $i \in \{0, 1, \dots, N_h\}$. In order to pass to the limit in (31), we multiply (31) by $\delta t \varphi_K^{i+1}$, introduce the global pressure variable by (44), (45) and sum over $K \in \mathcal{T}_h$ and $i \in \{0, 1, \dots, N_h - 1\}$ to obtain

$$S_1^h + S_2^h + S_3^h + S_4^h + S_5^h = 0,$$

where we have denoted

$$S_1^h = \sum_{i=0}^{N_h-1} \sum_{K \in \mathcal{T}_h} |K| \Phi_K \left(\rho_{n,K}^{i+1} S_{n,K}^{i+1} - \rho_{n,K}^i S_{n,K}^i \right) \varphi_K^{i+1} \quad (72)$$

$$S_2^h = \sum_{i=0}^{N_h-1} \delta t \sum_{K \in \mathcal{T}_h} \sum_{L \in N_D(K)} \tau_{K|L} k_{K|L} \lambda_{n,K|L}^{up,i+1} \rho_{n,K|L}^{up,i+1} \omega_{K|L}^{i+1} (p_K^{i+1} - p_L^{i+1}) \varphi_K^{i+1} \quad (73)$$

$$S_3^h = \sum_{i=0}^{N_h-1} \delta t \sum_{K \in \mathcal{T}_h} \sum_{L \in N_D(K)} \tau_{K|L} k_{K|L} \lambda_{n,K|L}^{up,i+1} \rho_{n,K|L}^{up,i+1} f_{w,K|L}^{i+1} (u_K^{i+1} - u_L^{i+1}) \varphi_K^{i+1} \quad (74)$$

$$S_4^h = \sum_{i=0}^{N_h-1} \delta t \sum_{K \in \mathcal{T}_h} |K| \left(\rho_{n,K}^{i+1} S_{n,K}^{i+1} F_{p,K}^{i+1} \varphi_K^{i+1} - \rho_{n,K}^{i+1} S_{n,K}^{I,i+1} F_{I,K}^{i+1} \varphi_K^{i+1} \right) \quad (75)$$

$$S_5^h = \sum_{i=0}^{N_h-1} \delta t \sum_{K \in \mathcal{T}_h} \sum_{L \in N_D(K)} |\sigma_{K|L}| k_{K|L} \lambda_{n,K|L}^{G,i+1} \left(\rho_{n,K|L}^{G,i+1} \right)^2 g_{K|L} \varphi_K^{i+1}. \quad (76)$$

By applying standard technique (see [16, 60]) we get

$$\lim_{h \rightarrow 0} S_1^h = - \int_{Q_T} \Phi(x) \rho_n(p_n(x, t)) S_n(x, t) \partial_t \varphi(x, t) dx dt - \int_{\Omega} \Phi(x) \rho_n(p_n^0(x)) S_n^0(x) \varphi(x, 0) dx.$$

By applying gathering by edges and simple calculation we can rewrite the term S_2^h as

$$S_2^h = \frac{1}{2} \sum_{i=0}^{N_h-1} \delta t \sum_{K \in \mathcal{T}_h} \sum_{L \in N_D(K)} |\tilde{T}_{K|L}| k_{K|L} \lambda_{n,K|L}^{up,i+1} \rho_{n,K|L}^{up,i+1} \omega_{K|L}^{i+1} \nabla_{K|L} p_h^{i+1} \cdot \nabla \varphi(\bar{x}_{K|L}, t^{i+1}),$$

where $\bar{x}_{K|L}$ is some point on the segment with the endpoints x_K and x_L .

By introducing the corresponding piecewise constant functions $S_{w,h}^{up}$, $\bar{S}_{w,h}$, \bar{p}_h , $\tilde{S}_{w,h}$, and \tilde{p}_h defined on the dual mesh we can write

$$S_2^h = \int_0^T \int_{\Omega} k_h(x) \lambda_n(S_{w,h}^{up}) \rho_n(p_n(\bar{S}_{w,h}, \bar{p}_h)) \omega(\tilde{S}_{w,h}, \tilde{p}_h) \nabla_h p_h \cdot (\nabla \varphi)_h dx dt.$$

Now, by Theorem 5.5, Lemma 5.6, Lemma 6.3, and $\|k - k_h\|_{L^2(\Omega)} \rightarrow 0$ as $h \rightarrow 0$ we get

$$\lim_{h \rightarrow 0} S_2^h = \int_0^T \int_{\Omega} k(x) \lambda_n(S_w) \rho_n(p_n(S_w, p)) \omega(S_w, p) \nabla p \cdot \nabla \varphi \, dx dt.$$

After applying gathering by edges and Lemma 6.4 we can rewrite the term S_3^h as

$$\begin{aligned} S_3^h &= \frac{1}{2} \sum_{i=0}^{N_h-1} \delta t \sum_{K \in \mathcal{T}_h} \sum_{L \in N_D(K)} |\tilde{T}_{K|L}| k_{K|L} \tilde{\alpha}(S_{w,K|L}^{i+1}, \underline{p}_{K|L}^{i+1}) \nabla_{K|L} \beta(S_{w,h}^{i+1}) \cdot \nabla \varphi(\overline{x_{K|L}}, t^{i+1}) \\ &+ \frac{1}{2} \sum_{i=0}^{N_h-1} \delta t \sum_{K \in \mathcal{T}_h} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} k_{K|L} \Delta_{K|L}^{i+1} (\varphi_K^{i+1} - \varphi_L^{i+1}) := c_I + c_{II}. \end{aligned}$$

Then using the estimate (71) and by Cauchy-Schwarz's and Hölder's inequalities we get the following estimate:

$$\begin{aligned} |c_{II}| &\leq C \left\{ \left(\sum_{i=0}^{N_h-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} |\beta(S_{w,L}^{i+1}) - \beta(S_{w,K}^{i+1})|^2 \right)^\tau \right. \\ &\quad \times \left. \left(\sum_{i=0}^{N_h-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} |\varphi_L^{i+1} - \varphi_K^{i+1}|^{\frac{1}{1-\tau}} \right)^{1-\tau} \right. \\ &\quad + \|\nabla \varphi\|_\infty \|\nabla_h \beta(S_{w,h})\|_{L^2(Q_T)} \left(\sum_{n=0}^{N_h-1} \delta t \int_{\Omega} |\overline{S_{w,h}^{i+1}} - S_{w,h}^{i+1}|^2 dx \right)^{1/2} \\ &\quad \left. + \|\nabla \varphi\|_\infty \|\nabla_h \beta(S_{w,h})\|_{L^2(Q_T)} \left(\sum_{n=0}^{N_h-1} \delta t \int_{\Omega} |\overline{p_h^{i+1}} - p_h^{i+1}|^2 dx \right)^{1/2} \right\}. \end{aligned}$$

We can estimate

$$\begin{aligned} &\left(\sum_{i=0}^{N_h-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} |\varphi_L^{i+1} - \varphi_K^{i+1}|^{\frac{1}{1-\tau}} \right)^{1-\tau} \\ &\leq \|\nabla \varphi\|_\infty \left(\sum_{i=0}^{N_h-1} \delta t \sum_{K \in \mathcal{T}} \sum_{L \in N_D(K)} l |\tilde{T}_{K|L}| |d_{K|L}|^{\frac{1}{1-\tau}-2} \right)^{1-\tau} \leq C \|\nabla \varphi\|_\infty h^{1-2(1-\tau)}, \end{aligned}$$

which gives us $|c_{II}| \leq C(h^{2\tau-1} + h)$ and due to (A.7) the term c_{II} tends to zero as $h \rightarrow 0$.

Using the same reasoning as for S_2^h we get

$$\lim_{h \rightarrow 0} S_3^h = \int_{Q_T} k(x) \tilde{\alpha}(S_w, p) \nabla \beta(S_w) \cdot \nabla \varphi \, dx dt. \quad (77)$$

Using (64) and (65) it is easy to pass to the limit in S_4^h and get

$$\lim_{h \rightarrow 0} S_4^h = \int_0^T \int_{\Omega} (\rho_n S_n F_P \varphi - \rho_n S_n^I F_I \varphi) \, dx dt. \quad (78)$$

The term S_5^h can be written as

$$S_5^h = -\frac{1}{2} \sum_{i=0}^{N_h-1} \delta t \sum_{K \in \mathcal{T}_h} \sum_{L \in N_D(K)} |\tilde{T}_{K|L}| k_{K|L} \lambda_{n,K|L}^{G,i+1} (\rho_{n,K|L}^{G,i+1})^2 \mathbf{g} \cdot \nabla_{K|L} \varphi(t^{i+1})$$

$$= - \int_0^T \int_{\Omega} k_h(x) \lambda_n(S_{w,h}^{G,up}) \rho_n^2(p_n(S_{w,h}^G, p_h^G)) \mathbf{g} \cdot \nabla_h \varphi \, dx \, dt$$

where $S_{w,h}^{G,up}$, $S_{w,h}^G$, and p_h^G are suitable piecewise constant function such that $\underline{S}_{w,h} \leq S_{w,h}^{G,up}$, $S_{w,h}^G \leq \bar{S}_{w,h}$ and $\underline{p}_h \leq p_h^G \leq \bar{p}_h$. We note that for smooth test function φ , by Lemma 3.4, $\nabla_h \varphi \rightarrow \nabla \varphi$ weakly in $L^2(Q_T)$. Then the same arguments as in S_2^h and S_3^h ensure

$$\lim_{h \rightarrow 0} S_5^h = - \int_0^T \int_{\Omega} k(x) \lambda_n(S_w) \rho_n^2(p_n) \mathbf{g} \cdot \nabla \varphi \, dx \, dt. \quad (79)$$

We can perform similar calculations and reasoning in all terms of the equation (32) and after passing to the limit as $h \rightarrow 0$ we obtain the following variational equations:

$$\begin{aligned} & - \int_0^T \Phi \rho_w(p_w) S_w \partial_t \varphi \, dx \, dt - \int_{\Omega} \Phi(x) \rho_w(p_w^0(x)) S_w^0(x) \varphi(0, x) \, dx \\ & + \int_{Q_T} [\mathbb{K}(\lambda_w(S_w) \rho_w(p_w) \omega(S_w, p) \nabla p - \tilde{\alpha}(S_w, p) \nabla \beta(S_w)) - \lambda_w(S_w) \rho_w^2(p_w) \mathbb{K} \mathbf{g}] \cdot \nabla \varphi \, dx \, dt \end{aligned} \quad (80)$$

$$\begin{aligned} & + \int_{Q_T} \rho_w(p_w) S_w F_P \varphi \, dx \, dt = \int_{Q_T} \rho_w(p_w) S_w^I F_P \varphi \, dx \, dt; \\ & - \int_0^T \Phi \rho_n(p_n) S_n \partial_t \psi \, dx \, dt - \int_{\Omega} \Phi(x) \rho_n(p_n^0(x)) (1 - S_w^0(x)) \psi(0, x) \, dx \\ & + \int_{Q_T} [\mathbb{K}(\lambda_n(S_w) \rho_n(p_n) \omega(S_w, p) \nabla p + \tilde{\alpha}(S_w, p) \nabla \beta(S_w)) - \lambda_n(S_w) \rho_n^2(p_n) \mathbb{K} \mathbf{g}] \cdot \nabla \psi \, dx \, dt \end{aligned} \quad (81)$$

$$+ \int_{Q_T} \rho_n(p_n) S_n F_P \psi \, dx \, dt = \int_{Q_T} \rho_n(p_n) S_n^I F_P \psi \, dx \, dt,$$

for all $\varphi, \psi \in C^1([0, T]; V)$ with $\psi(T, \cdot) = \varphi(T, \cdot) = 0$.

Starting from the limit global pressure p and the wetting phase saturation S_w one can define the limit phase pressures p_n and p_w by (7). From (13) and (14) we can reintroduce the gradients of the phase pressures into the previous variational formulation which then reduces to the variational problem from Definition 2.3. Theorem 6.1 is proved.

7 Numerical results

In this section, we present the numerical results for test cases modeling different scenarios of immiscible compressible two-phase flow in porous media. The first test case is a 2D simulation of the gas migration inside a nuclear waste repository. The second test case is the injection of gas (CO₂) in a 3D homogeneous porous domain fully saturated with water.

All our developments have been implemented in DuMu^X. It provides many tools to solve numerically PDEs and allowing, among other things, the management of mesh, discretization or linear and nonlinear solvers. The code is an object-oriented software written in C++ and has massively parallel computation capability. The modular concept of DuMu^X makes it easy to integrate new modules adapted to our numerical scheme. [Using the scheme \(31\)-\(32\), we have developed a new module, named 2p-global, which allows to numerically solve the coupled system \(1\)–\(2\) with a fully implicit scheme in time and a cell-centered FV method in space.](#) We have a set of nonlinear equations which are solved implicitly using Newton's method with variable time stepping. The control of the time-step is based on the number of iterations required by the Newton method to achieve convergence for the last time iteration. The time-step is reduced, if the number of iterations exceeds a specified threshold, whereas it is increased if the method converges within less iterations. Let us

mention that throughout all numerical experiments, we observed that in no instance more than a maximum of 10 iterations was needed for the convergence of Newton’s method. Consequently, for this study the adopted strategy for the management of the time step is sufficient. Therefore, there is no need to use other types of local time-stepping strategies proposed in the literature. Numerical differentiation techniques are used to approximate the derivatives in the calculation of the Jacobian matrix. This allows to transform the nonlinear system of equations for each iteration step into a linear system of equations. For solving the occurring linearized systems of equations, an iterative linear solver is used, namely, BiConjugate Gradient STABILized (BiCGSTAB) method, preconditioned by an Algebraic Multigrid (AMG) solver. This solver is integrated in the ISTL-Library of DUNE.

Our approach has been validated by solving several tests in 1D including the MoMaS benchmark [18] on multiphase flow, where hydrogen (H_2) flow in nuclear waste repositories was examined, the numerical results are satisfactory and replicated to those in the literature. The results of these simulations are omitted since nothing startling was found. Instead, we concentrate on the results obtained in realistic two test cases. The first example proposed in the framework of the multiphase flow simulation benchmark Couplex-Gaz [10] which was launched to improve the understanding of gas migration in a repository situated in clay formation. The benchmark was designed to compare the performance of the numerical methods and to increase the confidence into the numerical tools used for two-phase flow modeling and evaluation of critical parameters such the peak gas pressure in a repository, the saturation around the canisters, and water flux induced by gas. The second test case is adapted from a test case described in [56] and simulates CO_2 sequestration scenario in 3D and shows that our approach can handle a large number of unknowns. Both test cases show that our fully implicit approach is suitable to simulate immiscible compressible two-phase flow in heterogeneous porous media.

All computations were performed on a laptop with Intel(R) Core(TM) i5-4590 CPU Processor (3.30GHz x4) with 8GB RAM. One of the objectives of this paper is to deliver computational performance also suitable for limited computational resources. Let us mention that in view of the CPU times required for the examples treated in this paper, all the simulations were performed sequentially. However, the new module developed can be used on multicore/multinode systems. The parallelization in DuMu^X is carried out using the DUNE parallel library package based on MPI providing high parallel efficiency and allowing simulations with several tens of millions of degrees of freedom to be carried out, ideal for large-scale field applications. DuMu^X has the ability to run on anything from single processor systems to highly parallel supercomputers with specialized hardware architectures.

7.1 Example 1: Couplex–Gaz Benchmark

The first test case is an example from the Couplex–Gaz Benchmark [10]. It deals with a simulation of H_2 migration out of intermediate-level radioactive waste disposal drifts for at least 100000 years after the closure of the facility. The model configuration considers, a cross-section (2D) through the disposal drift, a heterogeneous domain $\Omega = (0, 200 \text{ m}) \times (0, 130 \text{ m})$ composed of seven different materials as shown in Figure 1. Main challenging issues arise as lots of different materials were taken into account at scales between 10 cm and several tens of meters and due to high contrasts in permeability (up to 8 orders of magnitude) of the different materials.

For all media we have used Van Genuchten’s capillary pressure curves,

$$p_c(S_{we}) = P_r \left(\frac{1}{S_{we}^{1/m}} - 1 \right)^{1/n},$$

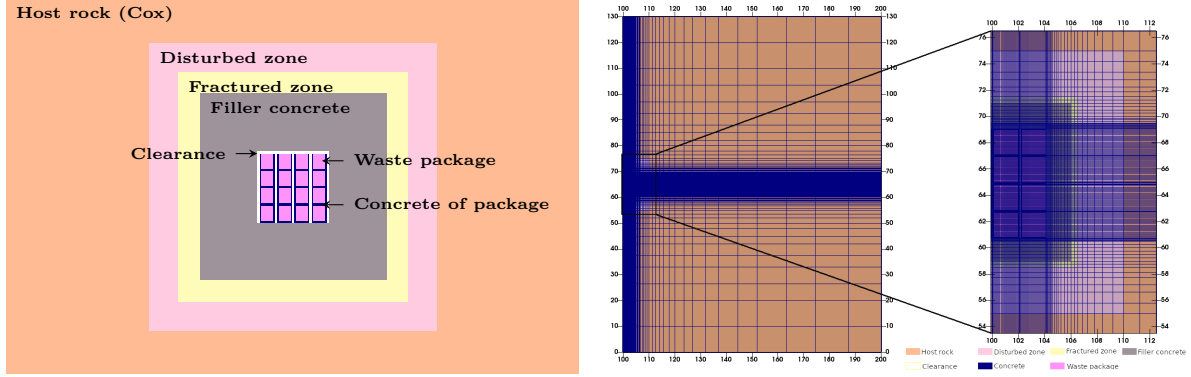


Figure 1: Schematic of the geometry of the 2D domain (left) and the mesh (right) for test case 1.

and the relative permeability curves

$$kr_w(S_{we}) = \sqrt{S_{we}} \left(1 - \left(1 - S_{we}^{1/m}\right)^m\right)^2, \quad kr_n(S_{we}) = (1 - S_{we})^{1/2} \left(1 - S_{we}^{1/m}\right)^{2m},$$

but with different parameters. The parameters used in the simulation are given in Table 1. Rock properties are also given in the same table. A simplification in comparison to the original test case is that we impose the same vertical and horizontal permeability in the Cox layer. We find that this simplification does not severely impact overall the behavior. It is assumed that a gas (H_2) is produced inside each waste package. For the first 500 years 6.25 mol/years of H_2 per waste package is produced, and for the next 9500 years it is produced 0.5 mol/years of H_2 per waste package. After 10000 years the gas source term is set to 0.0.

	Waste package	Concrete of package	Clearance	Filler concrete	Fractured zone	Disturbed zone	Host rock
$K[m^2]$	10^{-15}	10^{-19}	10^{-12}	10^{-18}	$5 \cdot 10^{-16}$	$5 \cdot 10^{-18}$	$5 \cdot 10^{-21}$
$\Phi[-]$	0.25	0.15	1.0	0.3	0.16	0.15	0.15
$S_{nr}[-]$	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$S_{wr}[-]$	0.01	0.01	0.01	0.01	0.1	0.2	0.4
$n[-]$	1.5	1.54	1.5	1.54	1.5	1.5	1.49
$Pr[Pa]$	$3 \cdot 10^4$	$2 \cdot 10^6$	$5 \cdot 10^4$	$2 \cdot 10^6$	$2 \cdot 10^6$	$5 \cdot 10^6$	$15 \cdot 10^6$

Table 1: Van Genuchten's parameters and rock properties.

We consider two-phase flow composed of H_2 and water. The water phase is assumed incompressible with density $\rho_w = 1000 \text{ kg/m}^3$ and viscosity $\mu_w = 10^{-3} \text{ Pa} \cdot \text{s}$. The H_2 density is modeled by the ideal gas law, precisely $\rho_n = Mp_n/(RT)$, with H_2 molar mass set to $2 \cdot 10^{-3} \text{ kg/mol}$ and the temperature to 303.15 K . Additionally we impose H_2 viscosity as $\mu_n = 10^{-6} \text{ Pa} \cdot \text{s}$. The initial conditions for the water saturation are imposed as shown in Table 2. In the fully saturated parts of the domain we impose hydrostatic wetting phase pressure. In the remaining parts of the domain the initial gas pressure is set to 1 atm. The duration of the simulation is equal to 100000 years.

On the top and the bottom of the domain we impose the following boundary conditions

$$p_w(x, z = 0, t) = 5.5 \cdot 10^6 \text{ Pa}, \quad S_w(x, z = 0, t) = 1, \quad x \in [0, 200], t \in [0, t_{end}],$$

	Waste package	Concrete of package	Clearance	Filer concrete	Fractured zone	Disturbed zone	Host rock
S_w	0.2	0.6	0.1	0.7	1.0	1.0	1.0

Table 2: Initial condition for the water saturation.

$$p_w(x, z = 130, t) = 4.2 \cdot 10^6 \text{Pa}, \quad S_w(x, z = 130, t) = 1, \quad x \in [0, 200], t \in [0, t_{end}].$$

The left and the right parts of the domain are assumed impermeable.

For this simulation we have used a rectangular grid with 96 cells in the horizontal direction and 90 cells in the vertical direction, for the half of the domain, with cells more densely set around the disposal system as shown in Figure 1. The mesh was generated manually using The Dune Grid Format. The convergence was achieved with an initial time step of 1 s and a maximum time-step equal to 100 years have been considered. The tolerances for the Newton method and the BICGSTAB method are respectively 10^{-8} and 10^{-13} . In this case, Newton’s method converges rapidly in less than 9 iterations.

The obtained results are given in the left part of Figures 2 - 3. We compare our results with those obtained by other teams that took part in the Couplex–Gaz Benchmark given in [65] (right part of the presented figures). Figure 2 displays the evolution of the gas pressure in the point (101, 62) defined by the benchmark. We can see that we obtain the same physical behavior for the gas phase pressure inside the waste package. We obtain the maximum gas pressure of 8.65 MPa at 10000 years, which represents a major indicator to investigate possible pressure buildup, which may introduce a risk of damage to the host rock.

In Figure 3 we can see that we again have the same physical behavior for the water saturation as shown in the figure on the right with somewhat higher values. There is a slight desaturation of this part of the domain in the beginning of the simulation followed by an increase of the saturation values until 10000 years. For the next 10000 years we again have slight desaturation, and afterwards the water saturation value rises until the end of the simulation when it reaches the value of 0.36.

To get an idea of how fluid flows through the domain, the gas pressure, the water pressure and the water saturation contours from the simulation are presented. In Figure 4 we can see a significant increase of the gas pressure around the waste packages due to H_2 production. It is also interesting to observe in Figure 5 that the water pressure is modified 50 meters away from the disposal system since the low permeability of the host rock prevents rapid water flow in this area. Notice that the evolution of the front behaves in a physically realistic manner. The saturation front is very sharp due to the strong and sharp localized variation of the permeability, this is remarkably captured (see Figure 6).

We terminate by noting that the general trends of the system behavior are in good agreement with the results obtained by other groups. The results show that locally the differences between the simulations can be slightly different but the global behavior is similar enough to confirm the same conclusions about the response of the system to the migration of generated gas.

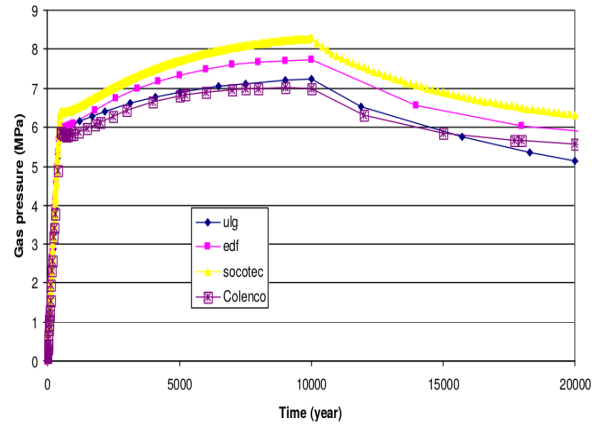
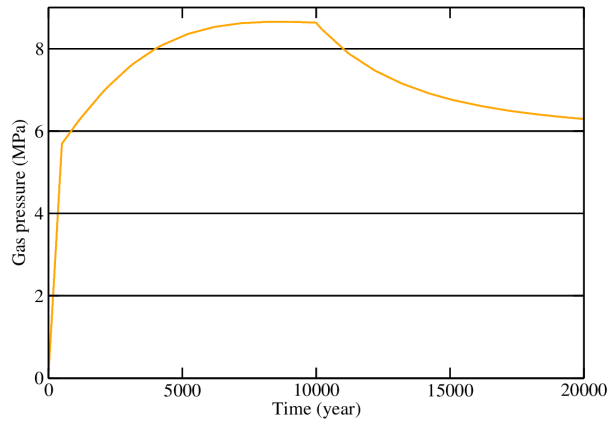


Figure 2: Comparison of the gas pressure in the waste package.

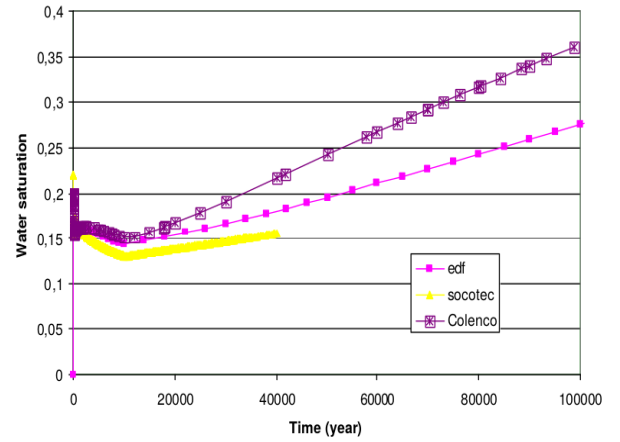
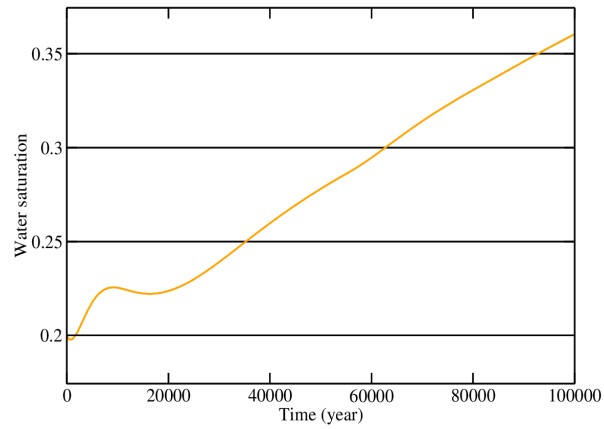


Figure 3: Comparison of the water saturation in the waste package.

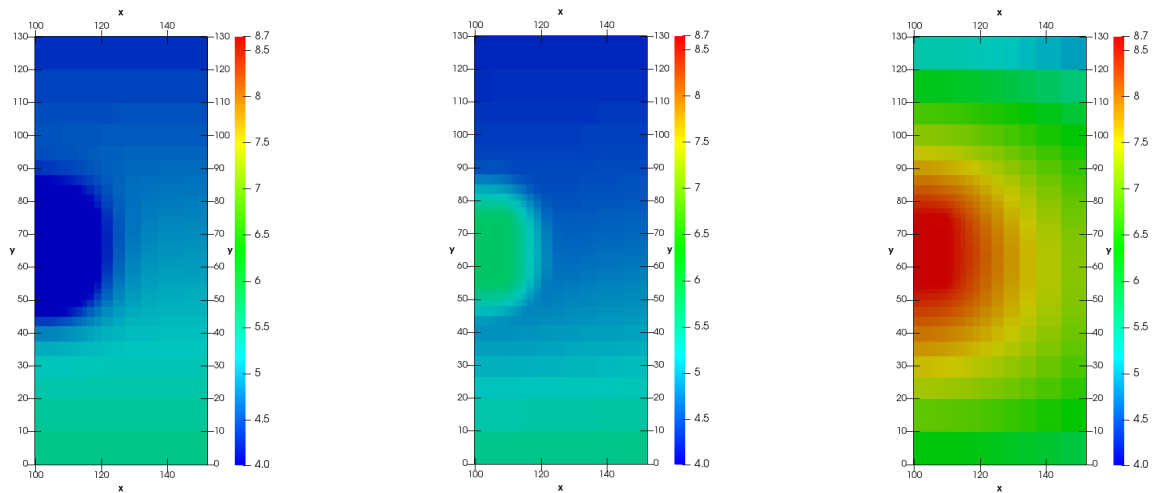


Figure 4: Gas pressure (MPa) at 1 year, 500 years, and 10000 years.

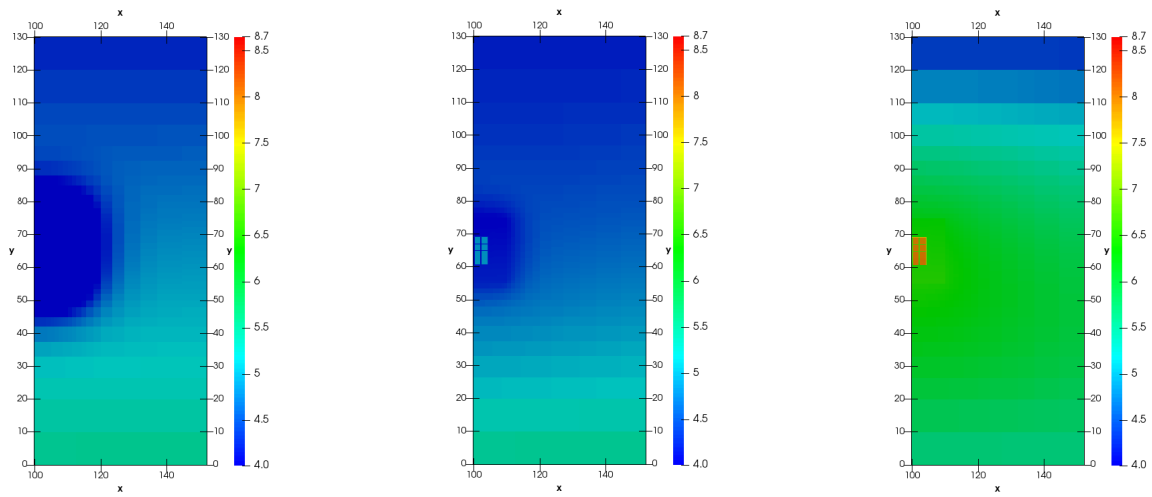


Figure 5: Water pressure (MPa) at 1 year, 500 years, and 10000 years.

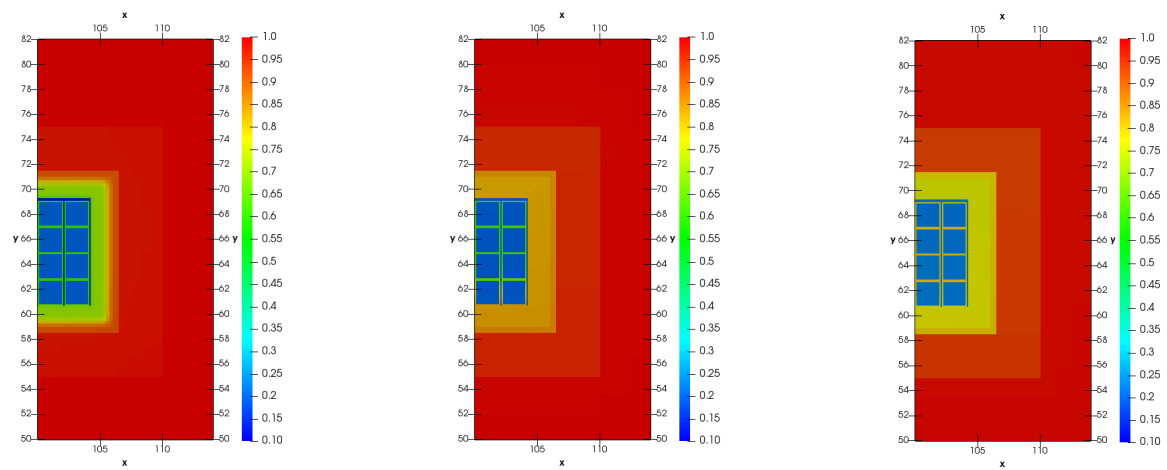


Figure 6: Water saturation at 1 year, 500 years, and 10000 years.

7.2 Example 2: CO₂ injection in a fully water-saturated domain

This test case concerns a 3D scenario of injection of CO₂ adapted from an example proposed in [56], where we consider two-phase flow model instead of two-phase two-component flow. The porous domain is a cube with dimensions 100 × 100 × 100 m³ which is located 800 m under the surface. In this test case the Brooks–Corey model is used for the capillary pressure and for the relative permeabilities:

$$p_c(S_{we}) = p_{entry} S_{we}^{-\frac{1}{\lambda}}, \quad kr_w(S_{we}) = S_{we}^{\frac{2+3\lambda}{\lambda}}, \quad kr_n(S_{we}) = (1 - S_{we})^2 \left(1 - S_{we}^{\frac{2+\lambda}{\lambda}}\right).$$

The parameters for the Brooks–Corey model and the properties of the porous domain are given in Table 3.

$\lambda(-)$	$p_{entry}(\text{Pa})$	$S_{wr}(-)$	$S_{nr}(-)$	Φ	$k(\text{m}^2)$	$T(\text{K})$
2	$1 \cdot 10^3$	0.0	0.0	0.2	10^{-12}	313.15

Table 3: Brooks Corey’s parameters and rock properties

The domain is initially fully saturated with water and CO₂ is injected into the lower left part of the cube as shown in Figure 7 by rate $q_n^{in} = 4 \cdot 10^{-2}$ kg/(m²s). The remaining parts of the boundary are assumed impermeable except of the side denoted by Γ_{out} where hydrostatic pressure for the water phase and zero gas saturation are imposed. The initial pressure for the wetting phase is also hydrostatic. The duration of the simulation is 18 days. **For the 3–D domain we have used a structured grid composed of 60 × 60 × 60 cubes of the same dimensions.** The initial time step δt is set to 1 s and the maximum time step is set to 5000 s. The tolerances for the Newton method and the BICGSTAB method are respectively 10^{-8} and 10^{-10} . In this case, Newton’s method converges rapidly in less than 6 iterations.

The results of this test case are given in Figures 8 - 11 which illustrate the evolution of CO₂ at different times. As expected, CO₂ which is less dense than the liquid phase, migrates upwards and when it reaches the impervious top of the domain it spreads laterally. Good agreement between our results and those of [56] was achieved. This test case shows the effectiveness and practicability of the method and that our approach can handle large number of unknowns.

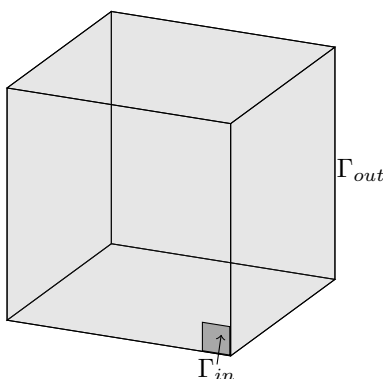


Figure 7: Computational domain for test case 2.

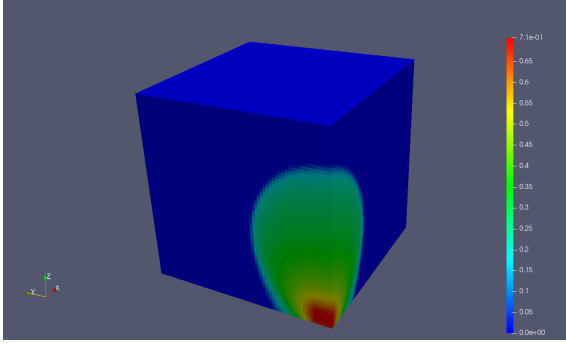


Figure 8: CO₂ saturation after 4 days.

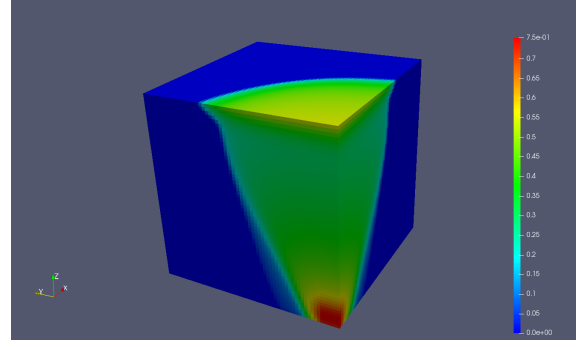


Figure 9: CO₂ saturation after 9 days.

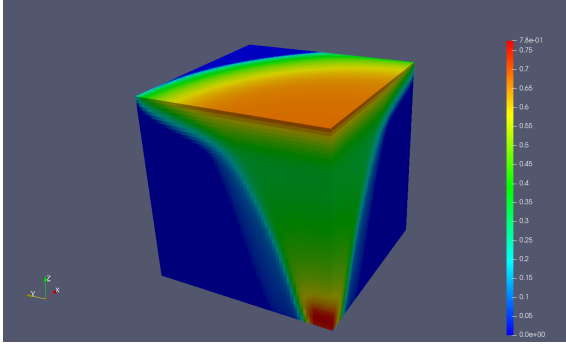


Figure 10: CO₂ saturation after 14 days.

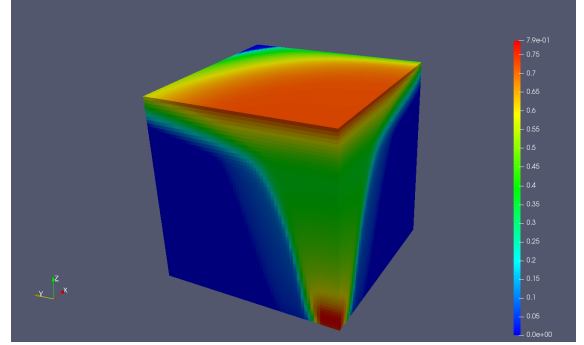


Figure 11: CO₂ saturation after 18 days.

8 Concluding remarks

In this article, we have presented a mathematical formulation and FV approximation for a system of coupled degenerate PDEs modeling immiscible compressible two-phase in the subsurface. Based on a priori estimates and compactness arguments, we prove the convergence of the numerical approximation to the weak solution using [the concept of the global pressure developed specially for compressible flows in heterogeneous porous media](#). The results improve upon previously derived schemes to heterogeneous porous media. A fully implicit approach has been developed and implemented in the framework of the parallel open-source platform DuMu^X. Numerical results concerning scenarios of gas migration through engineered and geological barriers for a deep repository of radioactive waste and geological storage of CO₂ validated the method. The study still needs to be improved in several areas such as the case of discontinuous capillary pressures. More precisely, this paper treats the case of a single rock-type model, i.e. we assume here that the capillary pressure and relative permeabilities depend on the saturation solely. Our future study will focus on extension of these results to the case of porous media with several rock types: capillary pressure and relative permeability curves being different in each type of porous media. Let us note that all the aforementioned works are restricted to the case where the gas density is bounded from below and above. This assumption is too restrictive for some realistic problems. In this case the gas obeys the ideal gas law, i.e. the equation of state is given by $\rho_g(p_g) \stackrel{\text{def}}{=} \sigma p_g$ where ρ_g is the gas density, p_g is the gas pressure and σ is a given constant. Then a new degeneracy appears in the evolution term of the gas pressure equation. These more complicated cases appear in the applications. Further work on these important issues is in progress. Finally, we believe that our convergence analysis also can be extended to a compositional compressible two-phase flow model based on the concept of the global pressure [7], but more research remains to verify this.

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