Mathematical modeling and numerical simulation of multiphase multicomponent flow in porous media

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Summary

Two-phase flow in porous media appears in many petroleum and environment engineering problems, like secondary and tertiary oil recovery, the disposal of radioactive waste, sequestration of CO_2 etc. This thesis covers both mathematical and numerical analysis of this type of flows.

Significant part of this thesis is devoted to the mathematical modeling and analysis of multiphase flows, precisely to a formulation of a two-phase, two-component model with exchange of the mass between the phases and to study the existence of weak solutions to this model. Specifically, flow of the fluid composed of water and gas with possible dissolution of the gas in water is considered. The model is completed with the assumption of the low solubility of the gas.

Numerical simulation often represents the only viable approach to the mathematical modeling of multiphase flows due to the nonlinearity of equations governing these flows, as well as heterogeneity of the domains where these flows occur. Therefore, an important part of this thesis is devoted to numerical analysis of the model describing immiscible compressible two-phase flow in porous media by the concept of the global pressure. More precisely, the convergence of a fully coupled fully implicit petroleum engineering finite volume method based on the cell-centered discretization is studied and the result is proved under standard assumptions. A similar proof was given in [76] with different techniques.

As a groundwork for future research regarding compositional flow in this thesis we also consider the fractional flow formulation with the global pressure as a primary variable in the case of immiscible compressible flow. An efficient numerical method is obtained once again through a cell-centered finite volume discretization. The proposed method is verified on important 1D, 2D and 3D benchmark test cases modeling different scenarios of water-gas (hydrogen) flow in porous media. For the code development we have used the DuMu^x, programming framework for implementation of the models describing the flow and transport processes in porous media, see [43] and [66].

Keywords: porous media flow, two-phase immiscible compressible flow, compositional flow, persistent variables, low solubility, finite volume method, global pressure, discontinuous capillary pressures.

Prošireni sažetak

Dvofazni tok fluida u poroznoj sredini javlja se u brojnim problemima vezanim za naftno inženjerstvo i hidrologiju, kao i u brojnim problemima vezanim za zaštitu okoliša. Neki od primjera su sekundarno i tercijarno izvlačenje nafte, odlaganje radioaktivnog otpada, sekvestracija CO_2 itd. U ovoj disertaciji je dana matematička i numerička analiza matematičkih modela koji opisuju navedene tokove.

Značajan dio disertacije posvećen je matematičkom modeliranju i analizi višefaznih tokova, preciznije formulaciji dvofaznog, dvokomponentnog modela s izmjenom mase između faza te analizi egzistencije rješenja predloženog modela. Preciznije, proučavan je tok fluida sastavljenog od vode i plina uz mogućnost otapanja plina u vodi. Model je upotpunjen pretpostavkom slabe topljivosti plina koja se koristi u dokazu egzistencije rješenja predloženog modela. Ovoj pretpostavci je dano precizno matematičko značenje. Pretpostavka slabe topljivosti je ključna za izvod energetske ocjene bez ikakvih nefizikalnih pretpostavki na difuzijske članove u modelu. Prilikom proučavanja višekomponentnih modela poseban tretman zahtjeva nestanak i ponovno pojavljivanje pojedine faze. U ovom radu taj je problem riješen primjenom perzistentnih varijabli koje su dobro definirane i u jednofaznim i u dvofaznim područjima.

Numeričke simulacije često predstavljaju jedini izvedivi pristup matematičkom modeliranju višefaznih tokova zbog nelinearnosti jednadžbi koje opisuju dotične tokove, kao i izrazite heterogenosti domena u kojima se javljaju. Upravo iz tih razloga, dio ove radnje je posvećen numeričkoj analizi modela koji opisuju nemješivi, stlačivi, dvofazni tok fluida u poroznoj sredini. Jedna od najčešće korištenih diskretizacijskih tehnika pri simulacijama tokova u poroznoj sredini je metoda konačnih volumena, koja je korištena u ovom radu. Preciznije, proučavana je konvergencija metode konačnih volumena centriranih u središtu elemenata za klasičnu inženjersku shemu. Sličan problem je proučavan u radu [76], gdje je korištena druga verzija globalnog tlaka, definirana u [36]. Globalni tlak je umjetna varijabla koja je ključna za izvod energetske ocjene, i u tu svrhu se često koristi. Dokaz predstavljen u ovom radu se temelji na globalnom tlaku koji je definiran u [5].

Globalni tlak također ima veliku ulogu u modeliranju višekomponentnog toka zbog činjenice da se može korisiti kao perzistentna varijabla. U ovoj disertaciji globalni tlak je korišten za simulaciju nešto jednostavnijeg modela za nemješivi, stlačivi, dvofazni tok fluida. Taj dio radnje nam služi kao temelj za buduća istraživanja vezana za višefazni, višekomponentni tok. Primijenjena numerička metoda je dobivena korištenjem diskretizacije konačnim volumenima. Predložena metoda je verificirana na poznatim testnim primjerima iz literature.

Struktura ove radnje je sljedeća. U poglavlju 1 su dane osnovne definicije i svojstva porozne sredine. Također su predstavljeni modeli koji opisuju jednofazni i dvofazni tok u poroznoj sredini, kao i višekomponentni tok. U ovom poglavlju predstavljeni su i različiti sustavi koji se mogu koristiti za modeliranje toka fluida, temeljeni na različitom izboru primarnih nepoznanica.

U poglavlju 2 predstavljen je teorem egzistencije rješenja modela koji opisuje dvofazni, dvokomponentni tok fluida u poroznoj sredini uz pretpostavku slabe topljivosti plina. Dokaz teorema se sastoji od nekoliko koraka. U prvom koraku sustav je regulariziran zajedno s vremenskim derivacijama kako bi se dobio niz eliptičkih sustava. Teorem egzistencije rješenja spomenutih eliptičkih sustava je dokazan korištenjem Schauderovog teorema o fiksnoj točki. Uvedene su dodatne regularizacije i specijalne test funkcije su primijenjene s ciljem dobivanja energetske ocjene na kojoj se temelji dokaz teorema. Puštanjem limesa u regularizacijskim parametrima eliminirane su vremenska diskretizacija i inicijalna regularizacija kako bi se na limesu dobilo slabo rješenje inicijalo rubne zadaće za dvofazni, dvokomponentni tok fluida.

U poglavlju 3 analizirana je konvergencija klasične inženjerske numeričke metode za nemješivi, stlačivi, dvofazni tok fluida u poroznoj sredini. Na početku poglavlja je predstavljena prostorna diskretizacija konačnim volumenima centriranim u središtu elemenata, kao i vremenska diskretizacija temeljena na implicitnoj Eulerovoj metodi. Nakon toga je definiran globalni tlak koji je ključan za izvod energetske ocjene. Sljedeći korak u dokazu konvergencije je dokaz principa maksimuma za zasićenje. Primjenom odgovarajućih test funkcija izvedena je energetska ocjena, koja je među ostalim korištena i u dokazu egzistencije rješenja sustava diskretnih jednadžbi. Nakon toga je predstavljen dokaz kompaktnosti diskretnog rješenja čime je omogućen prijelaz na limes u diskretnim jednadžbama. Na limesu je dobivena slaba formulacija polazne kontinuirane zadaće.

U poglavlju 4 je predstavljena numerička metoda koja direktno koristi globalni tlak. Predstavljeni su numerički rezultati dobiveni metodom konačnih volumena primjenjenom na nemješivi, stlačivi, dvofazni model. Na početku poglavlja opisana je korištena numerička metoda.

Nakon toga su predstavljeni numerički rezultati za testne primjere u kojima je domena homogena. Predstavljeni testovi su insipirirani poznatim primjerima iz literature. Zatim je promatran slučaj heterogene domene, odnosno domene koja je sastavljena od više različitih tipova stijena. Kod ovakvih testnih primjera javlja se potreba za specijalnim tretmanom granice koja razdvaja pod-domene sastavljene od različitih tipova stijena, koji je potanko opisan u ovom poglavlju. Nakon toga su predstavljeni numerički rezultati dobiveni za testne primjere s heterogenom domenom. Na samom kraju disertacije dan je kratki opis implementacije numeričke metode u biblioteci DuMu^{x} ([43], [66]).

Ključne riječi: tok u poroznoj sredini, dvofazni,nemješivi, stlačivi tok, mješivi tok, perzistentne varijable, slaba topljivost, metoda konačnih volumena, globalni tlak, diskontinuitet u kapilarnom tlaku.

Contents

Introduction

This thesis is closely related to the area of modeling, analysis, and numerical simulations of two-phase flow in porous media. This type of flow appears in many petroleum and environment engineering problems. Some of these problems are secondary and tertiary oil recovery, the disposal of radioactive waste, sequestration of CO_2 etc. Main focus of this work will be on problems regarding nuclear waste management, based on the disposal of the nuclear waste in deep geological formations, see [2]. The design of these storage units is based on the series of impervious barriers which are made from engineered and natural materials. The resulting repository is then a highly heterogeneous porous medium which is almost fully saturated with water. In such conditions the corrosion of the ferrous materials, which are used for manufacturing waste containers, will appear in time. As a result of the corrosion significant amount of the gas, most commonly hydrogen, will appear in the repository. In order to prevent overpressure and possible damage of the metal canisters, which could cause entering of the radionuclides into the biosphere, water-hydrogen flow in host rock should be considered. There are two approaches in modeling water-hydrogen flow in the host rock. Simplified version consists in considering immiscible two-phase flow, but it is also important to note that even though the gas component (hydrogen) is weakly soluble in water, the solubility is still highly important for long term gas migration and the repository pressurization. Therefore, a more complex approach would be to take exchange of the mass between phases into account which leads to partially miscible flow models. When studying the partially miscible fluid flow, the Henry law will be used to determine the amount of the dissolved gas in the liquid.

The mass balance law and the Darcy-Muskat law for each phase are used for modeling two-phase immiscible flow in porous media. The system is completed by adding the equation of state, in order to take compressibility of the fluid into consideration, and the capillary pressure law, which describes the phase pressure difference. In the proposed system there are various options for primary variables choice, such as phase pressures or phase pressure of the one phase and the saturation of the other phase. Another possibility is an introduction of the artificial variable called the global pressure, which can be used as a primary variable, alongside for example the saturation of one phase. The latter variable is of special importance in models describing two-phase flow with exchange of the mass between phases, due to the possible phase disappearance and appearance. In such systems the global pressure can be used as one of the persistent variables, meaning it is well defined even in the case when only one phase is present.

The mathematical theory of incompressible, immiscible, and isothermal two-phase flow through porous media is developed in extensive literature and summarized in several monographs [15, 36, 49] and articles [37, 38, 33, 16]. An analysis of a nonisothermal immiscible incompressible model is presented in [11] where we can find a recent review on the subject. Development of a mathematical theory for compressible, immiscible two-phase flow started with the work of Galusinski and Saad [50, 52, 53] and is further developed in [3, 6, 8, 9, 63, 64, 69, 41, 78, 65]. For the two-phase partially miscible flow model there are far fewer publications. First results for simplified models were obtained in [80] and [71]. More complete two-phase, two-component models were considered in articles [34] and [35]. In [34] the authors replace the phase equilibrium by the first order chemical reactions which are supposed to model the mass exchange between the phases. In [35] the phase equilibrium model is taken into account but the degeneracy of the diffusion terms is eliminated by some nonphysical assumptions. As the diffusion terms in the flow equations are multiplied by the liquid saturation they can be arbitrary small, therefore they do not add sufficient regularity to the system. In this work this degeneracy of the diffusive terms is compensated by the low solubility of the gas component in the liquid phase which keeps the liquid phase composed mostly of the liquid component (water). This compensation allows us to treat the complete two-phase two-component model without any unphysical assumptions on the diffusive parts of the model.

Numerical simulations of two-phase fluid flows have been a subject of an extensive scientific research for a long time. One of the most commonly used discretization technique is the finite volume method. The basic theory and mathematical analysis of the finite volume method on admissible orthogonal meshes is given in [45]. In this thesis the cell-centered finite volume method is used for the discretization of the system of equations describing two-phase flow in porous media. A convergence analysis of the cell-centered finite volume method for classical phase-by-phase upwind scheme in the case of compressible two-phase flow was given in [76], and also in [22] for a simplified model where the gas density depends on the global pressure. In these two references the authors use the global pressure based on the total velocity, defined in

[36]. Here we address the question of the convergence of the classical phase-by-phase upwind scheme by a different technique, using the new compressible model introduced in [5] based on the concept of the global pressure. Additionally, we use an upwind approximation of the phase density, which is more natural approximation than the one presented in [76]. We show convergence of the method for an isotropic model with a piecewise continuous function with finitely many surfaces of discontinuity for absolute permeability, while an isotropic model with constant absolute permeability throughout domain was considered in [76]. We also mention two important articles where authors consider anisotropic model [77, 56].

Final topic covered by this work is a cell-centered finite volume discretization of the two-phase flow equations based on the fractional flow formulation which was introduced in [5]. The main difference between this formulation and the classical engineering formulation is that the upwind is performed with respect to the total flux instead of the phase fluxes. It was expected that such formulation would outperform the classical one in terms of numerical efficiency, since the use of the global pressure reduces the coupling between the partial differential equations in the fractional flow formulation. However, up to now, this formulation did not perform as expected in the case of immiscible compressible two-phase flow. Despite some shortcomings regarding running times seen in numerical simulations in the case of immiscible flow, due to the computation of the global pressure, it is strongly believed that these shortcomings will be insignificant in comparison to the advantages that the global pressure as a persistent variable can bring in case of the two-phase flow with mass exchange between the phases. With this motivation, we present the method, its implementation in DuMu^{x} and results of numerical simulations for immiscible compressible two-phase flow in homogeneous and heterogeneous domains. Numerical methods for heterogeneous domains may need special treatment of the interfaces between control volumes. These kinds of methods are presented in numerous papers, and here we mention the two most relevant for our work. In [30] the authors present the cell-centered finite volume approximation for an immiscible incompressible two-phase flow with discontinuous capillary pressure and in [7] the authors consider a compressible case with vertex-centered finite volume approximation. We also address the question of discontinuous capillary pressure in the numerical model based on the fractional flow formulation with the global pressure as primary variable, which brings additional complexity to the model.

The outline of this thesis is as follows: Chapter 1 contains the basic definitions and properties of a porous medium. Since fluid flow through porous media can be modeled at different scales, a short description of the main differences and connections between these approaches is given. The models describing one-phase and two-phase flow in porous media are also presented, both in case of a single component flow and multicomponent flow. Different choices of primary variables are also discussed in this chapter.

Chapter 2 contains an existence result for two-phase two-component flow in porous media with the low solubility assumption. This result was published in [61]. The main result is proved in several steps. First, the system is regularized and the time derivatives are discretized, obtaining thus a sequence of elliptic problems. Then an existence theorem for the elliptic problems is proved by an application of the Schauder fixed point theorem. Some additional regularizations are performed and special test functions are applied in order to obtain the energy estimate on which the existence theorem is based. By passing to zero in the regularization parameters, the time discretization and the initial regularization of the system are eliminated. At the limit, a weak solution to the initial boundary value problem for two-phase, two-component flow model is obtained.

Chapter 3 contains the convergence analysis of the classical engineering numerical finite volume method for immiscible, compressible, two-phase flow in porous media model. First, the spatial discretization based on the cell-centered finite volume method is presented, along the implicit Euler method for the time discretization leading to a fully coupled fully implicit scheme. Then, a discretization of the corresponding fractional flow formulation is developed, which is used in the convergence proof. In the following section the maximum principle for the water saturation is proved. By applying suitable test functions the energy estimate is derived, and it is used to prove the existence of a solution to discrete equations. Afterwards, the compactness of the solution vector is proved and after passing to the limit in the discrete equations, the weak formulation for the initial boundary value problem for immiscible, compressible, two-phase flow model is obtained.

At the beginning of Chapter 4 a cell-centered finite volume method for the fractional flow formulation describing immiscible, compressible, two-phase fluid flow through porous media is developed. The method is based on the global pressure as a primary variable. Afterwards, numerical results obtained by the proposed method are presented in tests involving homogeneous domains. Presented test cases are inspired by some known benchmark problems from [28, 56, 58, 13]. Domains composed of multiple rock types are then considered and a special treatment of the interface between different rock types is developed. The method is tested on test cases from the literature [28]. At the end, in the Appendix, we give a brief description of implementation of the numerical method in the platform DuMu^{x}.

Chapter 1

Modeling two-phase flow in porous media

This chapter gives the basic definitions and equations for modeling immiscible compressible two-phase flow in porous media. In section 1.1 we give the definition of a porous medium and its basic properties and in section 1.2 we give main laws for modeling one-phase flow in porous media. In section 1.3 we present model describing two-phase flow, both for immiscible and partially miscible fluid flows. This chapter follows references [18], [19], [20], [36], and [84].

1.1 Porous media

In this section we describe the main properties of porous media. We also give few examples of porous media domains and introduce different scales that can be used to model fluid flow through porous media.

1.1.1 Basic definitions

A porous medium is a medium composed of a *solid matrix* and a *void space* or *pore space*. The solid matrix represents a persistent solid part, while the pore space can be occupied by a single fluid, or by a number of fluids. Some of the examples are soil, sand, fissured rock, cemented sandstone, etc.

In [20] a *phase* is defined as a chemically homogeneous portion of a system under consideration that is separated from other such portions by a definite physical boundary (interface, or interphase boundary). This definition allows us to consider the solid matrix as a solid phase. When studying single phase flow we distinguish the case when the system is composed of only one fluid and the case when the system is composed of several fluids completely *miscible* with each other (e.g. several gases). If the void space is occupied by two or more fluids which are *immiscible* with each other, we talk about multiphase flow.

A *component* is defined as part of a phase that is composed of an identifiable homogeneous chemical species, or of an assembly of species, see [20]. It is also noted that each phase can be a molecular mixture of several identifiable components, e.g., ions or molecules of different chemical species in a liquid solution, or in a mixture of gases, or labelled particles of a phase.

The main properties that need to be satisfied in order to derive mathematical models for fluid flow through porous media are given in [40] and [18]:

- *The void space is interconnected.*
- *The dimensions of the void space must be large compared to the mean free path length of the fluid molecules.* This property allows application of the continuum approach to modeling of fluid flow.
- *The dimensions of the void space must be small enough so that the fluid flow is controlled by adhesive forces at fluid–solid interfaces and cohesive forces at fluid–fluid interfaces (multiphase systems).* This property eliminates network pipes from domains considered to be a porous medium.

1.1.2 Continuum approach

The basic definitions and concepts modeling fluid flow through porous media can be given at *molecular*, *microscopic* and *macroscopic* scale. A discussion about the main differences and connections between these approaches is given in [59] and we here present a brief summary of the given ideas.

Some fluid properties, such as viscosity, density, binary diffusion coefficients, are based on molecular variables, which means that they are determined at the molecular scale. Due to the large number of molecules, consideration of individual molecules for description of fluid flow is not feasible. Therefore, consideration of the continuum is taken into account. This concept is based on the averaging process, which consists of replacement of the properties that are important for molecular consideration by combined properties of a larger number of molecules. This means that the individual molecules on the molecular scale are replaced by a hypothetical continuum on the microscopic scale, as explained in [18]. This process leads to Navier-Stokes equations, with assigned boundary conditions. The solving of the Navier-Stokes equations at the microscopic scale is also not practical, since the pore space geometry is unknown. Therefore, one usually used is the macroscopic scale model. In this model a different kind of continuum is considered. Instead of averaging over a large number of molecules, averaging is done over elementary volume. In the macroscopic scale model each point in the continuum is associated to the elementary volume which is composed of both solid matrix and pore space. Average values of quantities on the microscopic scale are assigned to the elementary volume. Process of averaging on the macroscopic scale is described more precisely in the next subsection 1.1.3 by defining *porosity* of the porous medium. The transition from microscopic to macroscopic scale leads to the new set of equation (e.g. Darcy's law) with new variables (e.g. saturation).

1.1.3 Porous medium properties

One of the basic macroscopic properties of porous media is *porosity*. In order to define this quantity, we first introduce the pore space indicator function on the microscopic scale

$$\varphi(x) = \begin{cases} 1 & \text{if } x \in \text{ pore space} \\ 0 & \text{if } x \in \text{ solid matrix} \end{cases} \qquad \forall x \in \Omega, \tag{1.1}$$

where we have supposed that a porous medium fills the domain Ω. Now we give the definition of the porosity $\Phi(x_0)$ at the position x_0

$$\Phi(x_0) = \frac{1}{\text{meas}(K(x_0,r))} \int_{K(x_0,r)} \varphi(x)dx. \tag{1.2}$$

The averaging volume $K(x_0,r)$ is called *representative elementary volume* (REV). In order to set fluid flow equations on the macroscopic level, REV has to be identified. This rises a question of the size of the radius of the averaging volume. In [19] it has been shown that if we denote the characteristic dimension of the REV by d (e.g. diameter of a sphere), the length characterizing the microscopic structure of the void space by l (e.g. the hydraulic radius which is equal to the reciprocal of the specific surface area of the void space), and by L a characteristic length of the porous medium domain, over which significant changes in averaged quantities of interest occur, we have upper and lower bound for size d:

$$l \leq d \leq L.$$

Another macroscopic property of the porous medium, which depends solely on properties of the solid matrix, is the absolute permeability $\mathbb{K}$. The absolute permeability measures the ability of the porous medium to transmit the fluid.

A porous medium is said to be *homogeneous* if its macroscopic properties do not vary in space or time. Otherwise, it is said to be *heterogeneous*. The absolute permeability $\mathbb{K}$ is usually a symmetric tensor. This quantity can vary with direction, and in that case the porous medium is said to be *anisotropic*. If the absolute permeability does not vary with direction, meaning $\mathbb{K} = k\mathbb{I}$, the porous medium is said to be *isotropic*.

1.2 One-phase flow in porous media

In this section macroscopic equations and laws describing flow and transport of the single-phase fluid in porous media are considered.

1.2.1 Mass conservation law

If only one phase is present in a porous medium $\Omega \subset \mathbb{R}^l$ the macroscopic mass conservation law is valid and it states [18], [36]:

$$\Phi \frac{\partial \rho(p)}{\partial t} + \operatorname{div}(\rho(p)\mathbf{q}) = F. \tag{1.3}$$

The quantities that appear in the previous equation, which have not been mentioned before are described here:

- ρ - mass density of the fluid in $\mathrm{kg/m^3}$. Mass density of the fluid generally depends also on the temperature of the fluid T, beside the fluid pressure p. Since, in this work only isothermal flow is considered, we omit writing dependence of density on the temperature. For incompressible fluid the mass density ρ is constant and in case of compressible fluid it will be given by the equation of state $\rho = \rho(p)$, where p is the fluid pressure. One of the possible equations of state for a gas phase is the ideal gas law which states

  $$\rho(p) = \frac{pM}{RT},$$

  where R is the universal gas constant ($R = 8.21\mathrm{JK^{-1}mol^{-1}}$) and M is the fluid molar mass.

- $\mathbf{q}$ - macroscopic apparent velocity. It is given by Darcy's law that will be described in subsection 1.2.2. Macroscopic velocity is given by $\mathbf{q}/\Phi$ since only pore space in REV is filled with fluid.

- F - source/sink term.

1.2.2 Darcy's law

Darcy's law gives the relation between the macroscopic apparent velocity, also called Darcy velocity, and the gradient of fluid pressure, see e.g. [82],

$$\mathbf{q} = -\frac{1}{\mu}\mathbb{K}(\nabla p - \rho \mathbf{g}), \tag{1.4}$$

where $\mathbf{g}$ is the gravitational, downward-pointing, constant vector and μ is *dynamic viscosity* of the fluid in $\mathrm{Pa}\cdot\mathrm{s}$. The dynamic viscosity can depend on temperature and pressure of the fluid, but in this work it will be taken as a constant value. Introducing (1.4) into (1.3) we obtain the model that describes single-phase flow in porous media

$$\Phi\frac{\partial \rho(p)}{\partial t} - \operatorname{div}\left(\frac{\rho(p)}{\mu}\mathbb{K}(\nabla p - \rho(p)\mathbf{g})\right) = F \quad \text{in } \Omega. \tag{1.5}$$

Initial and boundary conditions have to be assigned to this equation e.g.

$$p(x,0) = p^0(x), \quad p(x,t) = p^D(x,t) \text{ on } \Gamma_D, \quad \rho(p)\mathbf{q}\cdot\mathbf{n} = q^N \text{ on } \Gamma_N,$$

where the domain boundary is composed of the Dirichlet and the Neumann boundary $\partial\Omega = \Gamma_D \cup \Gamma_N$.

1.2.3 One-phase multicomponent flow

In this subsection we consider the flow of a single fluid which is a mixture of different components, e.g. mixture of different gases. Transport of each component in the mixture is a result of a phase transport and also interactions between components inside the mixture.

In order to describe a phase composition we introduce, like in [18], a *fraction of the component in the mixture*, precisely

- *volume fraction of the component i*

$$C^i(x,t) = \frac{\text{volume of the component } i \text{ in REV}}{\text{volume of the mixture in REV}},$$

- *mass fraction of the component i*

$$X^i(x,t) = \frac{\text{mass of the component } i \text{ in REV}}{\text{mass of the mixture in REV}}.$$

With the same purpose the *mass concentration of the component i* in the mixture in $\mathrm{kg/m^3}$ is defined as

$$\rho^i = \frac{\text{mass of the component } i \text{ in REV}}{\text{volume of the mixture in REV}}. \tag{1.6}$$

In this work we will mainly use the mass concentration of the component, therefore we will give here a governing equation in terms of this quantity.

Using definition (1.6) the mass density of the fluid composed of n components can be written as

$$\rho = \sum_{i=1}^{n} \rho^i.$$

Inside the mixture different components have different velocities, therefore the mass balance law for each component have to be taken into consideration. In order to simplify notation in the rest of the section, we will consider the fluid composed of only two components. Components will be denoted by upper indicies 1 and 2. If the Darcy velocity of the mixture is denoted by $\mathbf{q}$ the mixture flux is a sum of the fluxes of each component (see [24])

$$\rho \mathbf{q} = \rho^1 \mathbf{q}^1 + \rho^2 \mathbf{q}^2.$$

This equation enables as to rewrite the component fluxes in the following way

$$\rho^i \mathbf{q}^i = \rho^i \mathbf{q} + \mathbf{j}^i, \quad \mathbf{j}^i = \rho^i (\mathbf{q}^i - \mathbf{q}), \quad i = 1,2. \tag{1.7}$$

The first part in expression for $\rho^i \mathbf{q}$ is called *convective flux* and the remaining part $\mathbf{j}^i$ is called *diffusive flux*. The diffusive fluxes satisfy

$$\mathbf{j}^1 + \mathbf{j}^2 = 0,$$

and they can be given by the Fick law (see [24, 20])

$$\mathbf{j}^1 = -\Phi \rho D_{12} \nabla X^1, \quad \mathbf{j}^2 = \Phi \rho D_{21} \nabla X^2. \tag{1.8}$$

Since $\mathbf{j}^1 + \mathbf{j}^2 = 0$ and $X^1 + X^2 = 1$, we have $D_{12} = D_{21} = D$. The coefficient D is called diffusion coefficient. More elaborate description of the diffusion coefficient D can be found in [59].

The mass conservation law for component i is given by equation

$$\Phi\partial_t\rho^i + \mathrm{div}(\rho^i\mathbf{q}^i) = F^i, \tag{1.9}$$

where F^i is the source/sink term of the component i. Introducing (1.7), (1.8), and $\rho^i = \rho X^i$ in (1.9), the mass balance equation can be written as

$$\Phi\partial_t(\rho X^i) + \mathrm{div}\left(\rho X^i\mathbf{q} - \Phi\rho D\nabla X^i\right) = F^i. \tag{1.10}$$

By summing equations (1.10) over components, the mass conservation law for mixture is obtained:

$$\Phi\partial_t\rho + \mathrm{div}\,(\rho\mathbf{q}) = F^1 + F^2.$$

1.3 Two-phase flow in porous media

In this section we will consider flow of two different fluids, which fill the whole pore space. Since each point on the macroscopic scale represents one representative elementary volume, we will have the presence of two different fluids in the macroscopic point. In the rest of this section we will denote different phases by lower indices 1 and 2. In order to describe this kind of flow, additional quantities have to be introduced.

1.3.1 Saturation

Saturation S_i describes quantity of phase i at the point x_0 of the porous medium,

$$S_i = \frac{\text{volume of phase } i \text{ in REV}}{\text{volume of the pore space in REV}}.$$

We can rewrite more precisely this definition if we first define indicator function of phase i like in [18] and [84]

$$\gamma_i(x,t) = \begin{cases} 1 & \text{if } x \in \text{ phase } i \text{ at time } t \\ 0 & \text{otherwise} \end{cases}, \quad x \in \Omega.$$

With this definition we obtain

$$S_i(x_0,t) = \frac{\int_{K(x_0,r)} \gamma_i(x,t)dx}{\int_{K(x_0,r)} \varphi(x)dx}, \tag{1.11}$$

where the function φ is given by (1.1). Like it is already been said, in this work we will assume that there is no void space present, which means that

$$S_1 + S_2 = 1.$$

1.3.2 Capillary pressure

In a two-phase system considered on the microscopic scale, two fluids are separated by the curved interface. Shape of the interface is determined by the surface tension σ, which is defined (see [21]) as the ratio of the amount of work ΔW necessary to enlarge the area of the interface by ΔA,

$$\sigma = \frac{\Delta W}{\Delta A}. \tag{1.12}$$

Due to this phenomena we distinguish *wetting* and *nonwetting* phase in the two-phase system. The fluid on the concave side of the interface is called the nonwetting fluid because it is less attracted to the solid than the other fluid and the fluid on the convex side of the interface is called the wetting fluid since it preferentially wets the solid, see [21, 74]. In accordance with the previous definition, we will use indices w and n instead of the indices 1 and 2, in order to distinguish wetting and nonwetting fluid, and associated properties.

The interface between phases is related to the discontinuity in the microscopic pressure of the existing phases. This jump in the microscopic pressure is called the *capillary pressure*

$$p_c = p_n - p_w, \tag{1.13}$$

and it is given by the *Young–Laplace law*

$$p_c = \sigma \left(\frac{1}{R_1} + \frac{1}{R_2} \right), \tag{1.14}$$

where R_1 and R_2 are principal radii of the curvature of the interface between two fluids. As already mentioned, the macroscopic phase pressures represent average values over the representative elementary volume of the microscopic phase pressures. Therefore, (1.13) is also used as the definition of the macroscopic capillary pressure. Since there is no interface between phases on the macroscopic scale, the Young–Laplace law is not valid. The macroscopic capillary pressure is usually taken as a decreasing function of the wetting phase saturation (or an increasing function of the nonwetting phase saturation)

$$p_c = p_c(S_w).$$

This assumption can be justified as in [21, 74], if one considers the case when both phases are present in a porous medium made up of sand grains. Based on the microscopic consideration of the capillary pressure, one would expect that the wetting phase will be drawn into the smaller pores. When the wetting phase is in the smaller pores the curvature of the interface between two phases will be greater than when it is in the larger pores, therefore the capillary pressure will be higher. This also means that as the relative amount of wetting phase decreases, the more high curvature interfaces will appear between the phases.

An attempt of draining completely the wetting phase from the domain by introducing the nonwetting phase may leave some residual wetting phase in the pore space at some low saturation S_{wr}, usually greater than zero. This value is called the *wetting phase residual saturation*. The capillary pressure function has vertical asymptote at S_{wr}. Instead of drainage of the wetting phase, one can consider the opposite process, imbibition. Again, the complete displacement of the nonwetting phase is usually not possible, which means that the saturation of the nonwetting phase cannot be below *the nonwetting phase residual saturation* S_{nr}.

Driven by previous considerations the effective saturation of the phase can be defined with

$$S_{we} = \frac{S_w - S_{wr}}{1 - S_{wr} - S_{nr}}, \quad S_{ne} = \frac{S_n - S_{nr}}{1 - S_{wr} - S_{nr}}. \tag{1.15}$$

Let us note that for the effective saturation we also have $S_{we} + S_{ne} = 1$. The capillary pressure curve is usually given as a function of S_{we}. Most commonly used models for capillary pressure curve are the *Van Genuchten* model, see e.g. [81],

$$p_c(S_{we}) = \frac{1}{\alpha}(S_{we}^{-\frac{1}{m}} - 1)^{\frac{1}{n}}, \quad S_{we} \in (0,1], \tag{1.16}$$

where $m = 1 - \frac{1}{n}$, and the *Brooks–Corey* model, see e.g. [32],

$$p_c(S_{we}) = P_d S_{we}^{-\frac{1}{\lambda}}, \quad S_{we} \in (0,1]. \tag{1.17}$$

Remark 1.3.1. *For the purposes of numerical analysis we will assume for simplicity that the capillary pressure function satisfies $p_c \in C^1([0,1])$. Let us note that this assumption is not completely arbitrary, since it is standard procedure to regularize capillary pressure curve when performing numerical simulations, even though the physical capillary pressure has vertical asymptote at S_{wr}. By performing more detailed analysis this assumption can be eliminated in most of the applications.*

1.3.3 Darcy–Muskat's law

It has been shown experimentally that Darcy's law stays valid in the case of a two-phase flow, see e.g. [20, 21, 36], and has the form:

$$\mathbf{q}_n = -\frac{kr_n(S_w)}{\mu_n}\mathbb{K}\left(\nabla p_n - \rho_n \mathbf{g}\right), \tag{1.18}$$

$$\mathbf{q}_w = -\frac{kr_w(S_w)}{\mu_w}\mathbb{K}\left(\nabla p_w - \rho_w \mathbf{g}\right), \tag{1.19}$$

where $kr_n(S_w)$ and $kr_w(S_w)$ are the relative permeability functions. The ratio $\lambda_\alpha(S_w) = kr_\alpha(S_w)/\mu_\alpha$ is referred to as the *mobility of the phase* α, $\alpha = w, n$, and the sum of the mobilities $\lambda(S_w) = \lambda_n(S_w) + \lambda_w(S_w)$ as the *total mobility*. The relative permeability of the phase is used to model the fact that phase will be more mobile, as the phase saturation in a porous medium is increasing. If the phase is missing, its relative permeability function vanishes,

$$kr_w(S_{we} = 0) = 0, \quad kr_n(S_{ne} = 0) = 0.$$

The most commonly applied models are the *Brooks–Corey*:

$$\begin{aligned} kr_w(S_{we}) &= S_{we}^{\frac{2+3\lambda}{\lambda}}, \\ kr_n(S_{we}) &= (1 - S_{we})^2\left(1 - S_{we}^{\frac{2+\lambda}{\lambda}}\right), \end{aligned} \tag{1.20}$$

where λ is the coefficient from the Brooks–Corey $p_c - S_w$ relationship, and the *Van Genuchten* model,

$$\begin{aligned} kr_w(S_{we}) &= S_{we}^{\varepsilon}\left(1 - \left(1 - S_{we}^{\frac{1}{m}}\right)^m\right)^2, \\ kr_n(S_{we}) &= (1 - S_{we})^{\gamma}\left(1 - S_{we}^{\frac{1}{m}}\right)^{2m}, \end{aligned} \tag{1.21}$$

where the parameter m is the parameter from the Van Genuchten capillary pressure function. The remaining two parameters ε and γ describe the connectivity of the pores. The most commonly used values are $\varepsilon = \frac{1}{2}$ and $\gamma = \frac{1}{3}$, see more in [59].

Remark 1.3.2. *For simplicity we have assumed in mathematical and numerical analysis that* $S_{wr} = 0$ *and* $S_{nr} = 0$*, meaning* $S_w = S_{we}$ *and* $S_n = S_{ne}$*. It is also standard to assume that 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_j *is a nondecreasing functions of* S_j*. Moreover, we assume that there exist constants* $\lambda_M \geq \lambda_m > 0$ *such that for all* $S_w \in [0,1]$

$$0 < \lambda_m \leq \lambda_w(S_w) + \lambda_n(S_w) \leq \lambda_M.$$

1.3.4 Two-phase flow governing equations

Let the porous medium fills domain $\Omega \subset \mathbb{R}^l$. Two-phase flow in domain $Q_T = \Omega \times (0,T)$, for some $T > 0$, is modeled by the mass conservation law for each phase, the Darcy–Muskat law and the capillary pressure law

$$\Phi \frac{\partial(\rho_n S_n)}{\partial t} + \operatorname{div}(\rho_n \mathbf{q}_n) = F_n, \tag{1.22}$$

$$\Phi \frac{\partial(\rho_w S_w)}{\partial t} + \operatorname{div}(\rho_w \mathbf{q}_w) = F_w, \tag{1.23}$$

$$\mathbf{q}_n = -\lambda_n(S_w)\mathbb{K}(\nabla p_n - \rho_n \mathbf{g}), \tag{1.24}$$

$$\mathbf{q}_w = -\lambda_w(S_w)\mathbb{K}(\nabla p_w - \rho_w \mathbf{g}), \tag{1.25}$$

$$p_c(S_w) = p_n - p_w, \tag{1.26}$$

where F_n and F_w are the source terms. Additionally, we have $S_w + S_n = 1$.

If we look closely at the given system of equations, we observe that we can choose two primary variables and we can use them to compute the remaining unknowns. In [59] it is given an elaborate description of different choices of the primary variables. Most commonly used is, so-called saturation-pressure formulation, which uses pressure of the one phase and saturation of the other phase as primary unknowns. If we choose p_n and S_w as primary variables we will obtain following system of equations:

$$\Phi \frac{\partial(\rho_n(p_n)(1-S_w))}{\partial t} - \operatorname{div}(\rho_n(p_n)\lambda_n(S_w)\mathbb{K}(\nabla p_n - \rho_n(p_n)\mathbf{g})) = F_n, \tag{1.27}$$

$$\begin{aligned} \Phi \frac{\partial(\rho_w(p_n - p_c(S_w))S_w)}{\partial t} - \operatorname{div}\Big(&\rho_w(p_n - p_c(S_w))\lambda_w(S_w)\mathbb{K}(\nabla p_n - \nabla p_c(S_w)) \\ &-\rho_w(p_n - p_c(S_w))\mathbf{g})\Big) = F_w. \end{aligned} \tag{1.28}$$

This system has to be completed with initial and boundary conditions. The most commonly used choice is

$$\begin{aligned} p_n(x,0) = p_n^0(x), \quad S_w(x,0) = S_w^0(x), \\ p_n(x,t) = p_n^D(x,t), \quad S_w(x,t) = S_w^D(x,t) \text{ on } \Gamma_D, \\ \rho(p_n)\mathbf{q}_n \cdot \mathbf{n} = q_n^N, \quad \rho(p_w)\mathbf{q}_w \cdot \mathbf{n} = q_w^N \text{ on } \Gamma_N, \end{aligned}$$

where domain boundary is subdivided as $\partial\Omega = \Gamma_D \cup \Gamma_N$. One of the possible choices for the primary unknown is also an artificial variable called *global pressure*, which can be defined in two different ways. We will closely describe these two formulations in the next subsection.

1.3.5 Global pressure formulation

Global pressure definition based on the total velocity. In order to present the first definition of the global pressure from [15], we will first introduce the term *total velocity* $\mathbf{q} = \mathbf{q}_n + \mathbf{q}_w$. After introducing (1.18) and (1.19) in the total velocity definition we obtain

$$\mathbf{q} = -\lambda \mathbb{K} (\nabla p_w + f_n \nabla p_c - b_g \mathbf{g}), \tag{1.29}$$

where the following notation has been used

$$\begin{aligned} f_w(S_w) &= \lambda_w(S_w)/\lambda(S_w), \\ f_n(S_w) &= \lambda_n(S_w)/\lambda(S_w), \\ b_g(S_w, p_w, p_n) &= \frac{\rho_w(p_w)\lambda_w(S_w) + \rho_n(p_n)\lambda_n(S_w)}{\lambda(S_w)}. \end{aligned} \tag{1.30}$$

The functions $f_w(S_w)$ and $f_n(S_w)$ are called *fractional flow* functions. The equation (1.29) can be written as the Darcy law of some artificial pressure p, so-called global pressure, by imposing

$$\nabla p = \nabla p_w + f_n \nabla p_c.$$

For this equation to hold it is sufficient to define the global pressure p as,

$$p = p_w + \overline{P}(S_w), \quad \overline{P}(S_w) = -\int_{S_w}^{1} f_n(s) p_c'(s) ds. \tag{1.31}$$

It can easily be shown that the global pressure p given by (1.31) satisfies

$$p_w \leq p \leq p_n.$$

By introducing the functions

$$\gamma(S_w) = \sqrt{\frac{\lambda_w(S_w)\lambda_n(S_w)}{\lambda(S_w)}}, \quad \alpha(S_w) = -\gamma(S_w) p_c'(S_w) \text{ and } \beta(S_w) = \int_0^{S_w} \alpha(s)\, ds, \tag{1.32}$$

one can write formally

$$\begin{aligned} \lambda_n(S_w)\nabla p_n &= \lambda_n(S_w)\nabla p - \gamma(S_w)\nabla\beta(S_w), \\ \lambda_w(S_w)\nabla p_w &= \lambda_w(S_w)\nabla p + \gamma(S_w)\nabla\beta(S_w). \end{aligned} \tag{1.33}$$

These two equations hold true a.e. in Q_T if $p, \beta(S_w) \in H^1(\Omega)$ for a.e. $t \in (0,T)$. From here one can easily conclude that the equality (1.34) holds, which is of fundamental importance in the two-phase flow existence theory:

$$\lambda_w(S_w)\mathbb{K}\nabla p_w \cdot \nabla p_w + \lambda_n(S_w)\mathbb{K}\nabla p_n \cdot \nabla p_n = \lambda(S_w)\mathbb{K}\nabla p \cdot \nabla p + \mathbb{K}\nabla\beta(S_w) \cdot \nabla\beta(S_w). \tag{1.34}$$

By summing the equations (1.22) and (1.23) and introducing

$$\mathbf{q} = -\lambda \mathbb{K}(\nabla p - b_g \mathbf{g}),$$
$$\mathbf{q}_n = f_n \mathbf{q} - \mathbb{K}\left(\gamma(S_w)\nabla\beta(S_w) + \frac{\lambda_w(S_w)\lambda_n(S_w)}{\lambda(S_w)}(\rho_w - \rho_n)\mathbf{g}\right),$$
$$\mathbf{q}_w = f_w \mathbf{q} + \mathbb{K}\left(\gamma(S_w)\nabla\beta(S_w) + \frac{\lambda_w(S_w)\lambda_n(S_w)}{\lambda(S_w)}(\rho_w - \rho_n)\mathbf{g}\right),$$

we obtain the equation in terms of the global pressure and the saturation:

$$\Phi\partial_t(\rho_n S_n + \rho_w S_w) - \mathrm{div}((\rho_n\lambda_n + \rho_w\lambda_w)\nabla p - (\rho_w - \rho_n)\gamma(S_w)\mathbb{K}\nabla\beta(S_w)) + \mathrm{div}\left((\rho_w^2\lambda_w + \rho_n^2\lambda_n)\mathbb{K}\mathbf{g}\right) = F_n + F_w. \tag{1.35}$$

The equation (1.35) is usually referred to as the global pressure equation. The system is completed by the so-called saturation equation which can be taken as either one of the equations (1.22) and (1.23), where the phase pressures are expressed in terms of the global and capillary pressure. In that way the following system is obtained:

$$\Phi\partial_t(\rho_n S_n + \rho_w S_w) - \mathrm{div}((\rho_n\lambda_n + \rho_w\lambda_w)\nabla p - (\rho_w - \rho_n)\gamma(S_w)\mathbb{K}\nabla\beta(S_w)) + \mathrm{div}\left((\rho_w^2\lambda_w + \rho_n^2\lambda_n)\mathbb{K}\mathbf{g}\right) = F_n + F_w, \tag{1.36}$$

$$\Phi\partial_t(\rho_n S_n) + \mathrm{div}\Big(\rho_n\Big(f_n\mathbf{q} - \mathbb{K}\Big(\gamma(S_w)\nabla\beta(S_w) + \frac{\lambda_w(S_w)\lambda_n(S_w)}{\lambda(S_w)}(\rho_w - \rho_n)\mathbf{g}\Big)\Big)\Big) = F_n. \tag{1.37}$$

For the primary variables in the system one can take the global pressure and the capillary pressure or the saturation of one of the phases. Let us note that in the incompressible case the system (1.36)–(1.37) can be rewriten as:

$$-\mathrm{div}(\lambda\mathbb{K}(\nabla p - b_g\mathbf{g})) = \frac{F_n}{\rho_n} + \frac{F_w}{\rho_w}, \tag{1.38}$$

$$\Phi\frac{\partial S_n}{\partial t} + \mathrm{div}\left(f_n\mathbf{q} - \mathbb{K}\left(\gamma(S_w)\nabla\beta(S_w) + \frac{\lambda_w(S_w)\lambda_n(S_w)}{\lambda(S_w)}(\rho_w - \rho_n)\mathbf{g}\right)\right) = \frac{F_n}{\rho_n}. \tag{1.39}$$

The system (1.38)–(1.39) has a clear mathematical form: an elliptic equation, (1.38), for the pressure p and a convection-diffusion equation, (1.39), for the saturation S_w. In the compressible case this simple form is lost.

The global pressure based on total velocity has been used in the numerous scientific papers describing two-phase flow in porous media and here we will mention some of the most important results. In an analysis of the immiscible, incompressible two-phase flow we highlight [15, 16, 37, 38, 41]. In the immiscible, compressible fluid flow analysis we mention [50, 51, 53] where some approximate models based on the global pressure were considered. Some more general models were considered in [54, 63, 64], where the global pressure was used in the existence proof. Recently immiscible, compressible two phase flow with mass exchange between the phases has been considered in [34, 35, 61], where also the global pressure was used in the existence proof. For numerical simulations based on the concept of the global pressure we mention [56, 30, 72]. We would also want to highlight results from [46, 76, 22] where the global pressure was used in the convergence proof of numerical methods.

Global pressure definition based on the total flux. The second, slightly different, approach in defining global pressure from [5] is based on introducing *total flux*

$$\mathbf{Q}_t = \rho_w(p_w)\mathbf{q}_w + \rho_n(p_n)\mathbf{q}_n$$

and on summation of the equations (1.22)–(1.23) which leads to the following equations:

$$\begin{aligned}\Phi\partial_t(S_w\rho_w(p_w)+S_n\rho_n(p_n)) - \operatorname{div}(\lambda(S_w,p_n)\mathbb{K}(\nabla p_n - f_w(S_w,p_n)\nabla p_c(S_w)))&\\ +\operatorname{div}(\lambda(S_w,p_n)\rho(S_w,p_n)\mathbb{K}\mathbf{g}) = F_w+F_n&,\end{aligned} \tag{1.40}$$

$$\Phi\partial_t\left(S_n\rho_n(p_n)\right)+\operatorname{div}(f_n(S_w,p_n)\mathbf{Q}_t - b_g(S_w,p_n)\mathbb{K}\mathbf{g}) + \operatorname{div}(a(S_w,p_n)\mathbb{K}\nabla S_w) = F_w, \tag{1.41}$$

where we have denoted

$$\mathbf{Q}_t = -\lambda(S_w,p_n)\mathbb{K}\left(\nabla p_n - f_w(S_w,p_n)\nabla p_c(S_w) - \rho(S_w,p_n)\mathbf{g}\right). \tag{1.42}$$

In the system (1.40)–(1.41) following notation was used (for simplicity some notations are the same as in the first part of the subsection)

$$\begin{aligned}\lambda(S_w,p_n) &= \rho_w(p_w)\lambda_w(S_w)+\rho_n(p_n)\lambda_n(S_w),\\ f_w(S_w,p_n) &= \rho_w(p_w)\lambda_w(S_w)/\lambda(S_w,p_n),\\ f_n(S_w,p_n) &= \rho_n(p_n)\lambda_n(S_w)/\lambda(S_w,p_n),\\ \rho(S_w,p_n) &= (\lambda_w(S_w)\rho_w(p_w)^2+\lambda_n(S_w)\rho_n(p_n)^2)/\lambda(S_w,p_n),\\ \alpha(S_w,p_n) &= \rho_w(p_w)\rho_n(p_n)\lambda_w(S_w)\lambda_n(S_w)/\lambda(S_w,p),\\ b_g(S_w,p_n) &= (\rho_w(p_w)-\rho_n(p_n))\alpha(S_w,p_n),\\ a(S_w,p_n) &= -\alpha(S_w,p_n)p_c'(S_w).\end{aligned} \tag{1.43}$$

The phase fluxes can also be expressed as fractions of the total flux $\mathbf{Q}_t$:

$$\rho_w(p_w)\mathbf{q}_w = f_w(S_w,p_n)\mathbf{Q}_t - a(S_w,p_n)\mathbb{K}\nabla S_w + b_g(S_w,p_n)\mathbb{K}\mathbf{g}, \tag{1.44}$$

$$\rho_n(p_n)\mathbf{q}_n = f_n(S_w,p_n)\mathbf{Q}_t + a(S_w,p_n)\mathbb{K}\nabla S_w - b_g(S_w,p_n)\mathbb{K}\mathbf{g}. \tag{1.45}$$

By using the same reasoning as in the first part, one can take the following equality as the definition of the global pressure p:

$$\nabla p_n - f_w(S_w,p_n)p_c'(S_w)\nabla S_w = \omega(S_w,p)\nabla p, \tag{1.46}$$

where the function $\omega(S_w,p)$ is needed and will be defined later in this subsection. The equation (1.46) can be satisfied if the global pressure p and the nonwetting phase pressure p_n are related by

$$p_n = \pi(S_w,p),$$

where the function π is given as a solution to the Cauchy problem:

$$\begin{cases} \dfrac{d\pi(S_w,p)}{dS_w} = \dfrac{\rho_w(\pi(S_w,p)-p_c(S_w))\lambda_w(S_w)p_c'(S_w)}{\rho_w(\pi(S_w,p)-p_c(S_w))\lambda_w(S_w)+\rho_n(\pi(S_w,p)))\lambda_n(S_w)}, & S<1 \\ \pi(1,p) = p. \end{cases} \tag{1.47}$$

Here we assume that $p_c(S_w=1)=0$; for the case $p_c(S_w=1)\neq 0$ see Remark 1.3.5.

Remark 1.3.3. *From (1.47) and Remark 1.3.1 it easily follows that there exists a constant $M>0$ such that*

$$p - M \leq p_w \leq p, \quad p \leq p_n \leq p+M.$$

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

$$\omega(S_w,p) = \frac{\partial \pi(S_w,p)}{\partial p} = \frac{\partial p_w(S_w,p)}{\partial p}. \tag{1.48}$$

In [5] it is shown that $\omega(S_w,p)$ solves the problem

$$\begin{cases} \frac{\partial \omega(S_w,p)}{\partial S_w} = \partial_\pi f_w(S_w,\pi(S_w,p))p_c'(S_w)\omega(S_w,p) \\ \omega(1,p) = 1, \end{cases} \tag{1.49}$$

and it can be written as,

$$\omega(S_w,p) = \exp\left(\int_{S_w}^1 (\nu_n(s,p)-\nu_w(s,p))\frac{\rho_w(p_w(s,p))\rho_n(p_n(s,p))\lambda_n(s)\lambda_w(s)p_c'(s)}{(\rho_w(p_w(s,p))\lambda_w(s)+\rho_n(p_n(s,p))\lambda_n(s))^2}\,ds\right), \tag{1.50}$$

where the following notation is used

$$\nu_w(S_w,p) = \frac{\rho_w'(\pi(S_w,p)-p_c(S_w))}{\rho_w(\pi(S_w,p)-p_c(S_w))}, \quad \nu_n(S_w,p) = \frac{\rho_n'(\pi(S_w,p))}{\rho_n(\pi(S_w,p))}.$$

Remark 1.3.4. *For purposes of numerical analysis we assume that $\rho_n, \rho_w \in C^1(\mathbb{R})$ are increasing functions and that there are constants $\rho_m, \rho_M, \rho_M^d > 0$ such that for all $p \in \mathbb{R}$ it holds*

$$\rho_m \le \rho_\alpha(p) \le \rho_M, \quad \rho_\alpha'(p) \le \rho_M^d, \quad \alpha = w, n.$$

Then it is easy to see that there are constants ω_m, ω_M such that for all $S \in [0,1]$ and $p \in \mathbb{R}$, it holds

$$0 < \omega_m \le \omega(S,p) \le \omega_M < +\infty.$$

With this approach one has to define saturation potential in a slightly different way since in this case the total mobility λ depends on the global pressure. We set

$$\tilde{\beta}(S_w) = \int_0^{S_w} \sqrt{\lambda_n(s)\lambda_w(s)}\, p_c'(s)\, ds,$$

which leads to the following fundamental equality:

$$\begin{aligned} &\rho_n(p_n)\lambda_n(S_w)\mathbb{K}\nabla p_n \cdot \nabla p_n + \rho_w(p_w)\lambda_w(S_w)\mathbb{K}\nabla p_w \cdot \nabla p_w \\ &\quad = \lambda(S_w,p)\omega(S_w,p)\mathbb{K}\nabla p \cdot \nabla p + \frac{\rho_n(p_n)\rho_w(p_w)}{\lambda(S_w,p)}\mathbb{K}\nabla\tilde{\beta}(S_w) \cdot \nabla\tilde{\beta}(S_w). \end{aligned}$$

By solving differential equation (1.47) the nonwetting phase pressure p_n can be computed from the global pressure p and the wetting phase saturation S_w. This implies that the global pressure p and the wetting phase saturation S_w can be used as primary unknowns in the system (1.40)–(1.41). However, due to degeneracy of the system obtained in that way we replace the wetting phase saturation by the saturation potential $\tilde{\beta}(S_w)$ as a primary variable, which leads to the following equations:

$$\begin{aligned} &\Phi\partial_t(S_w\rho_w(p_w(S_w,p)) + S_n\rho_n(p_n(S_w,p))) \\ &\qquad - \operatorname{div}(\lambda(S_w,p)\mathbb{K}(\omega(S_w,p)\nabla p - \rho(S_w,p)\mathbf{g})) = F_w + F_n, \end{aligned} \tag{1.51}$$

$$\begin{aligned} &\Phi\partial_t\left(S_n\rho_n(p_n(S_w,p))\right) + \operatorname{div}(f_n(S_w,p)\mathbf{Q}_t - b_g(S_w,p)\mathbb{K}\mathbf{g}) \\ &\qquad - \operatorname{div}\left(\frac{\rho_w(p_w)\rho_n(p_n)\sqrt{\lambda_w(S_w)\lambda_g(S_w)}}{\lambda(S_w,p)}\mathbb{K}\nabla\tilde{\beta}(S_w)\right) = F_n, \end{aligned} \tag{1.52}$$

where the total flux $\mathbf{Q}_t$ becomes

$$\mathbf{Q}_t = -\lambda(S_w, p)\mathbb{K}\left(\omega(S_w, p)\nabla p - \rho(S_w, p)\mathbf{g}\right). \tag{1.53}$$

For simplicity the same notation is used for the most of the coefficients in the system as in (1.40)–(1.41), even though functional dependence on the pressure p_n is replaced by the dependence on the global pressure p. Let us also note that one can use the mass balance equation for the wetting phase instead of (1.52),

$$\begin{aligned} &\partial_t\left(\Phi S_w \rho_w(p_w(S_w, p))\right) + \operatorname{div}\left(f_w(S_w, p)\mathbf{Q}_t + b_g(S_w, p)\mathbb{K}\mathbf{g}\right) \\ &\qquad + \operatorname{div}\left(\frac{\rho_w(p_w)\rho_n(p_n)\sqrt{\lambda_w(S_w)\lambda_g(S_w)}}{\lambda(S_w, p)}\mathbb{K}\nabla\tilde{\beta}(S_w)\right) = F_w. \end{aligned} \tag{1.54}$$

Formulation (1.51)–(1.52) is sometimes referred to as a fractional flow formulation. Let us note that in the system (1.51)–(1.52) for compressible flow the coupling remains significant since the equation (1.51) does not have a clear type, although it can be interpreted as a nonlinear parabolic equation for the global pressure with some source terms. The saturation equation (1.52) is again of a nonlinear convection-diffusion type. However it is worth noticing that the coupling is clearly reduced in comparison to the system (1.36)–(1.37) since the saturation gradient is eliminated from (1.51).

Remark 1.3.5. *Previously defined relation between the global pressure p and the phase pressures p_w and p_n are given under the assumption $p_c(S_w = 1) = 0$. This is not the case for all known capillary pressure models, e.g. for the Brooks–Corey capillary pressure model. If this assumption is not satisfied, meaning $p_c(S_w = 1) = p_0$ for some entry pressure $p_0 > 0$, the initial condition in (1.47) is set to be $\pi(1, p) = p + p_0$.*

The existence result for the second global pressure formulation is given in [6] and numerical simulations of the water–gas flow in heterogeneous porous media with discontinuous capillary pressures are presented in [7]. An application of the global pressure to the modeling of the compositional, compressible, two-phase flow based on the concept of the global pressure is given in [10].

1.3.6 Two-phase multicomponent flow

In this subsection we consider flow of two different fluids, which are composed of different species. We have already given a brief description of a model for single-phase compositional flow. Similar relations are valid for the two-phase flow with additional complication due to possible exchange of the mass between phases.

We will start with definition of fraction of the component i, but this time in phase α, $\alpha = w,n$

- *volume fraction of the component i in phase* α

$$C^i_\alpha(x,t) = \frac{\text{volume of the component } i \text{ in phase } \alpha \text{ in REV}}{\text{volume of phase } \alpha \text{ in REV}},$$

- *mass fraction of the component i*

$$X^i_\alpha(x,t) = \frac{\text{mass of the component } i \text{ in phase } \alpha \text{ in REV}}{\text{mass of the phase } \alpha \text{ in REV}}.$$

Mass concentration of the component i in phase α is defined by

$$\rho^i_\alpha(x,t) = \frac{\text{mass of the component } i \text{ in phase } \alpha \text{ in REV}}{\text{volume of the phase } \alpha \text{ in REV}},$$

and the mass density of the phase α composed of k_α species is obtained as the sum of mass concentrations

$$\rho_\alpha = \sum_{i=1}^{k_\alpha} \rho^i_\alpha.$$

Now we state the mass conservation law for the component i in form (see [59])

$$\Phi\partial_t \left(\sum_\alpha \rho_\alpha X^i_\alpha S_\alpha \right) + \sum_\alpha \operatorname{div}\left(\rho_\alpha X^i_\alpha \mathbf{q}_\alpha + \mathbf{j}^i_\alpha\right) = F^i, \tag{1.55}$$

where F^i represents the source and sink term with respect to the component i. Phase velocities are given by the Darcy-Muskat law

$$\mathbf{q}_\alpha = -\lambda_\alpha(S_w)\mathbb{K}\left(\nabla p_\alpha - \rho_\alpha(p_\alpha)\mathbf{g}\right), \tag{1.56}$$

and diffusive fluxes are given by the Fick law

$$\mathbf{j}^i_\alpha = -\Phi S_\alpha D^i_\alpha \rho_\alpha \nabla X^i_\alpha. \tag{1.57}$$

We will give a more elaborate description of the model of compositional flow for particular case of the two-phase two-component in the next subsection since it will be the subject of the next chapter in this thesis.

1.3.7 Two-phase two-component flow

Here we give a detailed description of the system of equations governing *liquid* and *gas* flow in porous media. According to the application we have in mind (see [26]), we consider a fluid mixture of two components *water* and *hydrogen*. In order to emphasize the fluid system that we are considering we will denote the phases by the indices, l for liquid and g for gas. The components will be denoted by upper indices w and h, suggesting water and hydrogen. In this case (1.55) becomes

$$\Phi\partial_t\left(S_l\rho_l^w + S_g\rho_g^w\right) + \mathrm{div}\left(\rho_l^w\mathbf{q}_l + \rho_g^w\mathbf{q}_g + \mathbf{j}_l^w + \mathbf{j}_g^w\right) = F^w, \tag{1.58}$$

$$\Phi\partial_t\left(S_l\rho_l^h + S_g\rho_g^h\right) + \mathrm{div}\left(\rho_l^h\mathbf{q}_l + \rho_g^h\mathbf{q}_g + \mathbf{j}_l^h + \mathbf{j}_g^h\right) = F^h. \tag{1.59}$$

The phase velocities are given by (1.56) and diffusive fluxes are given by (1.57). Combining (1.58) and (1.59) with $S_l + S_g = 1$ and with capillary pressure law $p_c(S_l) = p_g - p_l$ we obtain totally four equations with eight unknowns: S_l, S_g, p_g, p_l, ρ_l^w, ρ_l^h, ρ_g^w, and ρ_g^h. To close the system we use thermodynamic properties of the phases, meaning the composition of the both phases is assumed to be in a local thermodynamic equilibrium. *Dalton's law* states that the total gas pressure is equal to the sum of the partial pressures of the individual gases,

$$p_g = p_g^w + p_g^h, \tag{1.60}$$

where p_g^w and p_g^h are the vaporized water and hydrogen partial pressures in the gas phase. Additionally we assume that the ideal gas law is applicable,

$$p_g^w = \frac{\rho_g^w}{M^w}RT, \quad p_g^h = \frac{\rho_g^h}{M^h}RT, \tag{1.61}$$

where T is the temperature, R is the universal gas constant, and M^w and M^h are the water and hydrogen molar masses. In order to determine the quantity of the dissolved hydrogen in water, one can apply *Henry's law*, which states that the amount of the dissolved gas is proportional to the partial pressure of that same gas in the gas phase

$$\rho_l^h = H(T)M^h p_g^h, \tag{1.62}$$

where $H(T)$ is Henry's law constant, which depends only on the temperature. For the liquid phase, one can apply *Raoult's law*, which states that the water vapor pressure is equal to the vapor pressure of the pure solvent at given temperature $\hat{p}_g^w(T)$ multiplied by the mole fraction of the solvent,

$$p_g^w = \hat{p}_g^w(T)\frac{\rho_l^w}{\rho_l^w + (M^w/M^h)\rho_l^h}. \tag{1.63}$$

By adding relations $\rho_l^h + \rho_l^w = \rho_l$ and $\rho_g^h + \rho_g^w = \rho_g$ and assuming water compressibility $\rho_l = \rho_l^{std}/B_l(p_l)$, the initial system is completed.

The main difficulty of the previously stated formulation is a treatment of the phase disappearance and reappearance, precisely adequate primary variable choice, which can be different in the saturated (only one phase present) and unsaturated (both phases present) zones. If the quantity of the dissolved gas is smaller than the hydrogen quantity at equilibrium, then the Henry law does not apply. In this case S_g is equal to the zero and S_g can not be taken as an unknown. Instead of the saturation S_g one could take ρ_l^h as an independent variable. Similar observations apply when the liquid phase is missing. One of the possible solution to this problem is primary variable switch based on the phase presence like in [75, 39]. The main challenge with this approach is detection of the unsaturated flow.

In [60] and [55] a model with neglected water vaporization was considered. Authors propose closing the system of nonlinear partial differential equations (conservation equations and Darcy-Muskat laws) by the *complementarity constraints*, which describe the transfer of hydrogen between the two phases

$$(1-S_l)(H(T)M^h p_g - \rho_l^h) = 0, \quad 1-S_l \geq 0, \quad H(T)M^h p_g - \rho_l^h \geq 0. \tag{1.64}$$

The main idea behind complementarity constraints is introduction of additional relations and variables in order to keep all natural variables of the system in saturated and unsaturated zones. In this example, alongside p_g and S_l one can introduce ρ_l^h as primary variable and use (1.64) to relate these variables. In [68] authors have used this model in terms of mole fractions, which are defined as the amount of the component i (expressed in moles), n_i, divided by the total amount of the phase α (also expressed in moles), n_α,

$$x_\alpha^i = \frac{n_i}{n_\alpha}, \quad \alpha = l,g, \quad i = w,h. \tag{1.65}$$

The system (1.58)-(1.59) can easily be written in terms of the mole fraction by introducing relation $\rho_\alpha^i = x_\alpha^i \rho_\alpha M_i/M_\alpha = x_\alpha^i M_i \rho_{\alpha,mol}$. Following system of equations is obtained

$$\Phi\partial_t\left(S_l\rho_{l,mol}x_l^w + S_g\rho_{g,mol}x_g^w\right) + \text{div}\left(\rho_{l,mol}x_l^w\mathbf{q}_l + \rho_{g,mol}x_g^w\mathbf{q}_g + \mathbf{j}_l^w + \mathbf{j}_g^w\right) = F^w/M_w, \tag{1.66}$$

$$\Phi\partial_t\left(S_l\rho_{l,mol}x_l^h + S_g\rho_{g,mol}x_g^h\right) + \text{div}\left(\rho_{l,mol}x_l^h\mathbf{q}_l + \rho_{g,mol}x_g^h\mathbf{q}_g + \mathbf{j}_l^h + \mathbf{j}_g^h\right) = F^h/M^h, \tag{1.67}$$

with Fick's law written as $\mathbf{j}^i_\alpha = -\Phi S_\alpha D^i_\alpha \rho_{\alpha,mol} \nabla x^i_\alpha$. In [68] following complementarity conditions have been imposed

$$1 - \sum_{i=1}^{2} x^i_\alpha \geq 0, \quad S_\alpha \geq 0, \quad S_\alpha \left(1 - \sum_{i=1}^{2} x^i_\alpha\right) = 0, \quad \alpha = l, g.$$

Another solution to the phase disappearance problem is definition of the new variables, so-called *persistent variables*, that will be well defined in both saturated and unsaturated regions. This approach was described in [26] for a simplified case without water vaporization. Authors propose liquid phase pressure p_l and total hydrogen mass density $X = S_l \rho^h_l + S_g \rho^h_g$ as the primary variables. Extension to this approach without simplification regarding water vaporization was presented in [10]. The main idea is to replace the liquid phase pressure p_l as the primary unknown, by the global pressure which is well defined in both one-phase and two-phase regions.

Similar way to address this issue is presented in [14] where the authors neglect evaporation, meaning that $p_g = p^h_g$. They propose a different set of persistent variables by using relation (1.62) to define the gas pressure even in the case where the gas phase is nonexistent. The *gas pseudopressure* defined by (1.62) is an artificial variable *proportional* to the concentration of the dissolved gas in the one-phase region and equal to the gas phase pressure in the two-phase region. In that way one avoids using directly the concentration of the dissolved gas ρ^h_l as a primary variable and uses more traditional gas pressure, suitably extended in one-phase region. For another primary unknown, one can take liquid phase pressure p_l that can be used as the persistent variable in case where there is no water vaporization. Let us note that this would not be a good approach in the general case with water vaporization. This choice of primary unknowns is also taken in this thesis in chapter 2.

Similar idea is presented in [73] where the capillary pressure p_c is taken as a primary variable. In this paper the authors have also used the governing equations in terms of molar fractions (1.66)–(1.67). The capillary pressure curve has an *entry pressure* $p_{entry} > 0$, which is a critical capillary pressure for appearance of the nonwetting phase. Authors distinguish the cases $p_c \leq p_{entry}$, where $S_g = 0$ and only wetting phase exists, and $p_c > p_{entry}$, where $S_g > 0$ and both phases exist. It has been shown that in both of these cases extended gas phase pressure p_g and the capillary pressure p_c can be used as persistent variables.

A different set of persistent variables was presented in [70]. The authors introduce mean pressure p, which equals the pressure of the remaining phase when one of them disappears

$$p = \gamma(S_w) p_g + (1 - \gamma(S_w)) p_l,$$

where $\gamma(S_w)$ is a weight function, e.g. $\gamma(S_w) = S_w$. Since the mole fraction formulation was used, the authors propose for the second primary unknown the total molar fraction of the gas component

$$x = \frac{M_g x_g^h S_g + M_l x_l^h S_l}{S_g M_g + S_l M_l}.$$

Both of these unknowns are well defined both in saturated and in unsaturated regions.

In [1] the standard variables S_w and p_g are used as persistent variables but they are given different meaning in saturated regions. Authors propose an extension of the phase saturation S_w allowing negative values and values greater than one in order to avoid degeneracy in the system (1.58)–(1.59) in the one-phase region. With this extension the saturation can also be used as a primary unkonwn.

1.4 Conclusion

In this chapter the basic properties of porous media were presented, alongside main models that are used for description of the one-phase and the two-phase flows. We have also presented models based on the concept of the global pressure which will be steadily referenced in this work. A special emphasis in this chapter was given to the description of the two-phase two-component flow, since the next chapter of this thesis deals with the existence proof of the proposed model in the case of the flow with low solubility of the gas component in the liquid phase where water vaporization is neglected.

Chapter 2

Mathematical analysis of two-phase two-component flow in porous media in low solubility regime

In this chapter we study a system of equations governing liquid and gas flow in porous media. The gas phase is homogeneous, while the liquid phase is composed of a liquid component and a dissolved gas component. It is assumed that the gas component is weakly soluble in the liquid. We formulate a weak solution of the initial boundary value problem and prove the existence theorem by passing to the limit in regularizations of the problem. This chapter mainly contains results published in [61].

Recently, two-phase, two-component models were considered in articles [34] and [35]. In [34] the authors replace the phase equilibrium by the first order chemical reactions which are supposed to model the mass exchange between the phases. In [35] the phase equilibrium model is taken into account but the degeneracy of the diffusion terms is eliminated by some nonphysical assumptions. As the diffusion terms in the flow equations are multiplied by the liquid saturation they can be arbitrary small, which can be seen in (2.8), therefore they do not add sufficient regularity to the system. In this work this degeneracy of the diffusive terms is compensated by the low solubility of the gas component in the liquid phase which keeps the liquid phase composed mostly of the liquid component (water). The hypothesis of low solubility is given precise mathematical meaning.

An important consideration in the modeling of fluid flow with mass exchange between phases is the choice of the primary variables that define the thermodynamic state of the fluid system [83].

When a phase appears or disappears, the set of appropriate thermodynamic variables may change. In mathematical analysis of the two-phase, two-component model presented in this chapter we choose a formulation based on persistent variable approach [26, 27, 14]. Namely, we use the liquid phase pressure and the gas pseudopressure (introduced in section 2.1) as two variables capable of describing the fluid system in both one-phase and two-phase regions.

The outline of this chapter is as follows. In Section 2.1 we give a short description of the physical and mathematical model of two-phase, two-component flow in porous media considered in this study. We also introduce the global pressure that plays an important role in mathematical study of the model, general assumptions on the data, and some auxiliary results. In Section 2.2 we present the main result of this chapter, the existence of a weak solution to an initial boundary value problem for the considered two-phase, two-component flow model. This theorem is proved in the following sections. In Section 2.3 we regularize the system and discretize the time derivatives, obtaining thus a sequence of elliptic problems. In Section 2.4 we prove the existence theorem for the elliptic problems by an application of the Schauder fixed point theorem. In this section we perform further regularizations and apply special test functions which lead to the energy estimate on which the existence theorem is based. In Sections 2.5 and 2.6 we eliminate the time discretization and the initial regularization of the system by passing to zero in the small parameters. At the limit we obtain a weak solution of the initial two-phase, two-component flow model.

2.1 Mathematical model

We consider herein the model described in 1.3.7, meaning we observe a porous medium saturated with a fluid composed of 2 phases, *liquid* and *gas*. The fluid is a mixture of two components: a *liquid component* which does not evaporate and a *low-soluble component* (such as hydrogen) which is present mostly in the gas phase and dissolves in the liquid phase. The porous medium is assumed to be rigid and in the thermal equilibrium, while the liquid component is assumed incompressible. The notation is the same as in Subsection 1.3.7. The phase volumetric fluxes $\mathbf{q}_\sigma$ are given by (1.56), and since we have assumed that there is no void space in the porous medium the phase saturations satisfy $S_l + S_g = 1$.

The phase pressures are connected through the *capillary pressure law* (see [21, 36])

$$p_c(S_l) = p_g - p_l, \tag{2.1}$$

where the function p_c is a strictly decreasing function of the liquid saturation, $p_c'(S_l) < 0$.

In the gas phase, we neglect the liquid component vapor such that the gas mass density depends only on the gas pressure:

$$\rho_g = \hat{\rho}_g(p_g), \tag{2.2}$$

where in the case of the ideal gas law we have $\hat{\rho}_g(p_g) = C_v p_g$ with $C_v = M^h/(RT)$, where M^h is the molar mass of the gas component, T is the temperature, and R is the universal gas constant.

In order to simplify notation we will denote ρ_l^h by u. The assumption of thermodynamic equilibrium leads to functional dependence,

$$u = \hat{u}(p_g), \tag{2.3}$$

if the gas phase is present. In the absence of the gas phase u must be considered as an independent variable. If the Henry law is applicable, then the function $\hat{u}$ can be taken as a linear function $u = C_h p_g$, where $C_h = HM^h$ and H is the Henry law constant. We suppose that the function $p_g \mapsto \hat{u}(p_g)$ is defined and invertible on $[0, \infty)$ and therefore we can express the gas pressure as a function of u,

$$p_g = \hat{p}_g(u), \tag{2.4}$$

where $\hat{p}_g$ is the inverse of $\hat{u}$. We use (2.4) to define the *gas pseudopressure* as an artificial variable *proportional* to the concentration of the dissolved gas in the one-phase region and equal to the gas phase pressure in the two-phase region. In that way one avoids using directly the concentration of the dissolved gas u as a primary variable and uses more traditional gas pressure, suitably extended in one phase region.

For the liquid density, due to the hypothesis of small solubility and the liquid incompressibility we may assume constant liquid component mass concentration, i.e.,

$$\rho_l^w = \rho_l^{std}, \tag{2.5}$$

where ρ_l^{std} is the standard liquid component mass density (a constant). The liquid mass density is then $\rho_l = \rho_l^{std} + u$.

Finally, the mass conservation for each component leads to the following partial differential equations:

$$\rho_l^{std} \Phi \frac{\partial S_l}{\partial t} + \text{div}\left(\rho_l^{std} \mathbf{q}_l + \mathbf{j}_l^w\right) = F^w, \tag{2.6}$$

$$\Phi\frac{\partial}{\partial t}(uS_l+\rho_g S_g)+\operatorname{div}\left(u\mathbf{q}_l+\rho_g\mathbf{q}_g+\mathbf{j}_l^h\right)=F^h, \tag{2.7}$$

where the phase flow velocities, $\mathbf{q}_l$ and $\mathbf{q}_g$, are given by the Darcy–Muskat law (1.56), F^k and $\mathbf{j}_l^k$, $k\in\{w,h\}$, are respectively the $k-$component source terms and the diffusive flux in the liquid phase. The diffusive fluxes are given by the Fick law, which can be expressed through the gradient of the mass fractions $X_l^h=u/\rho_l$ and $X_l^w=\rho_l^w/\rho_l$ as in [20, 26]:

$$\mathbf{j}_l^h=-\Phi S_l D\rho_l\nabla X_l^h,\quad \mathbf{j}_l^w=-\Phi S_l D\rho_l\nabla X_l^w, \tag{2.8}$$

where D is a molecular diffusion coefficient of dissolved gas in the liquid phase, possibly corrected by the tortuosity factor of the porous medium (see [20]). Note that we have $X_l^h+X_l^w=1$, leading to $\mathbf{j}_l^h+\mathbf{j}_l^w=0$. The source terms F^w and F^h will be taken in the usual form:

$$F^w=\rho_l^{std}F_I-\rho_l^{std}S_lF_P,\quad F^h=-(uS_l+\rho_gS_g)F_P,\quad F_I,F_P\geq 0, \tag{2.9}$$

where F_I is the rate of the fluid injection and F_P is the rate of the production. For simplicity we supposed that only the wetting phase is injected, while composition of the produced fluid is not a priori known.

We consider the liquid pressure p_l and the gas pseudopressure p_g as primary variables from which we calculate several *secondary* variables:

$$S_l=p_c^{-1}(p_g-p_l),\ S_g=1-S_l,\ u=\hat{u}(p_g),\ \rho_g=\hat{\rho}_g(p_g),\ \rho_l=\rho_l^{std}+\hat{u}(p_g). \tag{2.10}$$

Note that in the two-phase region we can recover the liquid saturation by inverting the capillary pressure curve, $S_l=p_c^{-1}(p_g-p_l)$. In the one-phase region we set the liquid saturation to one, which amounts to extending the inverse of the capillary pressure curve by one for negative pressures (see (A.4)), as described in [27]. As a consequence we have $0\leq S_l\leq 1$ by properties of the capillary pressure function (see (A.4)).

2.1.1 Problem formulation

Let $\Omega\subset\mathbb{R}^l$, for $l=1,2,3$, be a bounded Lipschitz domain and let $T>0$. We assume that $\partial\Omega=\Gamma_D\cup\Gamma_N$ is a regular partition of the boundary with $|\Gamma_D|>0$. We consider the following initial boundary value problem in $Q_T=\Omega\times(0,T)$ for the problem (2.6)–(2.9) written in selected variables:

$$\Phi\frac{\partial S_l}{\partial t}-\operatorname{div}\Big(\lambda_l(S_l)\mathbb{K}(\nabla p_l-\rho_l\mathbf{g})-\Phi S_l\frac{1}{\rho_l}D\nabla u\Big)+S_lF_P=F_I, \tag{2.11}$$

$$
\begin{aligned}
\Phi\frac{\partial}{\partial t}\big(uS_l+\rho_g S_g\big)-\operatorname{div}\Big(u\lambda_l(S_l)\mathbb{K}(\nabla p_l-\rho_l\mathbf{g})+\rho_g\lambda_g(S_l)\mathbb{K}(\nabla p_g-\rho_g\mathbf{g})\Big)\\
-\operatorname{div}\Big(\Phi S_l\frac{\rho_l^{std}}{\rho_l}D\nabla u\Big)+(uS_l+\rho_g S_g)F_P=0,
\end{aligned}
\tag{2.12}
$$

with homogeneous Neumann's boundary condition imposed,

$$
\begin{aligned}
\Big(\lambda_l(S_l)\mathbb{K}(\nabla p_l-\rho_l\mathbf{g})-\Phi S_l\frac{1}{\rho_l}D\nabla u\Big)\cdot\mathbf{n}=0,\\
\Big(u\lambda_l(S_l)\mathbb{K}\big(\nabla p_l-\rho_l\mathbf{g}\big)+\rho_g\lambda_g(S_g)\mathbb{K}\big(\nabla p_g-\rho_g\mathbf{g}\big)+\Phi S_l\frac{\rho_l^{std}}{\rho_l}D\nabla u\Big)\cdot\mathbf{n}=0,
\end{aligned}
\tag{2.13}
$$

on Γ_N and

$$
p_l=0,\quad p_g=0, \tag{2.14}
$$

on Γ_D. We impose initial conditions as follows:

$$
p_l(x,0)=p_l^0(x),\quad p_g(x,0)=p_g^0(x). \tag{2.15}
$$

All the secondary variables S_l, S_g, u, ρ_g, and ρ_l in (2.11), (2.12) are calculated from p_l and p_g by (2.10). The boundary condition $p_g=0$ on Γ_D is equivalent to the condition $u=0$, which impose that there is no dissolved gas on the boundary (see (A.5)).

2.1.2 Main assumptions

(A.1) The porosity Φ belongs to $L^\infty(\Omega)$, and there exist constants, $\phi_M\ge\phi_m>0$, such that $\phi_m\le\Phi(x)\le\phi_M$ a.e. in Ω. The diffusion coefficient D belongs to $L^\infty(\Omega)$, and there exists a constant $D_0>0$ such that $D(x)\ge D_0$ a.e. in Ω.

(A.2) The permeability tensor $\mathbb{K}$ belongs to $(L^\infty(\Omega))^{l\times l}$, and there exist constants $k_M\ge k_m>0$ such that for almost all $x\in\Omega$ and all $\xi\in\mathbb{R}^l$ it holds that

$$
k_m|\xi|^2\le\mathbb{K}(x)\xi\cdot\xi\le k_M|\xi|^2.
$$

(A.3) Relative mobilities λ_l,λ_g are defined as $\lambda_l(S_l)=kr_l(S_l)/\mu_l$ and $\lambda_g(S_l)=kr_g(S_l)/\mu_g$, where the constants $\mu_l>0$ and $\mu_g>0$ are the liquid and the gas viscosities, and $kr_l(S_l)$, $kr_g(S_l)$ are the relative permeability functions, satisfying $kr_l,kr_g\in C([0,1])$, $kr_l(0)=0$, and

$kr_g(1) = 0$; the function kr_l is a nondecreasing and kr_g is a nonincreasing function of S_l. Moreover, there is a constants $kr_m > 0$ such that for all $S_l \in [0,1]$

$$kr_m \leq kr_l(S_l) + kr_g(S_l).$$

We assume also that there exists a constant $a_l > 0$ such that for all $S_l \in [0,1]$

$$a_l S_l^2 \leq kr_l(S_l). \tag{2.16}$$

(A.4) The capillary pressure function, $p_c \in C^1(0,1) \cap C^0((0,1])$, is a strictly monotone decreasing function of $S_l \in (0,1]$, unbounded at $S_l = 0$, satisfying $p_c(1) = 0$, $p_c(S_l) > 0$ for $S_l \in (0,1)$ and $p_c'(S_l) \leq -M_0 < 0$ for $S_l \in (0,1)$ and some constant $M_0 > 0$. There exists a positive constant M_{p_c} such that

$$\int_0^1 p_c(s)\,ds = M_{p_c} < +\infty. \tag{2.17}$$

The inverse functions p_c^{-1} is extended as $p_c^{-1}(\sigma) = 1$ for $\sigma \leq 0$.

(A.5) The function $\hat{u}(p_g)$ is a strictly increasing C^1 function from $[0,+\infty)$ to $[0,+\infty)$ and $\hat{u}(0) = 0$. There exist constants $u_{max} > 0$ and $M_g > 0$ such that for all $\sigma \geq 0$ it holds that

$$|\hat{u}(\sigma)| \leq u_{max}, \quad 0 < \hat{u}'(\sigma) \leq M_g.$$

For $\sigma \leq 0$ we extend $\hat{u}(\sigma)$ as a smooth, sufficiently small, bounded monotone increasing function having global C^1 regularity. The main low solubility assumption is that the constant M_g is sufficiently small, namely, that the inequality (2.23) holds.

(A.6) The function $\hat{\rho}_g(p_g)$ is a C^1 strictly increasing function on $[0,\infty)$, and there exist constants $\rho_M > 0$ and $\rho_g^{max} > 0$ such that for all $p_g \geq 0$ it holds that

$$0 \leq \hat{\rho}_g(p_g) \leq \rho_M, \quad |\hat{\rho}_g'(p_g)| \leq \rho_g^{max}, \quad \hat{\rho}_g(0) = 0, \quad \int_0^1 \frac{d\sigma}{\hat{\rho}_g(\sigma)} < \infty.$$

For $\sigma \leq 0$ we set $\hat{\rho}_g(\sigma) = 0$ for all $\sigma \leq 0$.

(A.7) $F_I, F_P \in L^2(Q_T)$ and $F_I, F_P, p_g^0 \geq 0$ a.e. in Q_T.

(A.8) The function $\alpha(S_l)$ defined in (1.32) satisfies $\alpha \in C^0([0,1])$, $\alpha(0) = \alpha(1) = 0$, and $\alpha(S) > 0$ for $S \in (0,1)$. The inverse of the function $\beta(S_l)$, defined in (1.32), is a Hölder continuous function of order $\tau \in (0,1)$, which can be written as (for some positive constant $C \geq 0$.)

$$C\left|\int_{S_1}^{S_2} \alpha(s)\,ds\right|^{\tau} \geq |S_1 - S_2|. \tag{2.18}$$

Remark 2.1.1. *Boundedness of the function $\hat{u}$ from (A.5) is a simplification that is not restrictive since u_{max} can take arbitrary large values. The same is true for boundedness of the gas density in (A.6).*

Remark 2.1.2. *The function $\hat{u}(p_g)$ from (A.5) has a physical meaning only for nonnegative values of the pseudopressure p_g. Regularizations applied in section 2.4 destroy the minimum principle that enforces $p_g \geq 0$ and therefore we need to extend $\hat{u}(p_g)$ for negative values of p_g as a smooth function. This extension is arbitrary and we take it sufficiently small, such that*

$$0 < \rho_l^{std} - u_{min} \leq \rho_l = \rho_l^{std} + \hat{u}(p_g) \leq \rho_l^{std} + u_{max},$$

for some constant $0 < u_{min} < \rho_l^{std}$ and $u_{min} \leq u_{max}$. For reasons which appear in the proof of Lemma 2.1.6 we also suppose $u_{min} \leq \rho_l^{std}(1 - 1/\sqrt{2})$.

Remark 2.1.3. *By (A.4) the capillary pressure function is unbounded at $S_l = 0$ and consequently the wetting phase cannot be displaced completely by the non wetting phase. This assumption will be used in the proof of Lemma 2.4.8.*

2.1.3 The global pressure

We will use the notion of the global pressure p as given in [36], which was introduced in chapter 1 by (1.31). From (1.31) and (A.4) in section 2.1.2 it follows that $p_l \leq p$ and $p = p_l$ in the area where $p_g \leq p_l$. In other words, when the gas pseudopressure falls below the liquid pressure, and only the liquid phase remains, then the global pressure coincides with the liquid pressure.

In the part of the domain where $p_g \geq p_l$ we have another representation of the global pressure based on total velocity,

$$p = p_g + \hat{P}(S_l), \quad \hat{P}(S_l) = \int_{S_l}^{1} \frac{\lambda_l(s)}{\lambda(s)} p_c'(s) ds, \tag{2.19}$$

but in the domain area where $p_g < p_l$ formula (2.19) does not hold true as there the global pressure stays equal to the liquid pressure. From (1.31) we have a.e.

$$\nabla p_l = \nabla p - \frac{\lambda_g(S_l)}{\lambda(S_l)} \nabla p_c(S_l), \tag{2.20}$$

and from (2.19) it follows that

$$\nabla p_g = \nabla p + \frac{\lambda_l(S_l)}{\lambda(S_l)} \nabla p_c(S_l) \tag{2.21}$$

in the part of Q_T where $p_g \geq p_l$.

Lemma 2.1.4. *Under assumptions (A.4) and (A.8) there exists a constant $C > 0$ such that the following bounds hold true:*

$$p_g^+ \le |p| + C, \quad |S_l p_l| \le |p| + C, \quad |S_g p_g| \le |p| + C, \quad p_l \le p \le \max(p_l, p_g). \tag{2.22}$$

Proof. From (2.19) we have for $p_g \ge p_l$,

$$p_g^+ \le |p| - \int_0^{1/2} \frac{\lambda_l(s)}{\lambda(s)} p_c'(s) ds - \int_{1/2}^1 \frac{\lambda_l(s)}{\lambda(s)} p_c'(s) ds.$$

From (A.8) it follows that the first integral on the right-hand side is bounded and therefore we have

$$p_g^+ \le |p| + C + p_c(1/2).$$

The same inequality obviously holds also for $p_g < p_l = p$.

From (1.31) we have

$$|S_l p_l| \le |p| + |S_l \int_{S_l}^1 \frac{\lambda_g(s)}{\lambda(s)} p_c'(s) ds| \le |p| + \int_{S_l}^1 \frac{\lambda_g(s)}{\lambda(s)} s |p_c'(s)| ds.$$

Due to (A.4) the right-hand-side integral is bounded, which proves the second inequality. The third inequality follows in the same way from (2.19) and the fact that due to (A.4) and (A.8) the function $\hat{P}(S_l)$ is bounded on $(0,1)$. Finally, the last inequality follows directly from (2.19), (1.31). This proves the lemma. □

To the assumptions (A.1)–(A.8) we add the following assumption concerning the global pressure:

(A.9) The function $(1 - S_l)\hat{P}(S_l)$, where $\hat{P}(S_l)$ is defined in (2.19), is Hölder continuous for $S_l \in (0,1)$ with some exponent $\overline{\tau} \in (0,1]$.

Remark 2.1.5. *Assumptions on Hölder continuity in (A.8) and (A.9) are needed in the compactness proof in section 2.6. Assumption (A.8) is usual in the two-phase flow models, while assumption (A.9) is fulfilled if $(1 - S_l)p_c'(S_l)$ is an L^q function, for $q > 1$, away from $S_l = 0$. This assumption is a consequence of (A.8) ($\alpha(1) = 0$) if, for example, $kr_g(S_l) \ge C(1 - S_l)^\gamma$ for some $0 < \gamma < 2$.*

Lemma 2.1.6. *Let the assumptions (A.1)-(A.8) be fulfilled and let $u = \hat{u}(p_g)$ and $\rho_l = \rho_l^{std} + \hat{u}(p_g)$. By z we denote the number*

$$z = \min_{0 \le S_l \le 1} (kr_g(S_l) + S_l),$$

and we suppose that M_g *in (A.5) is sufficiently small, namely, we assume*

$$\frac{\Phi D}{\rho_l^{std} k_m/\mu_l} \max\left(\frac{\rho_M}{\rho_l^{std}}\frac{1}{a_l z}, \sqrt{\frac{\mu_g}{\mu_l}}\frac{1}{\sqrt{a_l z}}\right) < \frac{1}{M_g}. \tag{2.23}$$

Then the following inequalities hold:

$$c_D|\nabla u|^2 \le \lambda_g(S_l)\mathbb{K}\nabla p_g \cdot \nabla p_g + S_l \Phi D \frac{1}{\rho_g}\nabla p_g \cdot \nabla u, \tag{2.24}$$

$$\left|\frac{1}{\rho_l}\Phi S_l D \nabla u \cdot \nabla p_l\right| \le \frac{1}{2}\lambda_l(S_l)\mathbb{K}\nabla p_l \cdot \nabla p_l + q c_D |\nabla u|^2, \tag{2.25}$$

for some $0 < q < 1$*, where*

$$c_D = \frac{\Phi^2 D^2 \mu_l}{(\rho_l^{std})^2 k_m a_l}. \tag{2.26}$$

Proof. We have

$$\lambda_g(S_l)\mathbb{K}\nabla p_g \cdot \nabla p_g + S_l\Phi D\frac{1}{\rho_g}\nabla p_g \cdot \nabla u \ge \left(\frac{1}{\mu_g \hat{u}'(p_g)^2} kr_g(S_l)k_m + S_l \Phi D \frac{1}{\rho_g \hat{u}'(p_g)}\right)|\nabla u|^2,$$

from where it follows

$$\lambda_g(S_l)\mathbb{K}\nabla p_g \cdot \nabla p_g + S_l\Phi D\frac{1}{\rho_g}\nabla p_g \cdot \nabla u \ge z \min\left(\frac{k_m}{\mu_g M_g^2}, \frac{\Phi D}{\rho_M M_g}\right)|\nabla u|^2.$$

Estimates (2.24) and (2.26) follow immediately from

$$\frac{\Phi^2 D^2 \mu_l}{(\rho_l^{std})^2 k_m a_l} \le z \min\left(\frac{k_m}{\mu_g M_g^2}, \frac{\Phi D}{\rho_M M_g}\right). \tag{2.27}$$

It is easy to show that (2.27) follows from (2.23) and the fact that a_l can be taken arbitrary small, such that $a_l z \le 1$; this proves (2.24).

To prove (2.25) we note that since the extension of the function $\hat{u}$ into negative pseudopressures can be taken arbitrary small, we have $\rho_l \ge \rho_l^{std}(1-\varepsilon)$, for $0 < \varepsilon = u_{min}/\rho_l^{std} < 1 - 1/\sqrt{2}$ (see Remark 2.1.2). Therefore we can estimate

$$\begin{aligned}
\left|\frac{1}{\rho_l}\Phi S_l D\nabla u \cdot \nabla p_l\right| &\le \left|\frac{1}{\rho_l^{std}(1-\varepsilon)\sqrt{k_m \lambda_l(S_l)}}\Phi S_l D \sqrt{k_m\lambda_l(S_l)}\hat{u}'(p_g)\nabla p_g \cdot \nabla p_l\right| \\
&\le \frac{1}{2}k_m\lambda_l(S_l)\nabla p_l \cdot \nabla p_l + \frac{1}{2(1-\varepsilon)^2}\frac{\Phi^2 S_l^2 D^2}{(\rho_l^{std})^2 k_m \lambda_l(S_l)}\hat{u}'(p_g)^2 \nabla p_g \cdot \nabla p_g \\
&\le \frac{1}{2}\lambda_l(S_l)\mathbb{K}\nabla p_l \cdot \nabla p_l + q c_D |\nabla u|^2,
\end{aligned}$$

where in the last step we have used (2.16), and $q = 0.5/(1-\varepsilon)^2 < 1$. Lemma 2.1.6 is proved. □

Remark 2.1.7. *Exact meaning of the low solubility hypothesis is given by (2.23). The* solubility bound M_g *must be small enough so that* $1/M_g$ *is larger than a ratio of diffusivity* ΦD *and hydraulic conductivity* $\rho_l^{std} k_m/\mu_l$ *multiplied by generally small nondimensional factor.*

Remark 2.1.8. *If we take as an example the flow of water and hydrogen modeled by the Henry law,* $\hat{u}(p_g) = H(T)M^h p_g$*, we can check that the inequality (2.23) is realistic. Some typical values for corresponding parameters (at* $T = 303K$*) are the following:* $H(T) = 7.65 \cdot 10^{-6}$ mol/m^{2}Pa*,* $\rho_l^{std} = 10^3$ kg/m^3*,* $M^h = 2 \cdot 10^{-3}$ kg/mol*,* $\mu_l = 10^{-3}$ *and* $\mu_g = 6 \cdot 10^{-6}$ Pa $\cdot$ s*,* $k_m = 10^{-19}$ m^2*,* $\Phi = 0.1$*,* $D = 3 \cdot 10^{-9}$ m^2/s*,* $a_l = 1$*, and* $z = 0.1$*. With these values of the parameters we get that* $1/M_g$ *should be bigger than* $3 \cdot 10^4$*, while* $M_g = H(T)M^h = 15.3 \cdot 10^{-9}$ *(see [2]).*

2.2 Existence theorem

Let us recall that the primary variables are p_l and p_g. The secondary variables are the global pressure p defined by (1.31) and the functions u, ρ_g, S_l, and S_g defined as $u = \hat{u}(p_g)$, $\rho_g = \hat{\rho}_g(p_g)$, $S_l = p_c^{-1}(p_g - p_l)$, and $S_g = 1 - S_l$. By (A.5) and (A.6) the functions u and ρ_g are bounded and for S_l, due to (A.4) (see also Remark 2.1.3), we have

$$0 < S_l \leq 1. \tag{2.28}$$

A variational formulation is obtained by standard arguments. Taking test functions $\varphi, \psi \in C^1([0,T],V)$ where

$$V = \{\varphi \in H^1(\Omega) \colon \varphi = 0 \text{ on } \Gamma_D\}$$

we get the following theorem.

Theorem 2.2.1. *Let (A.1)-(A.9) hold true and assume* $(p_l^0, p_g^0) \in L^2(\Omega) \times L^2(\Omega)$*,* $p_g^0 \geq 0$ *a.e. in* Ω*. Then there exist functions* p_l *and* p_g *satisfying*

$$\begin{aligned} p_l, p_g \in L^2(Q_T), \quad p, u, \beta(S_l) \in L^2(0,T;V), \\ \Phi\partial_t(uS_l + \rho_g S_g),\ \Phi\partial_t S_l \in L^2(0,T;V'), \\ \sqrt{\lambda_l(S_l)}\nabla p_l,\ \sqrt{\lambda_g(S_l)}\nabla p_g \in L^2(Q_T)^l, \end{aligned}$$

such that for all $\varphi \in L^2(0,T;V)$

$$\begin{aligned} \int_0^T \left\langle \Phi\frac{\partial S_l}{\partial t}, \varphi \right\rangle dt + \int_{Q_T} \left[\lambda_l(S_l)\mathbb{K}\nabla p_l - \Phi S_l \frac{1}{\rho_l} D\nabla u \right] \cdot \nabla\varphi dxdt \\ + \int_{Q_T} S_l F_P \varphi dxdt = \int_{Q_T} F_I \varphi dxdt + \int_{Q_T} \rho_l \lambda_l(S_l)\mathbb{K}\mathbf{g} \cdot \nabla\varphi dxdt; \end{aligned} \tag{2.29}$$

for all $\psi \in L^2(0,T;V)$

$$
\begin{aligned}
&\int_0^T \left\langle \Phi \frac{\partial}{\partial t}(uS_l + \rho_g S_g), \psi \right\rangle dt \\
&+ \int_{Q_T} \left[u\lambda_l(S_l)\mathbb{K}\nabla p_l + \rho_g \lambda_g(S_l)\mathbb{K}\nabla p_g + \Phi S_l \frac{\rho_l^{std}}{\rho_l} D\nabla u \right] \cdot \nabla \psi dxdt \qquad (2.30)\\
&+ \int_{Q_T} (uS_l + \rho_g S_g) F_P \psi dxdt = \int_{Q_T} \left(\rho_l u \lambda_l(S_l) + \rho_g^2 \lambda_g(S_l)\right) \mathbb{K}\mathbf{g} \cdot \nabla \psi dxdt.
\end{aligned}
$$

Furthermore, for all $\psi \in V$ *the functions*

$$
t \mapsto \int_\Omega \Phi S_l \psi dx, \quad t \mapsto \int_\Omega \Phi((u-\rho_g)S_l + \rho_g)\psi dx
$$

are continuous in $[0,T]$ *and the initial condition is satisfied in the following sense:*

$$
\left(\int_\Omega \Phi S_l \psi dx \right)(0) = \int_\Omega \Phi s_0 \psi dx, \qquad (2.31)
$$

$$
\left(\int_\Omega \Phi(uS_l + \rho_g S_g)\psi dx \right)(0) = \int_\Omega \Phi(\hat{u}(p_g^0)s_0 + \hat{\rho}_g(p_g^0)(1-s_0))\psi dx \qquad (2.32)
$$

for all $\psi \in V$*, where* $s_0 = p_c^{-1}(p_g^0 - p_l^0)$.

The first step in proving correctness of the proposed model for the two-phase compositional flow is to show that the weak solution defined in Theorem 2.2.1 satisfies $p_g \geq 0$ a.e. in Q_T if the initial and the boundary conditions satisfy the corresponding inequality.

Lemma 2.2.2. *Let* p_l *and* p_g *be given by Theorem 2.2.1. Then,* $p_g \geq 0$ *a.e. in* Q_T.

Lemma 2.2.2 can be proved by a standard technique using the test function $\varphi = \frac{(\min(\hat{u}(p_g),0))^2}{2}$ in (2.29) and the function $\psi = \min(\hat{u}(p_g),0)$ in (2.30). The proof is omitted here since it will be given in the discrete case in Lemma 2.4.8.

The proof of Theorem 2.2.1 is based on an energy estimate obtained by the use of test functions

$$
\varphi = p_l - N(p_g), \quad \psi = M(p_g),
$$

with

$$
M(p_g) = \int_0^{p_g^+} \frac{1}{\hat{\rho}_g(\sigma)} d\sigma \quad N(p_g) = \int_0^{p_g^+} \frac{\hat{u}(\sigma)}{\hat{\rho}_g(\sigma)} d\sigma. \qquad (2.33)
$$

It is assumed that the functions M and N are extended by zero for negative pressures. For M and N we have the following bounds.

Lemma 2.2.3. *The functions (2.33) satisfy*

$$|N(p_g)| \leq \hat{C}_g u_{max}(p_g^+ + 1), \quad |M(p_g)| \leq \hat{C}_g(p_g^+ + 1), \tag{2.34}$$

where $\hat{C}_g = \max(\int_0^1 d\sigma/\hat{\rho}_g(\sigma), 1/\hat{\rho}_g(1))$.

Proof. Due to (A.5) and (A.6) we have

$$|N(p_g)| \leq \int_0^1 \frac{\hat{u}(\sigma)}{\hat{\rho}_g(\sigma)} d\sigma + \int_1^{\max(p_g^+,1)} \frac{\hat{u}(\sigma)}{\hat{\rho}_g(\sigma)} d\sigma \leq u_{max} \left(\int_0^1 \frac{1}{\hat{\rho}_g(\sigma)} d\sigma + \frac{1}{\hat{\rho}_g(1)} p_g^+ \right),$$

$$|M(p_g)| \leq \int_0^1 \frac{1}{\hat{\rho}_g(\sigma)} d\sigma + \int_1^{\max(p_g^+,1)} \frac{1}{\hat{\rho}_g(\sigma)} d\sigma \leq \int_0^1 \frac{1}{\hat{\rho}_g(\sigma)} d\sigma + \frac{1}{\hat{\rho}_g(1)} p_g^+.$$

Lemma 2.2.3 is proved. □

The key property of the test functions $p_l - N(p_g)$ and $M(p_g)$ is given by the relation

$$\frac{\partial S_l}{\partial t}(p_l - N(p_g)) + \frac{\partial}{\partial t}(uS_l + \rho_g S_g) M(p_g) = \frac{\partial}{\partial t} \mathscr{E}(p_l, p_g), \tag{2.35}$$

where the function $\mathscr{E}$ is given by

$$\mathscr{E}(p_l, p_g) = S_l (\hat{u}(p_g) M(p_g) - N(p_g)) + S_g (\hat{\rho}_g(p_g) M(p_g) - p_g) - \int_0^{S_l} p_c(s) ds. \tag{2.36}$$

Lemma 2.2.4. *The function $\mathscr{E}$ defined in (2.36) satisfies*

$$-M_{p_c} \leq \mathscr{E}(p_l, p_g) \leq C(|p_g| + 1) \tag{2.37}$$

for all $p_l \in \mathbb{R}$ and $p_g \geq 0$, where the constant C depends on u_{max}, ρ_M, $\hat{C}_g$, and M_{p_c}.

Proof. Using monotonicity of the gas mass density we have

$$\hat{u}(p_g) \int_0^{p_g} \frac{1}{\hat{\rho}_g(\sigma)} d\sigma - \int_0^{p_g} \frac{\hat{u}(\sigma)}{\hat{\rho}_g(\sigma)} d\sigma \geq u \int_0^{p_g} \frac{1}{\hat{\rho}_g(\sigma)} d\sigma - u \int_0^{p_g} \frac{1}{\hat{\rho}_g(\sigma)} d\sigma = 0.$$

By the same argument,

$$S_g \hat{\rho}_g(p_g) \int_0^{p_g} \frac{1}{\hat{\rho}_g(\sigma)} d\sigma \geq S_g \hat{\rho}_g(p_g) \cdot \frac{1}{\hat{\rho}_g(p_g)} \int_0^{p_g} d\sigma = S_g p_g.$$

Therefore, we have the estimate

$$\mathscr{E}(p_l, p_g) \geq -\int_0^{S_l} p_c(s) \, ds \geq -M_{p_c}.$$

The upper bound follows directly from the estimates on the functions M and N in Lemma 2.2.3. Lemma 2.2.4 is proved. □

By the use of above test functions one can formally prove the following a priori estimates:

Lemma 2.2.5. *Let the assumptions (A.1)-(A.8) be fulfilled and let the initial conditions p_l^0 and p_g^0 be such that $\mathscr{E}(p_l^0, p_g^0) \in L^1(\Omega)$. Then there is a constant C such that each solution of* (2.29), (2.30) *satisfies:*

$$\int_{Q_T} \left\{\lambda_l(S_l)|\nabla p_l|^2 + \lambda_g(S_l)|\nabla p_g|^2 + |\nabla u|^2\right\} \leq C, \tag{2.38}$$

$$\int_{Q_T} \left\{|\nabla p|^2 + |\nabla \beta(S_l)|^2 + |\nabla u|^2\right\} \leq C, \tag{2.39}$$

$$\left\|\partial_t(\Phi[uS_l + \rho_g S_g])\right\|_{L^2(0,T;H^{-1}(\Omega))} + \|\partial_t(\Phi S_l)\|_{L^2(0,T;H^{-1}(\Omega))} \leq C. \tag{2.40}$$

We shall not give a direct proof of Lemma 2.2.5 since it will be proved for the regularized problem and then inferred by passing to the limit in a regularization parameter.

2.3 Regularized η-problem and time discretization

The system of (2.11), (2.12) contains several degeneracies and, as a consequence, the phase pressures do not belong to $L^2(0,T;H^1(\Omega))$ space; the same is true for the capillary pressure and the saturation. As in [35], in the first regularization step we will add some terms into the governing equations that will make the capillary pressure $L^2(0,T;H^1(\Omega))$ function. Then, using (2.20), we may conclude that the regularized phase pressures are also $L^2(0,T;H^1(\Omega))$ functions. The regularized system is as follows:

$$\Phi \frac{\partial S_l^\eta}{\partial t} + \operatorname{div}\mathbf{Q}^{w,\eta} + S_l^\eta F_p = F_I, \tag{2.41}$$

$$\Phi \frac{\partial}{\partial t}\left(u^\eta S_l^\eta + \rho_g^\eta S_g^\eta\right) + \operatorname{div}\mathbf{Q}^{h,\eta} + (u^\eta S_l^\eta + \rho_g^\eta S_g^\eta)F_P = 0, \tag{2.42}$$

where the fluxes are given by

$$\mathbf{Q}^{w,\eta} = -\lambda_l(S_l^\eta)\mathbb{K}(\nabla p_l^\eta - \rho_l^\eta \mathbf{g}) + \Phi S_l^\eta \frac{1}{\rho_l^\eta} D\nabla u^\eta + \eta\nabla(p_g^\eta - p_l^\eta), \tag{2.43}$$

$$\begin{aligned}\mathbf{Q}^{h,\eta} = &- u^\eta \lambda_l(S_l^\eta)\mathbb{K}\left(\nabla p_l^\eta - \rho_l^\eta \mathbf{g}\right) - \rho_g^\eta \lambda_g(S_l^\eta)\mathbb{K}\left(\nabla p_g^\eta - \rho_g^\eta \mathbf{g}\right)\\ &- \Phi S_l^\eta \frac{\rho_l^{std}}{\rho_l^\eta} D\nabla u^\eta - \eta(\rho_g^\eta - u^\eta)\nabla(p_g^\eta - p_l^\eta).\end{aligned} \tag{2.44}$$

The system is completed with the initial and the boundary conditions:

$$
\begin{aligned}
p_l^\eta(x,0) = p_l^0(x), \quad p_g^\eta(x,0) = p_g^0(x) \qquad & \text{in } \Omega, \\
p_l^\eta(x,t) = 0, \quad p_g^\eta(x,t) = 0 \qquad & \text{on } (0,T)\times\Gamma_D, \\
\mathbf{Q}^{h,\eta}\cdot\mathbf{n} = 0, \quad \mathbf{Q}^{w,\eta}\cdot\mathbf{n} = 0 \qquad & \text{on } (0,T)\times\Gamma_N.
\end{aligned}
\tag{2.45}
$$

The secondary variables used in (2.41)–(2.44) are defined as

$$
u^\eta = \hat{u}(p_g^\eta),\ \rho_l^\eta = \rho_l^{std} + u^\eta,\ \rho_g^\eta = \hat{\rho}_g(p_g^\eta),\ S_l^\eta = p_c^{-1}(p_g^\eta - p_l^\eta),\ S_g^\eta = 1 - S_l^\eta.
$$

We shall first prove the following theorem, which states the existence of a weak solution to the problem (2.41)–(2.45) and then, by passing to the limit as small parameter η tends to zero, the existence of a weak solution to the degenerated system (2.11)–(2.15).

Theorem 2.3.1. *Let (A.1)-(A.8) hold and assume $(p_l^0, p_g^0) \in H^1(\Omega)\times H^1(\Omega)$, $p_g^0 \geq 0$. Then for all $\eta > 0$ there exists (p_l^η, p_g^η) with $p_g^\eta \geq 0$ a.e. in Q_T, satisfying*

$$
\begin{aligned}
p_l^\eta, p_g^\eta, u^\eta \in L^2(0,T;V), \\
\Phi\partial_t(u^\eta S_l^\eta + \rho_g^\eta S_g^\eta), \Phi\partial_t(S_l^\eta) \in L^2(0,T;V'), \\
u^\eta S_l^\eta + \rho_g^\eta S_g^\eta \in C^0([0,T];L^2(\Omega)), S_l^\eta \in C^0([0,T];L^2(\Omega)).
\end{aligned}
$$

For all $\varphi \in L^2(0,T;V)$,

$$
\begin{aligned}
\int_0^T \left\langle \Phi\frac{\partial S_l^\eta}{\partial t}, \varphi \right\rangle dt + \int_{Q_T} \left[\lambda_l(S_l^\eta)\mathbb{K}\nabla p_l^\eta - \Phi S_l^\eta \frac{1}{\rho_l^\eta} D\nabla u^\eta - \eta\nabla(p_g^\eta - p_l^\eta)\right]\cdot\nabla\varphi dxdt \\
+ \int_{Q_T} S_l^\eta F_p \varphi\, dxdt = \int_{Q_T} F_I \varphi\, dxdt + \int_{Q_T} \rho_l^\eta \lambda_l(S_l^\eta)\mathbb{K}\mathbf{g}\cdot\nabla\varphi dxdt.
\end{aligned}
\tag{2.46}
$$

For all $\psi \in L^2(0,T;V)$,

$$
\begin{aligned}
& \int_0^T \left\langle \Phi\frac{\partial}{\partial t}\left(u^\eta S_l^\eta + \rho_g^\eta S_g^\eta\right), \psi \right\rangle dt \\
& + \int_{Q_T} \left[u^\eta \lambda_l(S_l^\eta)\mathbb{K}\nabla p_l^\eta + \rho_g^\eta \lambda_g(S_l^\eta)\mathbb{K}\nabla p_g^\eta + \Phi S_l^\eta \frac{\rho_l^{std}}{\rho_l^\eta} D\nabla u^\eta\right]\cdot\nabla\psi dxdt \\
& + \eta\int_{Q_T} (\rho_g^\eta - u^\eta)\nabla(p_g^\eta - p_l^\eta)\cdot\nabla\psi dxdt \\
& + \int_{Q_T} (u^\eta S_l^\eta + \rho_g^\eta S_g^\eta) F_P \psi\, dxdt = \int_{Q_T} \left(\rho_l^\eta u^\eta \lambda_l(S_l^\eta) + (\rho_g^\eta)^2\lambda_g(S_l^\eta)\right)\mathbb{K}\mathbf{g}\cdot\nabla\psi dxdt.
\end{aligned}
\tag{2.47}
$$

Furthermore, $u^\eta S_l^\eta + \rho_g^\eta(1 - S_l^\eta) = \hat{u}(p_g^0)S_l^0 + \hat{\rho}_g(p_g^0)(1 - S_l^0)$ a.e. in Ω for $t = 0$, and $S_l^\eta(x,0) = S_l^0$ a.e. in Ω.

In the proof of Theorem 2.3.1 we will first discretize the time derivative (see [35]), reducing the problem to a sequence of elliptic problems, which will be solved by an application of the Schauder fixed point theorem. In order to simplify the notation we will omit writing the dependence on the small parameter η until the passage to the limit as $\eta \to 0$.

The time derivative is discretized in the following way. For each positive integer M we divide $[0,T]$ into M subintervals of equal length $\delta t = T/M$. We set $t_n = n\delta t$ and $J_n = (t_{n-1}, t_n]$ for $1 \leq n \leq M$, and we denote the time difference operator by

$$\partial^{\delta t} v(t) = \frac{v(t+\delta t) - v(t)}{\delta t}.$$

For any Hilbert space $\mathscr{H}$ we denote

$$l_{\delta t}(\mathscr{H}) = \{v \in L^\infty(0,T;\mathscr{H}) \colon v \text{ is constant in time on each subinterval } J_n \subset [0,T]\}.$$

For $v^{\delta t} \in l_{\delta t}(\mathscr{H})$ we set $v^n = v^{\delta t}|_{J_n}$ and, therefore, we can write

$$v^{\delta t} = \sum_{n=1}^{M} v^n \chi_{(t_{n-1},t_n]}(t), \quad v^{\delta t}(0) = v^0.$$

To function $v^{\delta t} \in l_{\delta t}(\mathscr{H})$ one can assign a piecewise linear in time function

$$\tilde{v}^{\delta t} = \sum_{n=1}^{M} \left(\frac{t_n - t}{\delta t} v^{n-1} + \frac{t - t_{n-1}}{\delta t} v^n \right) \chi_{(t_{n-1},t_n]}(t), \quad \tilde{v}^{\delta t}(0) = v^0. \tag{2.48}$$

Then we have $\partial_t \tilde{v}^{\delta t}(t) = \partial^{-\delta t} v^{\delta t}(t)$ for $t \neq n\delta t, n = 0,1,\ldots,N$. Finally, for any function $f \in L^1(0,T;\mathscr{H})$ we define $f^{\delta t} \in l_{\delta t}(\mathscr{H})$ by

$$f^{\delta t}(t) = \frac{1}{\delta t} \int_{J_n} f(\tau) d\tau, \quad t \in J_n.$$

The discrete secondary variables are denoted as before by

$$u^{\delta t} = \hat{u}(p_g^{\delta t}),\ \rho_l^{\delta t} = \rho_l^{std} + u^{\delta t},\ \rho_g^{\delta t} = \hat{\rho}_g(p_g^{\delta t}),\ S_l^{\delta t} = p_c^{-1}(p_g^{\delta t} - p_l^{\delta t}).$$

The weak formulation of the discrete in time system is as follows. For given p_l^0 and p_g^0 find $p_l^{\delta t} \in l_{\delta t}(V)$ and $p_g^{\delta t} \in l_{\delta t}(V)$ satisfying

$$\int_{Q_T} \Phi \partial^{-\delta t}(S_l^{\delta t}) \varphi \, dx\, dt + \int_{Q_T} \left[\lambda_l(S_l^{\delta t}) \mathbb{K} \nabla p_l^{\delta t} - \Phi S_l^{\delta t} \frac{1}{\rho_l^{\delta t}} D \nabla u^{\delta t} \right] \cdot \nabla \varphi \, dx\, dt$$
$$- \eta \int_{Q_T} [\nabla (p_g^{\delta t} - p_l^{\delta t})] \cdot \nabla \varphi \, dx\, dt + \int_{Q_T} S_l^{\delta t} F_P^{\delta t} \varphi \, dx\, dt \tag{2.49}$$

$$= \int_{Q_T} F_l^{\delta t} \varphi\, dx\, dt + \int_{Q_T} \rho_l^{\delta t} \lambda_l(S_l^{\delta t}) \mathbb{K} \mathbf{g} \cdot \nabla \varphi\, dx\, dt$$

for all $\varphi \in l_{\delta t}(V)$;

$$\begin{aligned}
&\int_{Q_T} \Phi \partial^{-\delta t} \left(u^{\delta t} S_l^{\delta t} + \rho_g^{\delta t}(1 - S_l^{\delta t}) \right) \psi\, dx\, dt \\
&\quad + \int_{Q_T} \left(u^{\delta t} \lambda_l(S_l^{\delta t}) \mathbb{K} \nabla p_l^{\delta t} + \rho_g^{\delta t} \lambda_g(S_l^{\delta t}) \mathbb{K} \nabla p_g^{\delta t} \right) \cdot \nabla \psi\, dx\, dt \\
&\quad + \int_{Q_T} \left(\Phi S_l^{\delta t} \frac{\rho_l^{std}}{\rho_l^{\delta t}} D \nabla u^{\delta t} \right) \cdot \nabla \psi\, dx\, dt + \eta \int_{Q_T} \left((\rho_g^{\delta t} - u^{\delta t}) \nabla (p_g^{\delta t} - p_l^{\delta t}) \right) \cdot \nabla \psi\, dx\, dt \\
&\quad + \int_{Q_T} (u^{\delta} S_l^{\delta t} + \rho_g^{\delta t} S_g^{\delta t}) F_P^{\delta t} \psi\, dx\, dt \\
&\quad = \int_{Q_T} \left(\rho_l^{\delta t} u^{\delta t} \lambda_l(S_l^{\delta t}) + (\rho_g^{\delta t})^2 \lambda_g(S_l^{\delta t}) \right) \mathbb{K} \mathbf{g} \cdot \nabla \psi dx dt
\end{aligned} \tag{2.50}$$

for all $\psi \in l_{\delta t}(V)$. For $t \le 0$ we set $p_l^{\delta t} = p_l^0$, $p_g^{\delta t} = p_g^0$.

We will prove the following theorem, Theorem 2.3.2, and then, by passing to the limit as $\delta t \to 0$, we will establish Theorem 2.3.1.

Theorem 2.3.2. *Assume (A.1)–(A.8), $p_g^0, p_l^0 \in L^2(\Omega)$, and $p_g^0 \ge 0$. Then for all δt there exist functions $p_l^{\delta t}, p_g^{\delta t} \in l_{\delta t}(V)$, $p_g^{\delta t} \ge 0$ a.e. in Q_T, satisfying (2.49), (2.50).*

The solution of the problem (2.49), (2.50) is built from a sequence of elliptic problems that we write here explicitly for the readers convenience. Let us fix $1 \le k \le M$. We need to establish the existence of functions $p_l^k, p_g^k \in V$ that satisfy

$$\begin{aligned}
\frac{1}{\delta t} \int_\Omega \Phi (S_l^k - S_l^{k-1}) \varphi\, dx + \int_\Omega \left[\lambda_l(S_l^k) \mathbb{K} \nabla p_l^k - \Phi S_l^k \frac{1}{\rho_l^k} D \nabla u^k \right] \cdot \nabla \varphi\, dx \\
- \eta \int_\Omega [\nabla p_g^k - \nabla p_l^k] \cdot \nabla \varphi\, dx + \int_\Omega S_l^k F_P^k \varphi\, dx \\
= \int_\Omega F_I^k \varphi\, dx + \int_\Omega \rho_l^k \lambda_l(S_l^k) \mathbb{K} \mathbf{g} \cdot \nabla \varphi\, dx
\end{aligned} \tag{2.51}$$

for all $\varphi \in V$ and

$$\begin{aligned}
&\frac{1}{\delta t} \int_\Omega \Phi \left(\left(u^k S_l^k + \rho_g^k (1 - S_l^k) \right) - \left(u^{k-1} S_l^{k-1} + \rho_g^{k-1}(1 - S_l^{k-1}) \right) \right) \psi\, dx \\
&\quad + \int_\Omega \left(u^k \lambda_l(S_l^k) \mathbb{K} \nabla p_l^k + \rho_g^k \lambda_g(S_l^k) \mathbb{K} \nabla p_g^k \right) \cdot \nabla \psi\, dx \\
&\quad + \int_\Omega \left(\Phi S_l^k \frac{\rho_l^{std}}{\rho_l^k} D \nabla u^k \right) \cdot \nabla \psi\, dx
\end{aligned} \tag{2.52}$$

$$+\eta\int_\Omega\left(\rho_g^k-u^k\right)\left(\nabla(p_g^k-p_l^k)\right)\cdot\nabla\psi\,dx+\int_\Omega(u^kS_l^k+\rho_g^kS_g^k)F_P^k\psi\,dx$$
$$=\int_\Omega\left(\rho_l^ku^k\lambda_l(S_l^k)+(\rho_g^k)^2\lambda_g(S_l^k)\right)\mathbb{K}\mathbf{g}\cdot\nabla\psi dx$$

for all $\psi\in V$. Here, as always, we use the notation

$$u^k=\hat{u}(p_g^k),\ \rho_l^k=\rho_l^{std}+\hat{u}(p_g^k),\ \rho_g^k=\hat{\rho}_g(p_g^k),\ S_l^k=p_c^{-1}(p_g^k-p_l^k).$$

2.4 Application of the Schauder fixed point theorem

In this section we prove Theorem 2.3.2 by proving the existence of at least one solution to the problem (2.51)–(2.52). The existence of the solution (p_l^k,p_g^k) for the system (2.51)–(2.52) will be proved by the Leray–Schauder fixed point theorem. This technique is common and is used in [11], [35], [63] and similar papers. We cite the Leray–Schauder theorem formulation from [11].

Theorem 2.4.1. *Let $\mathscr{T}$ be a continuous and compact map of a Banach $\mathscr{B}$ space into itself. Suppose that a set of $x\in\mathscr{B}$ such that $x=\sigma\mathscr{T}x$ is bounded for some $\sigma\in[0,1]$. Then the map $\mathscr{T}$ has a fixed point.*

In the construction of the fixed point map $\mathscr{T}$ we use several regularizations. First, we introduce a small parameter $\varepsilon>0$ and replace $\lambda_l(S_l)$ and $\hat{\rho}_g(p_g)$ by

$$\lambda_l^\varepsilon(S_l)=\lambda_l(S_l)+\varepsilon,\quad \hat{\rho}_g^\varepsilon(p_g)=\hat{\rho}_g(p_g)+\varepsilon.$$

The function $\lambda_g(S_l)$ is implicitly regularized with the parameter ε by the addition of a new term in the equation for the gas component (see (2.55)).

Finally, we use the operator $\mathcal{P}_N$ defined as an orthogonal projector in $L^2(\Omega)$ on the first N eigenvectors of the eigenproblem (see [63]),

$$\begin{aligned}-\Delta p_i&=\lambda_i p_i\quad\text{in}\quad\Omega;\\ p_i&=0\quad\text{on}\quad\Gamma_D;\\ \nabla p_i\cdot\mathbf{n}&=0\quad\text{on}\quad\Gamma_N,\end{aligned}\tag{2.53}$$

and replace several functions by its projections.

It is easy to verify that the operator $\mathcal{P}_N$ satisfies the following properties:

(P.1) There exists a constant C_N such that for all $p\in L^2(\Omega)$ and $q\in V$ it holds that

$$\|\nabla\mathcal{P}_N[p]\|_{L^2(\Omega)}\le C_N\|p\|_{L^2(\Omega)},\quad \|\nabla\mathcal{P}_N[q]\|_{L^2(\Omega)}\le\|\nabla q\|_{L^2(\Omega)}.$$

(P.2) For all $p \in V$ we have

$$\int_\Omega \nabla \mathcal{P}_N[p] \cdot \nabla p \, dx = \int_\Omega |\nabla \mathcal{P}_N[p]|^2 \, dx.$$

(P.3) For $p, \varphi \in L^2(\Omega)$ we have

$$\int_\Omega \mathcal{P}_N[p] \, \varphi \, dx = \int_\Omega p \mathcal{P}_N[\varphi] \, dx.$$

From now on, in order to simplify the notation we will omit the superscript k in (2.51)–(2.52) and assume k, δt, and η are fixed. All quantities on the preceding time level will be denoted by a star (u^{k-1} replaced by u^*, etc.). In order to simplify further notation we will denote the function S_l by S in the rest of the section.

Let p_l^* and p_g^* be given functions from $L^2(\Omega)$. We define secondary variables as

$$S^* = p_c^{-1}(p_g^* - p_l^*), \; u^* = \hat{u}(p_g^*), \; \rho_l^* = \rho_l^{std} + u^*, \; \rho_g^{\varepsilon,*} = \hat{\rho}_g^\varepsilon(p_g^*).$$

We define the mapping $\mathscr{T} : L^2(\Omega) \times L^2(\Omega) \to L^2(\Omega) \times L^2(\Omega)$ by $\mathscr{T}(\overline{p}_l, \overline{p}_g) = (p_l, p_g)$, where (p_l, p_g) is the unique solution of the linear system (2.54)–(2.55) below. In this system we use the following notation:

$$\overline{S} = p_c^{-1}(\overline{p}_g - \overline{p}_l), \quad \overline{u} = \hat{u}(\overline{p}_g), \quad \overline{\rho}_g^\varepsilon = \hat{\rho}_g^\varepsilon(\overline{p}_g), \quad \overline{\rho}_l = \rho_l^{std} + \overline{u}.$$

We also set $\tilde{p}_g = \mathcal{P}_N[p_g]$ and consequently $\tilde{\overline{p}}_g = \mathcal{P}_N[\overline{p}_g]$, which leads to the following shorthand notation:

$$\tilde{\overline{u}} = \hat{u}(\tilde{\overline{p}}_g), \quad \tilde{\overline{\rho}}_g^\varepsilon = \hat{\rho}_g^\varepsilon(\tilde{\overline{p}}_g), \quad \tilde{\overline{\rho}}_l = \rho_l^{std} + \tilde{\overline{u}}.$$

With this notation the linearized and regularized variational problem that defines the mapping $\mathscr{T}$ is given by the following set of equations:

$$\begin{aligned} \frac{1}{\delta t} \int_\Omega \Phi(\overline{S} - S^*) \varphi \, dx &+ \int_\Omega [\lambda_l^\varepsilon(\overline{S}) \mathbb{K} \nabla p_l - \Phi \overline{S} \frac{1}{\tilde{\overline{\rho}}_l} D \nabla \tilde{\overline{u}}] \cdot \nabla \varphi \, dx \\ &- \eta \int_\Omega [\nabla \tilde{\overline{p}}_g - \nabla \tilde{\overline{p}}_l] \cdot \nabla \varphi \, dx + \int_\Omega \overline{S} F_P \varphi \, dx \\ &= \int_\Omega F_l \varphi \, dx + \int_\Omega \overline{\rho}_l \lambda_l(\overline{S}) \mathbb{K} \mathbf{g} \cdot \nabla \varphi \, dx \end{aligned} \tag{2.54}$$

for all $\varphi \in V$ and

$$\frac{1}{\delta t} \int_\Omega \Phi \left(\left(\overline{u} \overline{S} + \overline{\rho}_g^\varepsilon (1 - \overline{S}) \right) - \left(u^* S^* + \rho_g^{\varepsilon,*}(1 - S^*) \right) \right) \psi \, dx$$

$$+\int_\Omega \left(\tilde{\bar{u}}\lambda_l^\varepsilon(\overline{S})\mathbb{K}\nabla p_l + \tilde{\bar{\rho}}_g^\varepsilon \lambda_g(\overline{S})\mathbb{K}\nabla\tilde{\overline{p}}_g + \varepsilon\tilde{\bar{\rho}}_g^\varepsilon\nabla p_g + \Phi\overline{S}\frac{\rho_l^{std}}{\tilde{\bar{\rho}}_l} D\nabla\tilde{\bar{u}} \right)\cdot\nabla\psi\, dx \tag{2.55}$$
$$+\eta\int_\Omega \left(\tilde{\bar{\rho}}_g^\varepsilon - \tilde{\bar{u}}\right)\left(\nabla\tilde{\overline{p}}_g - \nabla\tilde{\overline{p}}_l\right)\cdot\nabla\psi\, dx + \int_\Omega (\overline{u}\overline{S} + \overline{\rho}_g^\varepsilon(1-\overline{S}))F_P\psi\, dx$$
$$= \int_\Omega \left(\overline{\rho}_l\tilde{\bar{u}}\lambda_l(\overline{S}) + (\tilde{\bar{\rho}}_g^\varepsilon)^2\lambda_g(\overline{S})\right)\mathbb{K}\mathbf{g}\cdot\nabla\psi dx$$

for all $\psi \in V$. We note that (2.54) and (2.55) are linear and uncoupled. Different terms in these equations are carefully linearized in order to keep the symmetry present in original equations that allows us to use the test functions given by (2.59) and the orthogonality (P.2).

First we will show that the mapping $\mathscr{T}$ is well defined. Note that (2.54) is a linear elliptic problem for the function p_l, which can be written as $A_1(p_l, \varphi) = f_1(\varphi)$ with

$$A_1(p_l, \varphi) = \int_\Omega \lambda_l^\varepsilon(\overline{S}_l)\mathbb{K}\nabla p_l\cdot\nabla\varphi\, dx,$$

where the functional $f_1(\varphi)$ is given by the remaining terms in (2.54). Using boundedness of the functions $\hat{u}$ and $\hat{\rho}_g^\varepsilon, \tilde{\bar{\rho}}_l \geq \rho_l^{std} - u_{min} > 0$ and estimates $\|\nabla\tilde{\bar{\xi}}\|_{L^2(\Omega)} \leq C_N\|\overline{\xi}\|_{L^2(\Omega)}$ for $\xi = p_l, p_g, u$, one can easily prove the boundedness of the linear functional f_1:

$$|f_1(\varphi)| \leq C\|\varphi\|_V$$

for all $\varphi \in V$. By the Lax–Milgram lemma, (2.54) has a unique solution $p_l \in V$.

Similarly, since p_l is known from (2.54), (2.55) can be written as $A_2(p_g, \psi) = f_2(\psi)$ with

$$A_2(p_g, \psi) = \int_\Omega \varepsilon\tilde{\bar{\rho}}_g^\varepsilon\nabla p_g\cdot\nabla\psi\, dx, \tag{2.56}$$

where the linear functional $f_2(\psi)$ is given by the remaining terms in (2.55). Using the same arguments as in the estimate for f_1 we get the boundedness of f_2 and by the Lax–Milgram lemma the existence of a unique solution $p_g \in V$ to (2.55). This ensures that the map $\mathscr{T}$ is well defined on $L^2(\Omega)\times L^2(\Omega)$.

Continuity and compactness. Let $(\overline{p}_{l,n}, \overline{p}_{g,n})$ be a sequence in $(L^2(\Omega))^2$ that converges to some $(\overline{p}_l, \overline{p}_g)$ in $(L^2(\Omega))^2$. Then we can find a subsequence such that $(p_{l,n}, p_{g,n}) = \mathscr{T}(\overline{p}_{l,n}, \overline{p}_{g,n})$ converges weakly in $H^1(\Omega)^2$ to some functions (p_l, p_g). Using the continuity and the boundedness of all the coefficients in (2.54), (2.55), and the continuity of the operator $\mathcal{P}_N$, one can easily prove that $(p_l, p_g) = \mathscr{T}(\overline{p}_l, \overline{p}_g)$. The uniqueness of the solution to (2.54)–(2.55) gives the convergence of the whole sequence. This proves the continuity of the map $\mathscr{T}$; the compactness follows from the compact embedding of $H^1(\Omega)$ into $L^2(\Omega)$.

A priori estimate. Assume that for chosen $\sigma \in (0,1]$ there exists a pair (p_l, p_g) satisfying $(p_l, p_g) = \sigma \mathscr{T}(p_l, p_g)$, which can be written as

$$\begin{aligned}
&\frac{1}{\delta t}\int_\Omega \Phi(S-S^*)\varphi\,dx + \int_\Omega \left[\lambda_l^\varepsilon(S)\mathbb{K}\nabla\frac{p_l}{\sigma} - \Phi S\frac{1}{\tilde{\rho}_l}D\nabla\tilde{u}\right]\cdot\nabla\varphi\,dx \\
&\qquad -\eta\int_\Omega [\nabla\tilde{p}_g - \nabla\tilde{p}_l]\cdot\nabla\varphi\,dx + \int_\Omega SF_P\varphi\,dx \\
&\qquad = \int_\Omega F_I\varphi\,dx + \int_\Omega \rho_l\lambda_l(S)\mathbb{K}\mathbf{g}\cdot\nabla\varphi\,dx
\end{aligned} \tag{2.57}$$

for all $\varphi \in V$, and

$$\begin{aligned}
&\frac{1}{\delta t}\int_\Omega \Phi\left(\left(uS + \rho_g^\varepsilon(1-S)\right) - \left(u^*S^* + \rho_g^{\varepsilon,*}(1-S^*)\right)\right)\psi\,dx \\
&+\int_\Omega \left(\tilde{u}\lambda_l^\varepsilon(S)\mathbb{K}\nabla\frac{p_l}{\sigma} + \tilde{\rho}_g^\varepsilon\lambda_g(S)\mathbb{K}\nabla\tilde{p}_g + \varepsilon\tilde{\rho}_g^\varepsilon\nabla\frac{p_g}{\sigma} + \Phi S\frac{\rho_l^{std}}{\tilde{\rho}_l}D\nabla\tilde{u}\right)\cdot\nabla\psi\,dx \\
&+\eta\int_\Omega \left(\tilde{\rho}_g^\varepsilon - \tilde{u}\right)(\nabla\tilde{p}_g - \nabla\tilde{p}_l)\cdot\nabla\psi\,dx + \int_\Omega (uS + \rho_g^\varepsilon(1-S))F_P\psi\,dx \\
&= \int_\Omega \left(\rho_l\tilde{u}\lambda_l(S) + (\tilde{\rho}_g^\varepsilon)^2\lambda_g(S)\right)\mathbb{K}\mathbf{g}\cdot\nabla\psi dx
\end{aligned} \tag{2.58}$$

for all $\psi \in V$. Note that in the system (2.57)–(2.58) we have two kinds of secondary quantities:

$$u = \hat{u}(p_g), \quad \rho_g^\varepsilon = \hat{\rho}_g^\varepsilon(p_g), \quad \rho_l = \rho_l^{std} + u,$$

and

$$\tilde{u} = \hat{u}(\tilde{p}_g), \quad \tilde{\rho}_g^\varepsilon = \hat{\rho}_g^\varepsilon(\tilde{p}_g), \quad \tilde{\rho}_l = \rho_l^{std} + \tilde{u}.$$

We will use the test functions $\varphi = p_l - N^\varepsilon(\tilde{p}_g)$ and $\psi = M^\varepsilon(\tilde{p}_g)$ given by

$$N^\varepsilon(p_g) = \int_0^{p_g} \frac{\hat{u}(\sigma)}{\hat{\rho}_g^\varepsilon(\sigma)}d\sigma, \quad M^\varepsilon(p_g) = \int_0^{p_g} \frac{1}{\hat{\rho}_g^\varepsilon(\sigma)}d\sigma. \tag{2.59}$$

For any $p_g \in \mathbb{R}$ they satisfy ε dependent bounds:

$$|N^\varepsilon(p_g)| \le \frac{u_{max}}{\varepsilon}|p_g|, \quad |M^\varepsilon(p_g)| \le \frac{1}{\varepsilon}|p_g|. \tag{2.60}$$

We get

$$\begin{aligned}
&\frac{1}{\delta t}\int_\Omega \Phi(S-S^*)(p_l - N^\varepsilon(\tilde{p}_g))\,dx + \int_\Omega \left[\lambda_l^\varepsilon(S)\mathbb{K}\nabla\frac{p_l}{\sigma} - \Phi S\frac{1}{\tilde{\rho}_l}D\nabla\tilde{u}\right]\cdot\left(\nabla p_l - \frac{\tilde{u}}{\tilde{\rho}_g^\varepsilon}\nabla\tilde{p}_g\right)dx \\
&\qquad -\eta\int_\Omega [\nabla\tilde{p}_g - \nabla\tilde{p}_l]\cdot\left(\nabla p_l - \frac{\tilde{u}}{\tilde{\rho}_g^\varepsilon}\nabla\tilde{p}_g\right)dx + \int_\Omega SF_P\left(p_l - N^\varepsilon(\tilde{p}_g)\right)dx
\end{aligned}$$

$$= \int_\Omega F_l\left(p_l - N^\varepsilon(\tilde{p}_g)\right) dx + \int_\Omega \rho_l \lambda_l(S)\mathbb{K}\mathbf{g}\cdot\left(\nabla p_l - \frac{\tilde{u}}{\tilde{\rho}_g^\varepsilon}\nabla \tilde{p}_g\right) dx$$

and

$$\begin{aligned}
&\frac{1}{\delta t}\int_\Omega \Phi\left(\left(uS + \rho_g^\varepsilon(1-S)\right) - \left(u^*S^* + \rho_g^{\varepsilon,*}(1-S^*)\right)\right) M^\varepsilon(\tilde{p}_g)\, dx \\
&\quad + \int_\Omega \left(\tilde{u}\lambda_l^\varepsilon(S)\mathbb{K}\nabla\frac{p_l}{\sigma} + \tilde{\rho}_g^\varepsilon\lambda_g(S)\mathbb{K}\nabla\tilde{p}_g + \varepsilon\tilde{\rho}_g^\varepsilon\nabla\frac{p_g}{\sigma} + \Phi S\frac{\rho_l^{std}}{\tilde{\rho}_l}D\nabla\tilde{u}\right)\cdot\frac{1}{\tilde{\rho}_g^\varepsilon}\nabla\tilde{p}_g\, dx \\
&\quad + \eta\int_\Omega \left(\tilde{\rho}_g^\varepsilon - \tilde{u}\right)\left(\nabla\tilde{p}_g - \nabla\tilde{p}_l\right)\cdot\frac{1}{\tilde{\rho}_g^\varepsilon}\nabla\tilde{p}_g\, dx + \int_\Omega (uS + \rho_g^\varepsilon(1-S))F_P M^\varepsilon(\tilde{p}_g)\, dx \\
&\quad = \int_\Omega \left(\rho_l\tilde{u}\lambda_l(S) + (\tilde{\rho}_g^\varepsilon)^2\lambda_g(S)\right)\mathbb{K}\mathbf{g}\cdot\frac{1}{\tilde{\rho}_g^\varepsilon}\nabla\tilde{p}_g\, dx.
\end{aligned}$$

After summation we get (cancellation of four terms and summation of two terms)

$$\begin{aligned}
&\int_\Omega \left[\frac{1}{\sigma}\lambda_l^\varepsilon(S)\mathbb{K}\nabla p_l\cdot\nabla p_l + \frac{\varepsilon}{\sigma}\nabla p_g\cdot\nabla\tilde{p}_g\right] dx \\
&\int_\Omega \left[-\Phi S\frac{1}{\tilde{\rho}_l}D\nabla\tilde{u}\cdot\nabla p_l + \Phi S\frac{1}{\tilde{\rho}_g^\varepsilon}D\nabla\tilde{u}\cdot\nabla\tilde{p}_g + \lambda_g(S)\mathbb{K}\nabla\tilde{p}_g\cdot\nabla\tilde{p}_g\right] dx \\
&+ \eta\int_\Omega [\nabla\tilde{p}_g - \nabla\tilde{p}_l]\cdot(\nabla\tilde{p}_g - \nabla p_l)\, dx = -\int_\Omega SF_P(p_l - N^\varepsilon(\tilde{p}_g))\, dx \\
&+ \int_\Omega F_I(p_l - N^\varepsilon(\tilde{p}_g))\, dx + \int_\Omega \rho_l\lambda_l(S)\mathbb{K}\mathbf{g}\cdot\nabla p_l\, dx - \frac{1}{\delta t}\int_\Omega \Phi(S - S^*)(p_l - N^\varepsilon(\tilde{p}_g))\, dx \\
&- \frac{1}{\delta t}\int_\Omega \Phi\left(\left(uS + \rho_g^\varepsilon(1-S)\right) - \left(u^*S^* + \rho_g^{\varepsilon,*}(1-S^*)\right)\right) M^\varepsilon(\tilde{p}_g)\, dx \\
&+ \int_\Omega \tilde{\rho}_g^\varepsilon\lambda_g(S)\mathbb{K}\mathbf{g}\cdot\nabla\tilde{p}_g\, dx - \int_\Omega (uS + \rho_g^\varepsilon(1-S))F_P M^\varepsilon(\tilde{p}_g)\, dx.
\end{aligned}$$

By Lemma 2.1.6 we have for sufficiently small ε

$$\begin{aligned}
\Phi S\frac{1}{\tilde{\rho}_g^\varepsilon}D\nabla\tilde{u}\cdot\nabla\tilde{p}_g + \lambda_g(S)\mathbb{K}\nabla\tilde{p}_g\cdot\nabla\tilde{p}_g &\geq c_D|\nabla\tilde{u}|^2, \\
|\Phi S\frac{1}{\tilde{\rho}_l}D\nabla\tilde{u}\cdot\nabla p_l| &\leq \frac{1}{2}\lambda_l^\varepsilon(S)\mathbb{K}\nabla p_l\cdot\nabla p_l + qc_D|\nabla\tilde{u}|^2,
\end{aligned}$$

with $0 < q < 1$, which leads to

$$\begin{aligned}
&\int_\Omega \left[\left(\frac{1}{\sigma} - \frac{1}{2}\right))\lambda_l^\varepsilon(S)\mathbb{K}\nabla p_l\cdot\nabla p_l + (1-q)c_D|\nabla\tilde{u}|^2 + \frac{\varepsilon}{\sigma}\nabla p_g\cdot\nabla\tilde{p}_g\right] dx \\
&+ \eta\int_\Omega [\nabla\tilde{p}_g - \nabla\tilde{p}_l]\cdot(\nabla\tilde{p}_g - \nabla p_l)\, dx \leq RHS,
\end{aligned}$$

where

$$
\begin{aligned}
RHS = & -\int_\Omega SF_P(p_l - N^\varepsilon(\tilde{p}_g))\,dx + \int_\Omega F_I(p_l - N^\varepsilon(\tilde{p}_g))\,dx \\
& -\int_\Omega (uS + \rho_g^\varepsilon(1-S))F_P M^\varepsilon(\tilde{p}_g)\,dx - \frac{1}{\delta t}\int_\Omega \Phi(S - S^*)(p_l - N^\varepsilon(\tilde{p}_g))\,dx \\
& -\frac{1}{\delta t}\int_\Omega \Phi\left(\left(uS + \rho_g^\varepsilon(1-S)\right) - \left(u^* S^* + \rho_g^{\varepsilon,*}(1-S^*)\right)\right) M^\varepsilon(\tilde{p}_g)\,dx \\
& + \int_\Omega \rho_l \lambda_l(S)\mathbb{K}\mathbf{g}\cdot\nabla p_l\,dx + \int_\Omega \tilde{\rho}_g^\varepsilon \lambda_g(S)\mathbb{K}\mathbf{g}\cdot\nabla \tilde{p}_g\,dx.
\end{aligned}
$$

Using orthogonality of the spectral functions (P.2), multiplying by σ, and using $\sigma \leq 1$, we get

$$
\int_\Omega \left[\frac{1}{2}\varepsilon k_m|\nabla p_l|^2 + \sigma(1-q)c_D|\nabla\tilde{u}|^2 + \varepsilon|\nabla\tilde{p}_g|^2\right]dx + \eta\sigma\int_\Omega |\nabla\tilde{p}_g - \nabla\tilde{p}_l|^2\,dx \leq |RHS|.
$$

Since we need an estimate independent of σ it is enough to consider

$$
\frac{1}{2}\varepsilon\int_\Omega [k_m|\nabla p_l|^2 + |\nabla\tilde{p}_g|^2]\,dx \leq |RHS|. \tag{2.61}
$$

In the estimates of the right-hand side we use boundedness of the coefficients and bounds for function M^ε and N^ε given in (2.60). For example, we can estimate

$$
\begin{aligned}
\left|\int_\Omega SF_P(p_l - N^\varepsilon(\tilde{p}_g))\,dx\right| &\leq \int_\Omega \left(F_P|p_l| + F_P\frac{u_{max}}{\varepsilon}|\tilde{p}_g|\right)dx \\
&\leq \tilde{\varepsilon}\|\nabla p_l\|^2_{L^2(\Omega)} + \tilde{\varepsilon}\|\nabla\tilde{p}_g\|^2_{L^2(\Omega)} + C\|F_P\|^2_{L^2(\Omega)}
\end{aligned}
$$

with $\tilde{\varepsilon}$ small enough, depending on ε, and $C = C(u_{max}, C_\Omega, \varepsilon)$, where C_Ω is the constant from the Poincaré inequality. Note that C is independent of N and η. All the other integrals can be treated in similar way, obtaining

$$
|RHS| \leq \tilde{\varepsilon}\|\nabla p_l\|^2_{L^2(\Omega)} + \tilde{\varepsilon}\|\nabla\tilde{p}_g\|^2_{L^2(\Omega)} + C,
$$

where the constant C depends on ε, but it is independent of σ, N, and η. As a consequence we get from (2.61) (for $\tilde{\varepsilon}$ sufficiently small)

$$
\frac{1}{2}\varepsilon\int_\Omega [k_m|\nabla p_l|^2 + |\nabla\tilde{p}_g|^2]\,dx \leq C, \tag{2.62}
$$

with C independent of σ, N, and η.

By setting $\psi = p_g$ in (2.58) we get

$$
\int_\Omega \varepsilon\tilde{\rho}_g^\varepsilon|\nabla p_g|^2\,dx
$$

$$
\begin{aligned}
&= -\int_\Omega \left(\tilde{u}\lambda_l^\varepsilon(S)\mathbb{K}\nabla p_l + \sigma\tilde{\rho}_g^\varepsilon\lambda_g(S)\mathbb{K}\nabla\tilde{p}_g + \sigma\Phi S\frac{\rho_l^{std}}{\tilde{\rho}_l}D\nabla\tilde{u}\right)\cdot\nabla p_g\,dx \\
&- \frac{\sigma}{\delta t}\int_\Omega \Phi\left(\left(uS+\rho_g^\varepsilon(1-S)\right)-\left(u^*S^*+\rho_g^{\varepsilon,*}(1-S^*)\right)\right)p_g\,dx \\
&- \sigma\eta\int_\Omega \left(\tilde{\rho}_g^\varepsilon-\tilde{u}\right)(\nabla\tilde{p}_g-\nabla\tilde{p}_l)\cdot\nabla p_g\,dx - \sigma\int_\Omega (uS+\rho_g^\varepsilon(1-S))F_P p_g\,dx \\
&+ \sigma\int_\Omega \left(\rho_l\tilde{u}\lambda_l(S)+(\tilde{\rho}_g^\varepsilon)^2\lambda_g(S)\right)\mathbb{K}\mathbf{g}\cdot\nabla p_g\,dx.
\end{aligned}
$$

Using Hölder and Poincaré inequalities we get for any $\tilde{\varepsilon} > 0$,

$$
\varepsilon^2\int_\Omega |\nabla p_g|^2\,dx \le \tilde{\varepsilon}\int_\Omega |\nabla p_g|^2\,dx + C\left(\int_\Omega \left(|\nabla p_l|^2+|\nabla\tilde{u}|^2+|\nabla\tilde{p}_g|^2+|\nabla\tilde{p}_l|^2\right)dx+1\right).
$$

Using $\|\nabla\tilde{u}\|_{L^2(\Omega)} \le M_g\|\nabla\tilde{p}_g\|_{L^2(\Omega)}$, $\|\nabla\tilde{p}_l\|_{L^2(\Omega)} \le \|\nabla p_l\|_{L^2(\Omega)}$, and (2.62) we obtain

$$
\int_\Omega |\nabla p_g|^2\,dx \le C, \tag{2.63}
$$

where C depends on ε but it is independent of σ, N, and η. From (2.62) and (2.63) we conclude that all assumptions of the Schauder fixed point theorem are satisfied, which proves the following proposition.

Proposition 2.4.2. *For given $(p_l^*, p_g^*) \in L^2(\Omega)\times L^2(\Omega)$ there exists $(p_l, p_g) \in V\times V$ that solve (2.64), (2.65):*

$$
\begin{aligned}
&\frac{1}{\delta t}\int_\Omega \Phi(S-S^*)\varphi\,dx + \int_\Omega \left[\lambda_l^\varepsilon(S)\mathbb{K}\nabla p_l - \Phi S\frac{1}{\rho_l^{std}+\hat{u}(\mathcal{P}_N[p_g])}D\nabla\hat{u}(\mathcal{P}_N[p_g])\right]\cdot\nabla\varphi\,dx \\
&\quad - \eta\int_\Omega [\nabla\mathcal{P}_N[p_g]-\nabla\mathcal{P}_N[p_l]]\cdot\nabla\varphi\,dx + \int_\Omega SF_P\varphi\,dx \\
&\quad = \int_\Omega F_I\varphi\,dx + \int_\Omega \rho_l\lambda_l(S)\mathbb{K}\mathbf{g}\cdot\nabla\varphi\,dx
\end{aligned} \tag{2.64}
$$

for all $\varphi \in V$ and

$$
\begin{aligned}
&\frac{1}{\delta t}\int_\Omega \Phi\left(\left(uS+\rho_g^\varepsilon(1-S)\right)-\left(u^*S^*+\rho_g^{\varepsilon,*}(1-S^*)\right)\right)\psi\,dx + \int_\Omega \hat{u}(\mathcal{P}_N[p_g])\lambda_l^\varepsilon(S)\mathbb{K}\nabla p_l\cdot\nabla\psi\,dx \\
&\quad + \int_\Omega \left(\hat{\rho}_g^\varepsilon(\mathcal{P}_N[p_g])\lambda_g(S)\mathbb{K}\nabla\mathcal{P}_N[p_g] + \varepsilon\hat{\rho}_g^\varepsilon(\mathcal{P}_N[p_g])\nabla p_g\right)\cdot\nabla\psi\,dx \\
&\quad + \int_\Omega \Phi S\frac{\rho_l^{std}}{\rho_l^{std}+\hat{u}(\mathcal{P}_N[p_g])}D\nabla\hat{u}(\mathcal{P}_N[p_g])\cdot\nabla\psi\,dx \\
&\quad + \eta\int_\Omega \left(\hat{\rho}_g^\varepsilon(\mathcal{P}_N[p_g])-\hat{u}(\mathcal{P}_N[p_g])\right)(\nabla\mathcal{P}_N[p_g]-\nabla\mathcal{P}_N[p_l])\cdot\nabla\psi\,dx
\end{aligned} \tag{2.65}
$$

$$+\int_\Omega (uS+\rho_g^\varepsilon(1-S))F_P\psi\,dx$$
$$=\int_\Omega \big(\rho_l\hat{u}(\mathcal{P}_N[p_g])\lambda_l(S)+(\hat{\rho}_g^\varepsilon(\mathcal{P}_N[p_g]))^2\lambda_g(S)\big)\,\mathbb{K}\mathbf{g}\cdot\nabla\psi dx$$

for all $\psi\in V$. The secondary variables in equations (2.64), (2.65) are given by

$$S=p_c^{-1}(p_g-p_l),\quad u=\hat{u}(p_g),\quad \rho_g^\varepsilon=\hat{\rho}_g^\varepsilon(p_g),\quad \rho_l=\rho_l^{std}+\hat{u}(p_g).$$

Note that p_l and p_g depend on η, ε, and N. However, we omit this dependency in writing for simplicity until passing to the limit in some of the parameters, when the parameter of interest will be denoted explicitly.

2.4.1 Step 2. Limit as $N\to\infty$

By applying a priori estimates (2.62) and (2.63) given in the proof of Proposition 2.4.2 for $\sigma=1$ we get the following result.

Corollary 2.4.3. *There is a constant $C>0$ independent of N and η (but depending on ε) such that any solutions $(p_l^N,p_g^N)\in V\times V$ to the problem (2.64), (2.65) satisfy*

$$\int_\Omega|\nabla\mathcal{P}_N[p_g^N]|^2\,dx,\ \int_\Omega|\nabla p_g^N|^2\,dx,\ \int_\Omega|\nabla p_l^N|^2\,dx\le C.$$

We consider behavior of the solution to (2.64)–(2.65), p_l^N and p_g^N, as $N\to\infty$, while all other regularization parameters, ε, η, and δt, are kept constant. We also denote the secondary variables as

$$u^N=\hat{u}(p_g^N),\quad \rho_g^N=\hat{\rho}_g^\varepsilon(p_g^N),\quad \rho_l^N=\rho_l^{std}+\hat{u}(p_g^N),\quad S^N=p_c^{-1}(p_g^N-p_l^N).$$

The uniform bounds (with respect to N) from Corollary 2.4.3 imply that there is a subsequence, still denoted by N, such that as $N\to\infty$,

$$\begin{aligned}
p_g^N&\to p_g\quad \text{weakly in } V, \text{ strongly in } L^2(\Omega) \text{ and a.e. in } \Omega,\\
p_l^N&\to p_l\quad \text{weakly in } V, \text{ strongly in } L^2(\Omega) \text{ and a.e. in } \Omega,\\
\mathcal{P}_N[p_g^N]&\to\xi\quad \text{weakly in } V, \text{ strongly in } L^2(\Omega) \text{ and a.e. in } \Omega,
\end{aligned}$$

for some $p_l,p_g,\xi\in V$. Using the property (P.3) of the projection operator we find that $\xi=p_g$. Due to the properties (A.5) and (A.6) we have

$$S^N\to S=p_c^{-1}(p_g-p_l)\quad \text{a.e. in } \Omega,$$

$$\begin{aligned} u^N \to u = \hat{u}(p_g) &\quad \text{weakly in } V \text{ and a.e. in } \Omega, \\ \rho_g^N \to \rho_g^\varepsilon = \hat{\rho}_g^\varepsilon(p_g) &\quad \text{a.e. in } \Omega, \\ 1/\rho_l^N \to 1/\rho_l = 1/(\rho_l^{std} + \hat{u}(p_g)) &\quad \text{a.e. in } \Omega. \end{aligned}$$

These convergences are sufficient to pass to the limit as $N \to \infty$ in (2.64)–(2.65), and we get

$$\begin{aligned} &\frac{1}{\delta t}\int_\Omega \Phi(S - S^*)\varphi\, dx + \int_\Omega [\lambda_l^\varepsilon(S)\mathbb{K}\nabla p_l - \Phi S\frac{1}{\rho_l} D\nabla\hat{u}(p_g)]\cdot\nabla\varphi\, dx \\ &\qquad - \eta\int_\Omega [\nabla p_g - \nabla p_l]\cdot\nabla\varphi\, dx + \int_\Omega S F_P \varphi\, dx \\ &\qquad = \int_\Omega F_l \varphi\, dx + \int_\Omega \rho_l \lambda_l(S)\mathbb{K}\mathbf{g}\cdot\nabla\varphi\, dx \end{aligned} \tag{2.66}$$

for all $\varphi \in V$ and

$$\begin{aligned} &\frac{1}{\delta t}\int_\Omega \Phi\left(\left(uS + \rho_g^\varepsilon(1-S)\right) - \left(u^* S^* + \rho_g^{\varepsilon,*}(1-S^*)\right)\right)\psi\, dx \\ &+ \int_\Omega \left(u\lambda_l^\varepsilon(S)\mathbb{K}\nabla p_l + \rho_g^\varepsilon \lambda_g(S)\mathbb{K}\nabla p_g + \varepsilon\rho_g^\varepsilon\nabla p_g + \Phi S\frac{\rho_l^{std}}{\rho_l} D\nabla u\right)\cdot\nabla\psi\, dx \\ &+ \eta\int_\Omega \left(\rho_g^\varepsilon - u\right)(\nabla p_g - \nabla p_l)\cdot\nabla\psi\, dx + \int_\Omega (uS + \rho_g^\varepsilon(1-S))F_P\psi\, dx \\ &= \int_\Omega \left(\rho_l u \lambda_l(S) + (\rho_g^\varepsilon)^2\lambda_g(S)\right)\mathbb{K}\mathbf{g}\cdot\nabla\psi dx \end{aligned} \tag{2.67}$$

for all $\psi \in V$, where

$$u = \hat{u}(p_g), \quad \rho_g^\varepsilon = \hat{\rho}_g^\varepsilon(p_g), \quad \rho_l = \rho_l^{std} + \hat{u}(p_g), \quad S = p_c^{-1}(p_g - p_l). \tag{2.68}$$

We have proved the following result.

Proposition 2.4.4. *For given $(p_l^*, p_g^*) \in L^2(\Omega) \times L^2(\Omega)$ there exists $(p_l, p_g) \in V \times V$ that solve problem (2.66), (2.67), and (2.68).*

2.4.2 Step 3. Limit as $\varepsilon \to 0$

For the passage to the limit as $\varepsilon \to 0$ we need to refine a priori estimates since they are not independent of ε. This will be achieved by using the test functions $\varphi = p_l - N^\varepsilon(p_g)$ and $\psi = M^\varepsilon(p_g)$ in (2.66) and (2.67), which lead to the following estimate.

Lemma 2.4.5. *There is a constant C independent of δt, η, and ε such that each solution to the problem (2.66), (2.67), and (2.68) satisfies*

$$\frac{1}{\delta t}\int_\Omega \Phi[\mathscr{E}^\varepsilon(p_l, p_g) - \mathscr{E}^\varepsilon(p_l^*, p_g^*)]\, dx$$

$$
\begin{aligned}
&+\int_\Omega [\lambda_l(S)\mathbb{K}\nabla p_l\cdot\nabla p_l+\lambda_g(S)\mathbb{K}\nabla p_g\cdot\nabla p_g+c_D|\nabla u|^2+\varepsilon|\nabla p_g|^2]\,dx \\
&+\eta\int_\Omega |\nabla p_g-\nabla p_l|^2\,dx\le C,
\end{aligned}
\tag{2.69}
$$

where the function $\mathscr{E}^\varepsilon$ is given by

$$
\begin{aligned}
\mathscr{E}^\varepsilon(p_l,p_g)=S[\hat{u}(p_g)M^\varepsilon(p_g)-N^\varepsilon(p_g)]+(1-S)[\hat{\rho}_g^\varepsilon(p_g)M^\varepsilon(p_g)-p_g]\\
-\int_0^S p_c(\sigma)\,d\sigma.
\end{aligned}
\tag{2.70}
$$

Proof. After introducing the test functions $\varphi=p_l-N^\varepsilon(p_g)$ and $\psi=M^\varepsilon(p_g)$ in (2.66) and (2.67) and summation of the two equations, we get the following equation:

$$
\begin{aligned}
&\frac{1}{\delta t}\int_\Omega \Phi(S-S^*)(p_l-N^\varepsilon(p_g))\,dx\\
&\quad+\frac{1}{\delta t}\int_\Omega \Phi\left[\big(uS+\hat{\rho}_g^\varepsilon(p_g)(1-S)\big)-\big(u^*S^*+\rho_g^{\varepsilon,*}(1-S^*)\big)\right]M^\varepsilon(p_g)\,dx\\
&\quad+\int_\Omega\left[\lambda_l^\varepsilon(S)\mathbb{K}\nabla p_l\cdot\nabla p_l-\Phi\frac{S}{\rho_l}D\nabla u\cdot\nabla p_l+\lambda_g(S)\mathbb{K}\nabla p_g\cdot\nabla p_g+\varepsilon|\nabla p_g|^2\right]dx\\
&\quad+\int_\Omega\frac{\Phi SD}{\rho_g^\varepsilon}\nabla u\cdot\nabla p_g\,dx+\eta\int_\Omega|\nabla p_g-\nabla p_l|^2\,dx=RHS,
\end{aligned}
\tag{2.71}
$$

where $RHS=I_1+I_2+I_3$ with

$$
\begin{aligned}
I_1&=\int_\Omega F_I(p_l-N^\varepsilon(p_g))\,dx,\\
I_2&=-\int_\Omega SF_P(p_l-N^\varepsilon(p_g))\,dx-\int_\Omega(uS+\rho_g^\varepsilon(1-S))F_PM^\varepsilon(p_g)\,dx,\\
I_3&=\int_\Omega\rho_l\lambda_l(S)\mathbb{K}\mathbf{g}\cdot\nabla p_l\,dx+\int_\Omega\rho_g^\varepsilon\lambda_g(S)\mathbb{K}\mathbf{g}\cdot\nabla p_g dx.
\end{aligned}
\tag{2.72}
$$

First we consider the accumulation terms in (2.71) in which we will use shorthand notation:

$$
\mathscr{J}=(S-S^*)(p_l-N^\varepsilon(p_g))+\left[\big(uS+\hat{\rho}_g^\varepsilon(p_g)(1-S)\big)-\big(u^*S^*+\rho_g^{\varepsilon,*}(1-S^*)\big)\right]M^\varepsilon(p_g).
$$

Then, by simple manipulations we get

$$
\begin{aligned}
\mathscr{J}&=Sp_l+S(uM^\varepsilon(p_g)-N^\varepsilon(p_g))+(1-S)\hat{\rho}_g^\varepsilon(p_g)M^\varepsilon(p_g)\\
&\quad-\left[S^*p_l^*+S^*(u^*M^\varepsilon(p_g^*)-N^\varepsilon(p_g^*))+(1-S^*)\rho_g^{\varepsilon,*}M^\varepsilon(p_g^*)\right]\\
&\quad+S^*(p_l^*-p_l)+S^*\left([u^*M^\varepsilon(p_g^*)-N^\varepsilon(p_g^*)]-[u^*M^\varepsilon(p_g)-N^\varepsilon(p_g)]\right)\\
&\quad+(1-S^*)\rho_g^{\varepsilon,*}[M^\varepsilon(p_g^*)-M^\varepsilon(p_g)].
\end{aligned}
$$

Note that from (A.5) we get

$$[u^*M^\varepsilon(p_g^*)-N^\varepsilon(p_g^*)]-[u^*M^\varepsilon(p_g)-N^\varepsilon(p_g)]=\hat{u}(p_g^*)\int_{p_g}^{p_g^*}\frac{d\sigma}{\hat{\rho}_g^\varepsilon(\sigma)}-\int_{p_g}^{p_g^*}\frac{\hat{u}(\sigma)}{\hat{\rho}_g^\varepsilon(\sigma)}d\sigma\geq 0,$$

and from (A.6)

$$(1-S^*)\rho_g^*[M^\varepsilon(p_g^*)-M^\varepsilon(p_g)]=(1-S^*)\hat{\rho}_g^\varepsilon(p_g^*)\int_{p_g}^{p_g^*}\frac{d\sigma}{\hat{\rho}_g^\varepsilon(\sigma)}\geq(1-S^*)(p_g^*-p_g),$$

leading to

$$\begin{aligned}\mathscr{J}\geq{}& S(uM^\varepsilon(p_g)-N^\varepsilon(p_g))+(1-S)(\hat{\rho}_g^\varepsilon(p_g)M^\varepsilon(p_g)-p_g)\\&-\left[S^*(u^*M^\varepsilon(p_g^*)-N^\varepsilon(p_g^*))+(1-S^*)(\rho_g^{\varepsilon,*}M^\varepsilon(p_g^*)-p_g^*)\right]+(S^*-S)(p_g-p_l).\end{aligned}$$

Using (A.4) one can estimate

$$(S^*-S)(p_g-p_l)\geq(S^*-S)p_c(S)\geq\int_S^{S^*}p_c(\sigma)\,d\sigma,$$

and therefore we can estimate the accumulation term as follows:

$$\frac{1}{\delta t}\int_\Omega\Phi\mathscr{J}\,dx\geq\frac{1}{\delta t}\int_\Omega\Phi[\mathscr{E}^\varepsilon(p_l,p_g)-\mathscr{E}^\varepsilon(p_l^*,p_g^*)]\,dx, \tag{2.73}$$

where the function $\mathscr{E}^\varepsilon$ is given by (2.70).

We consider now the third and the fourth integrals in (2.71). Applying Lemma 2.1.6 we get

$$\begin{aligned}&\frac{\Phi SD}{\rho_g^\varepsilon}\nabla u\cdot\nabla p_g+\lambda_g(S)\mathbb{K}\nabla p_g\cdot\nabla p_g\geq c_D|\nabla u|^2,\\&\left|\Phi SD\frac{1}{\rho_l}\nabla u\cdot\nabla p_l\right|\leq\frac{1}{2}\lambda_l^\varepsilon(S)\mathbb{K}\nabla p_l\cdot\nabla p_l+qc_D|\nabla u|^2.\end{aligned}$$

If we denote the sum of the third and fourth integral in (2.71) by $\mathscr{I}$, then we easily get

$$\begin{aligned}\mathscr{I}\geq{}&\int_\Omega\left[\frac{1}{2}\lambda_l^\varepsilon(S)\mathbb{K}\nabla p_l\cdot\nabla p_l+\frac{1-q}{2}\lambda_g(S)\mathbb{K}\nabla p_g\cdot\nabla p_g\right]dx\\&+\int_\Omega\left[\frac{1-q}{2}c_D|\nabla u|^2+\varepsilon|\nabla p_g|^2\right]dx.\end{aligned} \tag{2.74}$$

Finally, let us estimate the right-hand side in (2.71). From $F_I\geq 0$, $p_l\leq p$ and since $N^\varepsilon(p_g)\geq 0$ for $p_g\in\mathbb{R}$ we can estimate

$$I_1=\int_{Q_T}F_I(p_l-N^\varepsilon(p_g))dxdt\leq\int_{Q_T}F_Ip\,dxdt\leq C_1+\frac{\tilde{\varepsilon}}{2}\|p\|_{L^2(Q_T)}^2 \tag{2.75}$$

for an arbitrary $\tilde{\varepsilon}$, and $C_1 = C_1(\|F_I\|_{L^2(Q_T)}, \tilde{\varepsilon})$.

The term I_2 can be rearranged as follows:

$$I_2 = -\int_\Omega SF_P p_l \, dx + \int_\Omega SF_P(N^\varepsilon(p_g) - \hat{u}(p_g)M^\varepsilon(p_g)) \, dx - \int_\Omega \rho_g^\varepsilon (1-S) F_P M^\varepsilon(p_g) \, dx.$$

Since the function $\hat{u}$ is nondecreasing on $\mathbb{R}$ we have $N^\varepsilon(p_g) - \hat{u}(p_g)M^\varepsilon(p_g) \leq 0$ and $F_P \geq 0$ gives

$$\int_{Q_T} SF_P \left(N^\varepsilon(p_g) - \hat{u}(p_g)M^\varepsilon(p_g)\right) dxdt \leq 0. \tag{2.76}$$

From Lemma 2.1.4 we can estimate the terms with the liquid pressure by the global pressure as follows:

$$-\int_{Q_T} SF_P p_l dxdt \leq \int_{Q_T} F_P(|p| + C) dxdt \leq C_2 + \frac{\tilde{\varepsilon}}{4}\|p\|^2_{L^2(Q_T)}$$

for some $\tilde{\varepsilon} > 0$ and $C_2 = C_2(\|F_P\|_{L^2(Q_T)}, \tilde{\varepsilon})$.

The last term in I_2 is nonpositive for $p_g \geq 0$, and in the region where $p_g < 0$ by Lemma 2.1.4 it holds that

$$\begin{aligned} -\int_{Q_T} \rho_g^\varepsilon(p_g) S_g F_P M^\varepsilon(p_g) dxdt &= \int_{Q_T} F_P |S_g p_g| dxdt \\ &\leq \int_{Q_T} F_P(|p| + C) dxdt \leq C_3 + \frac{\tilde{\varepsilon}}{4}\|p\|^2_{L^2(Q_T)} \end{aligned}$$

for arbitrary $\tilde{\varepsilon} > 0$ and $C_3 = C_3(\|F_P\|_{L^2(Q_T)}, \tilde{\varepsilon})$. Therefore, we conclude that for arbitrary $\tilde{\varepsilon} > 0$ we have the estimate

$$I_2 \leq C_4 + \frac{\tilde{\varepsilon}}{2}\|p\|^2_{L^2(Q_T)}, \tag{2.77}$$

where $C_4 = C_4(\|F_P\|_{L^2(Q_T)}, \tilde{\varepsilon})$.

A straightforward estimate, based on boundedness of the gas and the liquid densities, gives

$$I_3 \leq C_5 + \hat{\varepsilon} \int_{Q_T} \lambda_g(S) \mathbb{K} \nabla p_g \cdot \nabla p_g \, dxdt + \hat{\varepsilon} \int_{Q_T} \lambda_l(S) \mathbb{K} \nabla p_l \cdot \nabla p_l \, dxdt \tag{2.78}$$

for an arbitrary $\hat{\varepsilon}$.

The global pressure norm can be estimated by the Poincaré inequality and (1.34) as follows:

$$\|p\|^2_{L^2(Q_T)} \leq C \int_\Omega (\lambda_l(S) \mathbb{K} \nabla p_l \cdot \nabla p_l + \lambda_g(S) \mathbb{K} \nabla p_g \cdot \nabla p_g) \, dx. \tag{2.79}$$

From the estimates (2.73), (2.74), (2.75), (2.77), (2.78), and (2.79), taking sufficiently small $\tilde{\varepsilon}$ and $\hat{\varepsilon}$ we obtain the estimate (2.69). Lemma 2.4.5 is proved. □

Remark 2.4.6. *Note that by using Lemma 1.34 we can write the estimate (2.69) also as follows:*

$$\frac{1}{\delta t}\int_\Omega \Phi[\mathscr{E}^\varepsilon(p_l,p_g)-\mathscr{E}^\varepsilon(p_l^*,p_g^*)]\,dx$$
$$+\int_\Omega [\lambda(S)\mathbb{K}\nabla p\cdot\nabla p+\mathbb{K}\nabla\beta(S)\cdot\nabla\beta(S)+c_D|\nabla u|^2+\varepsilon|\nabla p_g|^2]\,dx$$
$$+\eta\int_\Omega |\nabla p_g-\nabla p_l|^2\,dx\le C.$$

Due to the monotonicity of the function $\hat{u}$ and the definition of the function $\hat{\rho}_g^\varepsilon$ we can carry out the same steps as in the proof of Lemma 2.2.4 to show

$$\mathscr{E}^\varepsilon(p_l,p_g)\ge -M_{p_c} \tag{2.80}$$

for $p_l,p_g\in\mathbb{R}$. Also, we have the upper bound

$$\mathscr{E}^\varepsilon(p_l^*,p_g^*)\le C(p_g^*+1) \tag{2.81}$$

since p_g^* satisfies $p_g^*\ge 0$. We can apply the previous estimates (2.80) and (2.81) to the estimate (2.69) and obtain that each solution to the problem (2.66), (2.67), and (2.68) with $p_g^*\ge 0$ satisfies the following bound:

$$\int_\Omega [|\nabla p|^2+|\nabla\beta(S)|^2+|\nabla u|^2+\varepsilon|\nabla p_g|^2]\,dx+\eta\int_\Omega |\nabla p_g-\nabla p_l|^2\,dx\le C, \tag{2.82}$$

where the constant C is independent of ε and η.

We shall now denote the solution to the problem (2.66), (2.67), and (2.68) by p_l^ε and p_g^ε. All secondary variables will also be denoted by ε,

$$u^\varepsilon=\hat{u}(p_g^\varepsilon),\quad \rho_g^\varepsilon=\hat{\rho}_g^\varepsilon(p_g^\varepsilon),\quad \rho_l^\varepsilon=\rho_l^{std}+\hat{u}(p_g^\varepsilon),\quad S^\varepsilon=p_c^{-1}(p_g^\varepsilon-p_l^\varepsilon), \tag{2.83}$$

and the global pressure defined by (1.31) is denoted p^ε.

The bounds (2.69) and (2.82) give the following bounds uniform with respect to ε:

$$(u^\varepsilon)_\varepsilon \text{ is uniformly bounded in } V, \tag{2.84}$$
$$(p^\varepsilon)_\varepsilon \text{ is uniformly bounded in } V, \tag{2.85}$$
$$(\beta(S^\varepsilon))_\varepsilon \text{ is uniformly bounded in } H^1(\Omega), \tag{2.86}$$
$$(\sqrt{\varepsilon}\nabla p_l^\varepsilon)_\varepsilon \text{ is uniformly bounded in } L^2(\Omega), \tag{2.87}$$
$$(\sqrt{\varepsilon}\nabla p_g^\varepsilon)_\varepsilon \text{ is uniformly bounded in } L^2(\Omega), \tag{2.88}$$
$$(\nabla p_c(S^\varepsilon))_\varepsilon \text{ is uniformly bounded in } L^2(\Omega). \tag{2.89}$$

Lemma 2.4.7. *Let p_l^ε and p_g^ε be a solution to (2.66), (2.67), and (2.68) and let the corresponding secondary variables be denoted as in (2.83). Then there exist functions $p_l, p_g \in L^2(\Omega)$, $S = p_c^{-1}(p_g - p_l)$, and $p = p_l + \overline{P}(S) \in V$ such that on a subsequence it holds that*

$$p^\varepsilon \longrightarrow p \quad \text{weakly in } V \text{ and a.e. in } \Omega, \tag{2.90}$$

$$p_c(S^\varepsilon) \longrightarrow p_c(S) \quad \text{weakly in } H^1(\Omega). \tag{2.91}$$

$$S^\varepsilon \longrightarrow S \quad \text{a.e. in } \Omega, \tag{2.92}$$

$$\beta(S^\varepsilon) \longrightarrow \beta(S) \quad \text{weakly in } H^1(\Omega) \text{ and a.e. in } \Omega, \tag{2.93}$$

$$p_l^\varepsilon \longrightarrow p_l \quad \text{a.e. in } \Omega, \tag{2.94}$$

$$p_g^\varepsilon \longrightarrow p_g \quad \text{a.e. in } \Omega, \tag{2.95}$$

$$\rho_g^\varepsilon = \hat{\rho}_g^\varepsilon(p_g^\varepsilon) \longrightarrow \rho_g = \hat{\rho}_g(p_g) \quad \text{a.e. in } \Omega, \tag{2.96}$$

$$\rho_l^\varepsilon = \rho_l^{std} + \hat{u}(p_g^\varepsilon) \longrightarrow \rho_l = \rho_l^{std} + \hat{u}(p_g) \quad \text{a.e. in } \Omega, \tag{2.97}$$

$$u^\varepsilon \longrightarrow u = \hat{u}(p_g) \quad \text{weakly in } V \text{ and a.e. in } \Omega, \tag{2.98}$$

Proof. The convergence (2.90) follows directly from (2.85). From (2.89) and the Dirichlet boundary condition we conclude that $\hat{p}_c(S^\varepsilon) \longrightarrow \xi$ weakly in $H^1(\Omega)$ and a.e. in Ω, for some $\xi \in H^1(\Omega)$, $\xi \geq 0$. Since the function p_c is invertible we can define $S = p_c^{-1}(\xi)$ and now (2.91) and (2.92) follow. From (2.86) and (2.92) we obtain (2.93).

Definition of the global pressure gives

$$p_l^\varepsilon = p^\varepsilon + \int_{S^\varepsilon}^1 \frac{\lambda_g(s)}{\lambda_l(s)+\lambda_g(s)} p_c'(s)ds \longrightarrow p + \int_S^1 \frac{\lambda_g(s)}{\lambda_l(s)+\lambda_g(s)} p_c'(s)ds =: p_l, \text{ a.e. in } \Omega,$$

where we define limiting liquid pressure p_l by its relation to the limiting global pressure. Similarly,

$$p_g^\varepsilon = p_l^\varepsilon + p_c(S^\varepsilon) \longrightarrow p_l + p_c(S) =: p_g \text{ a.e. in } \Omega.$$

Obviously, we have $S = p_c^{-1}(p_g - p_l)$. This proves (2.94), (2.95), and (2.96) and (2.97) follow from the continuity of the functions $\hat{\rho}_g$ and $\hat{u}$, and the uniform convergence of $\hat{\rho}_g^\varepsilon$ toward $\hat{\rho}_g$. Finally, (2.98) is a consequence of (2.84). □

2.4.3 End of the proof of Theorem 2.3.2

In order to prove Theorem 2.3.2 we need to pass to the limit as $\varepsilon \to 0$ in (2.66)–(2.67) using the convergences established in Lemma 2.4.7. This passage to the limit is evident in all terms except the terms containing the gradients of the phase pressures. In these terms we use relation (1.33). For example

$$\int_\Omega u^\varepsilon \lambda_l^\varepsilon(S^\varepsilon)\mathbb{K}\nabla p_l^\varepsilon \cdot \nabla\psi\,dx = \int_\Omega u^\varepsilon[\lambda_l(S^\varepsilon)\mathbb{K}\nabla p^\varepsilon + \gamma(S^\varepsilon)\mathbb{K}\nabla\beta(S^\varepsilon)]\cdot\nabla\psi\,dx$$
$$\to \int_\Omega u[\lambda_l(S)\mathbb{K}\nabla p + \gamma(S)\mathbb{K}\nabla\beta(S)]\cdot\nabla\psi\,dx = \int_\Omega u\lambda_l(S)\mathbb{K}\nabla p_l\cdot\nabla\psi\,dx,$$

where the limit liquid pressure p_l is defined from the limit global pressure p and the limit saturation S by (1.31). In this way we have proved that for given $p_l^{k-1}, p_g^{k-1} \in V$, $p_g^{k-1} \geq 0$, there exists at least one solution $p_l^k, p_g^k \in V$ of (2.51) and (2.52). In order to finish the proof of Theorem 2.3.2 we need to prove nonnegativity of the pseudo gas pressure p_g^k.

Lemma 2.4.8. *Let $p_l^{k-1}, p_g^{k-1} \in V$, $p_g^{k-1} \geq 0$. Then the solution to the problem (2.51), (2.52) satisfies $p_g^k \geq 0$.*

Proof. Let us define $X = \min(u^k, 0)$. We set $\varphi = X^2/2$ in the liquid component equation (2.51) and $\psi = X$ in the gas component equation (2.52). Note that the integration in these equations is performed only on the part of the domain where $p_g^k \leq 0$, which cancels the terms multiplied by ρ_g^k, since $\hat\rho_g(p_g) = 0$ for $p_g \leq 0$. By subtracting the liquid component equation from the gas component equation we get

$$\frac{1}{\delta t}\int_\Omega \Phi\left(X^2 S^k - \left(u^{k-1}S^{k-1} + \rho_g^{k-1}(1-S^{k-1})\right)X - (S^k - S^{k-1})\frac{X^2}{2}\right)dx$$
$$+\int_\Omega \Phi S^k D|\nabla X|^2\,dx + \int_\Omega S^k F_P^k\frac{X^2}{2}\,dx = -\int_\Omega F_I\frac{X^2}{2}\,dx.$$

Due to the fact $p_g^{k-1} \geq 0$ and $X \leq 0$ we have

$$-\left(u^{k-1}S^{k-1} + \rho_g^{k-1}(1-S^{k-1})\right)X \geq 0,$$

which leads to

$$\frac{1}{\delta t}\int_\Omega \Phi\frac{X^2}{2}\left(S^k + S^{k-1}\right)dx + \int_\Omega \Phi S^k D|\nabla X|^2\,dx + \int_\Omega S^k F_P^k\frac{X^2}{2}\,dx$$
$$\leq -\int_\Omega F_I\frac{X^2}{2}\,dx \leq 0.$$

Using the fact that the capillary pressure curve is unbounded at $S=0$ (see (A.4)) and $p_c(S^k) \in H^1(\Omega)$ it follows that $S^k > 0$ a.e. in Ω and therefore $X = 0$ a.e. in Ω. Lemma 2.4.8 is proved. □

This completes the proof of Theorem 2.3.2.

2.5 Uniform estimates with respect to δt

From Lemma 2.4.5 and Remark 2.4.6 it follows that there exists a constant C independent of δt, η, and ε such that each solution to the problem (2.66), (2.67) and (2.68) satisfies

$$\frac{1}{\delta t}\int_\Omega \Phi[\mathscr{E}^\varepsilon(p_l^\varepsilon,p_g^\varepsilon)-\mathscr{E}^\varepsilon(p_l^*,p_g^*)]\,dx+\int_\Omega[|\nabla p^\varepsilon|^2+|\nabla\beta(S^\varepsilon)|^2+|\nabla u^\varepsilon|^2]\,dx \\ +\eta\int_\Omega|\nabla p_g^\varepsilon-\nabla p_l^\varepsilon|^2\,dx\le C.$$

In this inequality p_g^ε is not necessarily positive, but due to monotonicity of the function $\hat{u}$ we have $\mathscr{E}^\varepsilon(p_l^\varepsilon,p_g^\varepsilon)\ge\mathscr{E}^\varepsilon(p_l^\varepsilon,(p_g^\varepsilon)^+)$. Then, it is easy to see that

$$\int_\Omega\Phi\mathscr{E}^\varepsilon(p_l^\varepsilon,(p_g^\varepsilon)^+)\,dx\longrightarrow\int_\Omega\Phi\mathscr{E}(p_l,p_g)\,dx,$$
$$\int_\Omega\Phi\mathscr{E}^\varepsilon(p_l^*,p_g^*)\,dx\longrightarrow\int_\Omega\Phi\mathscr{E}(p_l^*,p_g^*)\,dx$$

as $\varepsilon\to0$, where p_l and p_g are the limits from Lemma 2.4.7. Then, using the weak lower semi-continuity of norms, at the limit we get

$$\frac{1}{\delta t}\int_\Omega\Phi[\mathscr{E}(p_l,p_g)-\mathscr{E}(p_l^*,p_g^*)]\,dx+\int_\Omega[|\nabla p|^2+|\nabla\beta(S)|^2+|\nabla u|^2]\,dx \\ +\eta\int_\Omega|\nabla p_g-\nabla p_l|^2\,dx\le C,$$

where the constant C does not change and stays independent of δt and η. This bound can be applied to all time levels k, leading to

$$\frac{1}{\delta t}\int_\Omega\Phi[\mathscr{E}(p_l^k,p_g^k)-\mathscr{E}(p_l^{k-1},p_g^{k-1})]\,dx+\int_\Omega[|\nabla p^k|^2+|\nabla\beta(S^k)|^2+|\nabla u^k|^2]\,dx \\ +\eta\int_\Omega|\nabla p_g^k-\nabla p_l^k|^2\,dx\le C.$$

Multiplying this inequality by δt and summing from 1 to M we obtain

$$\int_\Omega\Phi\mathscr{E}(p_l^M,p_g^M)\,dx+\int_{Q_T}(|\nabla p^{\delta t}|^2+|\nabla\beta(S^{\delta t})|^2+|\nabla u^{\delta t}|^2)\,dx \\ +\eta\int_{Q_T}|\nabla p_g^{\delta t}-\nabla p_l^{\delta t}|^2\,dx\le C+\int_\Omega\Phi\mathscr{E}(p_l^0,p_g^0)\,dx.$$

From Lemma 2.2.4 and $p_g^0\in L^2(\Omega)$, $p_g^0\ge0$ we get the following bound.

Lemma 2.5.1. *Let $p_l^{\delta t}$ and $p_g^{\delta t}$ be a solution to (2.49), (2.50) and let the secondary variables be denoted by $S^{\delta t}$, $u^{\delta t}$, and $p^{\delta t}$. Then there exists a constant $C>0$, independent of δt and η, such that*

$$\int_{Q_T}(|\nabla p^{\delta t}|^2+|\nabla\beta(S^{\delta t})|^2+|\nabla u^{\delta t}|^2)\,dx\,dt+\eta\int_{Q_T}|\nabla p_g^{\delta t}-\nabla p_l^{\delta t}|^2\,dx\,dt\le C. \tag{2.99}$$

Let us introduce the function

$$r_g^k = \hat{u}(p_g^k)S^k + \hat{\rho}_g(p_g^k)(1-S^k)$$

and corresponding piecewise constant and piecewise linear time dependent functions which will be denoted by $r_g^{\delta t}$ and $\tilde{r}_g^{\delta t}$, respectively.

Lemma 2.5.2. *Let $p_l^{\delta t}$ and $p_g^{\delta t}$ be a solution to (2.49), (2.50) from Theorem 2.3.2. Then the following bounds uniform with respect to δt hold:*

$$(p^{\delta t})_{\delta t} \text{ is uniformly bounded in } L^2(0,T;V), \tag{2.100}$$

$$(\beta(S^{\delta t}))_{\delta t} \text{ is uniformly bounded in } L^2(0,T;H^1(\Omega)), \tag{2.101}$$

$$(u^{\delta t})_{\delta t} \text{ is uniformly bounded in } L^2(0,T;V), \tag{2.102}$$

$$(p_c(S^{\delta t}))_{\delta t} \text{ is uniformly bounded in } L^2(0,T;V), \tag{2.103}$$

$$(S^{\delta t})_{\delta t} \text{ is uniformly bounded in } L^2(0,T;H^1(\Omega)), \tag{2.104}$$

$$(\tilde{S}^{\delta t})_{\delta t} \text{ is uniformly bounded in } L^2(0,T;H^1(\Omega)), \tag{2.105}$$

$$(p_l^{\delta t})_{\delta t} \text{ is uniformly bounded in } L^2(0,T;V), \tag{2.106}$$

$$(p_g^{\delta t})_{\delta t} \text{ is uniformly bounded in } L^2(0,T;V), \tag{2.107}$$

$$(r_g^{\delta t})_{\delta t} \text{ is uniformly bounded in } L^2(0,T;H^1(\Omega)), \tag{2.108}$$

$$(\tilde{r}_g^{\delta t})_{\delta t} \text{ is uniformly bounded in } L^2(0,T;H^1(\Omega)), \tag{2.109}$$

$$(\Phi\partial_t\tilde{S}^{\delta t})_{\delta t} \text{ is uniformly bounded in } L^2(0,T;H^{-1}(\Omega)), \tag{2.110}$$

$$(\Phi\partial_t\tilde{r}_g^{\delta t})_{\delta t} \text{ is uniformly bounded in } L^2(0,T;H^{-1}(\Omega)). \tag{2.111}$$

Proof. The estimates (2.100), (2.101), (2.102), (2.103) are consequences of (2.99). Using (A.4) we get

$$\eta \int_{Q_T} |\nabla(p_g^{\delta t} - p_l^{\delta t})|^2 \, dx\,dt = \eta \int_{Q_T} |\nabla(p_c^{\delta t})|^2 \, dx\,dt \geq M_0^2 \eta \int_{Q_T} |\nabla S^{\delta t}|^2 \, dx\,dt,$$

and the estimate (2.104) follows from (2.99). The estimate (2.106) is a consequence of (2.20) and the estimates (2.100) and (2.103). The estimate (2.107) for $p_g^{\delta t}$ follow from the boundedness of the regularizing term in (2.99).

From the definition of function $r_g^{\delta t}$ we have

$$\nabla r_g^{\delta t} = \sum_{k=1}^{M} \left(S^k \nabla u^k + (u^k - \hat{\rho}_g(p_g^k))\nabla S^k + \hat{\rho}_g'(p_g^k)(1-S^k)\nabla p_g^k \right) \chi_{(t_{k-1},t_k]}(t).$$

Due to the fact that $\hat{\rho}_g$, $\hat{u}$, and $\hat{\rho}_g'$ are bounded functions we conclude

$$\|\nabla r_g^{\delta t}\|^2_{L^2(Q_T)} \leq C(\|\nabla u^{\delta t}\|^2_{L^2(Q_T)} + \|\nabla p_g^{\delta t}\|^2_{L^2(Q_T)} + \|\nabla S^{\delta t}\|^2_{L^2(Q_T)}),$$

where the constant C does not depend on δt. Applying (2.102), (2.104), and (2.107) we get the estimate (2.108). From the definitions of the functions $\tilde{S}^{\delta t}$ and $\tilde{r}_g^{\delta t}$, and the fact that $p_g^0, p_l^0 \in H^1(\Omega)$, we have

$$\|\nabla \tilde{S}^{\delta t}\|^2_{L^2(Q_T)} \leq C(\|\nabla S^{\delta t}\|^2_{L^2(Q_T)} + \|\nabla S^0\|^2_{L^2(\Omega)}),$$
$$\|\nabla \tilde{r}_g^{\delta t}\|^2_{L^2(Q_T)} \leq C(\|\nabla p_g^{\delta t}\|^2_{L^2(Q_T)} + \|\nabla S^{\delta t}\|^2_{L^2(Q_T)} + \|\nabla p_g^0\|^2_{L^2(\Omega)} + \|\nabla S^0\|^2_{L^2(\Omega)}),$$

and therefore we obtain the estimates (2.105) and (2.109). The estimates (2.110) and (2.111) follow from (2.102)–(2.108) and the variational equations (2.49) and (2.50). □

2.5.1 End of the proof of Theorem 2.3.1

In this section we pass to the limit as $\delta t \to 0$.

Proposition 2.5.3. *Let (A.1)–(A.8) hold and assume $(p_l^0, p_g^0) \in H^1(\Omega) \times H^1(\Omega)$, $p_g^0 \geq 0$. Then there is a subsequence, still denoted (δt), such that the following convergences hold when δt goes to zero:*

$$S^{\delta t} \to S \text{ strongly in } L^2(Q_T) \text{ and a.e. in } Q_T, \tag{2.112}$$
$$\beta(S^{\delta t}) \rightharpoonup \beta(S) \text{ weakly in } L^2(0,T;H^1(\Omega)) \text{ and a.e. in } Q_T, \tag{2.113}$$
$$p^{\delta t} \rightharpoonup p \text{ weakly in } L^2(0,T;V), \tag{2.114}$$
$$p_l^{\delta t} \rightharpoonup p_l \text{ weakly in } L^2(0,T;V), \tag{2.115}$$
$$p_g^{\delta t} \rightharpoonup p_g \text{ weakly in } L^2(0,T;V) \text{ and a.e. in } Q_T, \tag{2.116}$$
$$u^{\delta t} \rightharpoonup u = \hat{u}(p_g) \text{ weakly in } L^2(0,T;V), \tag{2.117}$$
$$r_g^{\delta t} \to \hat{u}(p_g)S + \hat{\rho}_g(p_g)(1-S) \text{ strongly in } L^2(Q_T) \text{ and a.e. in } Q_T. \tag{2.118}$$

Furthermore, $0 \leq S \leq 1$, and

$$\Phi\partial_t \tilde{S}^{\delta t} \rightharpoonup \Phi\partial_t S \quad \text{weakly in } L^2(0,T;H^{-1}(\Omega)), \tag{2.119}$$
$$\Phi\partial_t \tilde{r}_g^{\delta t} \rightharpoonup \Phi\partial_t(\hat{\rho}_g(p_g)(1-S) + \hat{u}(p_g)S) \quad \text{weakly in } L^2(0,T;H^{-1}(\Omega)). \tag{2.120}$$

Proof. From the estimates (2.110) and (2.105) we conclude that $(\tilde{S}^{\delta t})$ is relatively compact in $L^2(Q_T)$ and one can extract a subsequence converging strongly in $L^2(Q_T)$ and a.e. in Q_T to some $S \in L^2(Q_T)$. Obviously we have $0 \leq S \leq 1$. By applying Lemma 3.2 from [69] we find (2.112). The weak convergences in (2.113), (2.114), (2.115), (2.116), and (2.117) follow from Lemma 2.5.2.

The estimates (2.109) and (2.111) give relative compactness of the sequence $(\tilde{r}_g^{\delta t})_{\delta t}$ and, on a subsequence,

$$\tilde{r}_g^{\delta t} \to r_g \text{ strongly in } L^2(Q_T) \text{ and a.e. in } Q_T.$$

By applying Lemma 3.2 from [69] we also have the convergence

$$r_g^{\delta t} \to r_g \text{ strongly in } L^2(Q_T) \text{ and a.e. in } Q_T.$$

It remains to show that $r_g = \hat{u}(p_g)S + \hat{\rho}_g(p_g)(1-S)$. From the assumptions (A.5) and (A.6) we have for any $v \in L^2(Q_T)$

$$\int_{Q_T} \Big(\hat{u}(p_g^{\delta t})S^{\delta t} + \hat{\rho}_g(p_g^{\delta t})(1-S^{\delta t}) \\ - [\hat{u}(v)S^{\delta t} + \hat{\rho}_g(v)(1-S^{\delta t})] \Big)(p_g^{\delta t} - v)\, dxdt \geq 0.$$

After passing to the limit $\delta t \to 0$ we obtain for all $v \in L^2(Q_T)$,

$$\int_{Q_T} \Big(r_g - [\hat{u}(v)S + \hat{\rho}_g(v)(1-S)] \Big)(p_g - v)\, dxdt \geq 0.$$

By setting $v = p_g - \sigma v_1$ and passing to the limit $\sigma \to 0$ we get for all $v_1 \in L^2(Q_T)$

$$\int_{Q_T} \Big(r_g - [\hat{u}(p_g)S + \hat{\rho}_g(p_g)(1-S)] \Big) v_1\, dxdt \geq 0,$$

which gives $r_g = \hat{u}(p_g)S + \hat{\rho}_g(p_g)(1-S)$ and (2.118) is proved. Then obviously we also have $\hat{u}(p_g^{\delta t})S + \hat{\rho}_g(p_g^{\delta t})(1-S) \to \hat{u}(p_g)S + \hat{\rho}_g(p_g)(1-S)$ a.e. in Q_T. Since the functions $\hat{u}$ and $\hat{\rho}_g$ are C^1 increasing functions we have

$$\hat{u}'(p_g^{\delta t})S + \hat{\rho}_g'(p_g^{\delta t})(1-S) > 0,$$

which gives $p_g^{\delta t} \to p_g$ a.e. in Q_T. Consequently we conclude that $u = \hat{u}(p_g)$. The convergences (2.119) and (2.120) are consequences of the estimates (2.110), (2.111), and (2.118). □

Using the convergence results in Proposition 2.5.3 and the boundedness of all nonlinear coefficients, we can now pass to the limit as $\delta t \to 0$ in the variational equations (2.49), (2.50) and find that, for all $\varphi, \psi \in L^2(0,T;V)$, (2.46) and (2.47) hold.

Let us denote $r_g = \hat{\rho}_g(p_g)(1-S) + \hat{u}(p_g)S$. Then, from $S, r_g \in L^2(0,T;H^1(\Omega))$ and $\Phi\partial_t S$, $\Phi\partial_t r_g \in L^2(0,T;H^{-1}(\Omega))$ it follows immediately that $S,\ r_g \in C([0,T];L^2(\Omega))$. By a standard technique, using integration by parts, we see that the initial conditions, $S(0) = S^0$ and $r_g(0) = r_g^0$, are satisfied a.e. in Ω at $t = 0$. Finally, nonnegativity of the gas pseudopressure, $p_g \geq 0$, follows from the pointwise convergence. This concludes the proof of Theorem 2.3.1.

2.6 Proof of Theorem 2.2.1

Theorem 2.2.1 will be proved by passing to the limit as $\eta \to 0$ in the regularized problem (2.46), (2.47). We now denote explicitly the dependence of the regularized solution on the parameter η. In order to apply Theorem 2.3.1, we will regularize the initial conditions $p_l^0, p_g^0 \in L^2(\Omega)$ with the regularization parameter η and denote the regularized initial conditions by $p_l^{0,\eta}, p_g^{0,\eta} \in H^1(\Omega)$. We assume that $p_l^{0,\eta} \to p_l^0$ and $p_g^{0,\eta} \to p_g^0$ in $L^2(\Omega)$ and a.e. in Ω, when η tends to zero.

As before we introduce the notation:

$$r_g^\eta = \hat{u}(p_g^\eta)S^\eta + \hat{\rho}_g(p_g^\eta)(1-S^\eta). \tag{2.121}$$

By passing to the limit $\delta t \to 0$ to the estimate (2.99) and using the weak lower semi-continuity of the norms we find

$$\int_{Q_T} (|\nabla p^\eta|^2 + |\nabla \beta(S^\eta)|^2 + |\nabla u^\eta|^2)\, dx\, dt + \eta \int_{Q_T} |\nabla p_g^\eta - \nabla p_l^\eta|^2\, dx\, dt \leq C, \tag{2.122}$$

where $C > 0$ is independent of η. From this estimate we obtain the following bounds with respect to η:

$$(p^\eta)_\eta \text{ is uniformly bounded in } L^2(0,T;V), \tag{2.123}$$

$$(u^\eta)_\eta \text{ is uniformly bounded in } L^2(0,T;V), \tag{2.124}$$

$$(\beta^\eta(S^\eta))_\eta \text{ is uniformly bounded in } L^2(0,T;H^1(\Omega)), \tag{2.125}$$

$$(\sqrt{\eta}\nabla p_c(S^\eta))_\eta \text{ is uniformly bounded in } L^2(Q_T)^l, \tag{2.126}$$

$$(\Phi\partial_t(S^\eta))_\eta \text{ is uniformly bounded in } L^2(0,T;H^{-1}(\Omega)), \tag{2.127}$$

$$(\Phi\partial_t(r_g^\eta))_\eta \text{ is uniformly bounded in } L^2(0,T;H^{-1}(\Omega)). \tag{2.128}$$

Through the limit process are also conserved the following estimates:

$$0 \leq S^\eta \leq 1 \text{ a.e. in } Q_T, \tag{2.129}$$

$$p_g^\eta \geq 0 \ \text{ a.e. in } Q_T. \tag{2.130}$$

Due to Lemma 2.1.4, (1.34), and (2.130) we also have

$$(p_g^\eta)_\eta \ \text{ is uniformly bounded in } L^2(Q_T), \tag{2.131}$$

$$(\sqrt{\lambda_l(S_l^\eta)}\nabla p_l^\eta)_\eta)_\eta,\ (\sqrt{\lambda_g(S_l^\eta)}\nabla p_g^\eta)_\eta \ \text{ are uniformly bounded in } L^2(Q_T)^l. \tag{2.132}$$

For the passage to the limit as $\eta \to 0$ we need a compactness in $L^2(Q_T)$ of the sequences (S^η) and (r_g^η) which will be proved by an application of Lemma 4.2 in [4]. Therefore, we need the following estimates.

Lemma 2.6.1. *Under the assumptions (A.1)–(A.9), we have the following inequalities:*

$$\int_{Q_T} |S^\eta(x+\Delta x,t) - S^\eta(x,t)|^2\,dx\,dt \leq \omega(|\Delta x|), \tag{2.133}$$

$$\int_{Q_T} |r_g^\eta(x+\Delta x,t) - r_g^\eta(x,t)|^2\,dx\,dt \leq \tilde{\omega}(|\Delta x|), \tag{2.134}$$

for all $\Delta x \in \mathbb{R}^l$, *where the functions* ω *and* $\tilde{\omega}$ *are continuous and independent of* η *and satisfy* $\lim_{|\Delta x|\to 0} \omega(|\Delta x|) = 0$ *and* $\lim_{|\Delta x|\to 0} \tilde{\omega}(|\Delta x|) = 0$.

Proof. By using (A.8) and the bound (2.125) we obtain in a standard way

$$\int_{Q_T} |S^\eta(x+\Delta x,t) - S^\eta(x,t)|^2\,dx\,dt \leq C|\Delta x|^{2\tau}, \tag{2.135}$$

which proves (2.133). In order to obtain (2.134) we will consider the two parts of r_g^η separately. The first part, $\hat{u}(p_g)S$, is easy to estimate using (2.135) and the bound (2.124). We get

$$\int_{Q_T} |\hat{u}(p_g^\eta(x+\Delta x,t))S^\eta(x+\Delta x,t)) - \hat{u}(p_g^\eta(x,t))S^\eta(x,t)|^2\,dx\,dt \leq C(|\Delta x|^2 + |\Delta x|^{2\tau}). \tag{2.136}$$

The second term $(1-S^\eta)\hat{\rho}_g(p_g^\eta)$ can be written as $(1-S^\eta)\hat{\rho}_g(p^\eta - \hat{P}(S^\eta))$ in the whole domain Q_T since $1-S^\eta$ is equal to zero in the one phase region. We have

$$\begin{aligned}
&\int_{Q_T} |(1-S^\eta)(x+\Delta x,t)\hat{\rho}_g(p_g^\eta(x+\Delta x,t)) - (1-S^\eta)(x,t)\hat{\rho}_g(p_g^\eta(x,t))|^2\,dx\,dt \\
&\quad \leq \int_{Q_T} |(1-S^\eta)(x+\Delta x,t)\left(\hat{\rho}_g(p_g^\eta(x+\Delta x,t)) - \hat{\rho}_g(p_g^\eta(x,t))\right)|^2\,dx\,dt \\
&\quad + \int_{Q_T} |(S^\eta(x+\Delta x,t) - S^\eta(x,t))\hat{\rho}_g(p_g^\eta(x,t))|^2\,dx\,dt.
\end{aligned}$$

The second term on the right-hand side is estimated by using (2.135) and the boundedness of the function $\hat{\rho}_g$. In order to estimate the first term on the right-hand side we first note that by (A.6) the function $\hat{\rho}_g$ has bounded derivative. Then we can estimate

$$
\begin{aligned}
&\int_{Q_T} |(1-S^\eta)(x+\Delta x,t)\left(\hat{\rho}_g(p_g^\eta(x+\Delta x,t)) - \hat{\rho}_g(p_g^\eta(x,t))\right)|^2\,dx\,dt \\
&\quad \le C\int_{Q_T} |p^\eta(x+\Delta x,t) - p^\eta(x,t)|^2\,dx\,dt \\
&\quad + C\int_{Q_T} |(1-S^\eta)(x+\Delta x,t)\hat{P}(S^\eta(x+\Delta x,t)) - (1-S^\eta)(x,t)\hat{P}(S^\eta(x,t))|^2\,dx\,dt \\
&\quad + C\int_{Q_T} |(S^\eta(x+\Delta x,t) - S^\eta(x,t))\hat{P}(S^\eta(x,t))|^2\,dx\,dt.
\end{aligned}
$$

The first integral on the right-hand side is estimated due to (2.123), and the estimate for the third integral follows from the boundedness of the function $\hat{P}(S)$ and the bound (2.135). The second integral on the right-hand side is estimated using the assumption (A.9), which finally leads to the following estimate,

$$
\int_{Q_T} |r_g^\eta(x+\Delta x,t) - r_g^\eta(x,t)|^2 \le C(|\Delta x|^2 + |\Delta x|^{2\tau} + |\Delta x|^{2\bar{\tau}}),
$$

and (2.134) is proved. □

Lemma 2.6.2. *(Strong and weak convergences) Up to a subsequence the following convergence results hold:*

$$S^\eta \to S \ \text{ strongly in } L^2(Q_T) \text{ and a.e. in } Q_T, \tag{2.137}$$

$$r_g^\eta \to \hat{u}(p_g)S + \hat{\rho}_g(p_g)(1-S) \ \text{ strongly in } L^2(Q_T) \text{ and a.e. in } Q_T, \tag{2.138}$$

$$p_g^\eta \to p_g \text{ weakly and a.e. in } Q_T, \tag{2.139}$$

$$p^\eta \rightharpoonup p \ \text{ weakly in } L^2(0,T;V), \tag{2.140}$$

$$\beta(S^\eta) \rightharpoonup \beta(S) \ \text{ weakly in } L^2(0,T;H^1(\Omega)), \tag{2.141}$$

$$u^\eta \rightharpoonup \hat{u}(p_g) \ \text{ weakly in } L^2(0,T;V), \tag{2.142}$$

$$p_l^\eta \to p_l \text{ a.e. in } Q_T, \tag{2.143}$$

$$\Phi\partial_t S^\eta \rightharpoonup \Phi\partial_t S \text{ weakly in } L^2(0,T;H^{-1}(\Omega)), \tag{2.144}$$

$$\Phi\partial_t r_g^\eta \rightharpoonup \Phi\partial_t(\hat{u}(p_g)S + \hat{\rho}_g(p_g)(1-S)) \ \text{ weakly in } L^2(0,T;H^{-1}(\Omega)), \tag{2.145}$$

$$\lambda_l(S_l^\eta)\nabla p_l^\eta \rightharpoonup \lambda_l(S_l)\nabla p_l,\ \lambda_g(S_l^\eta)\nabla p_g^\eta \rightharpoonup \lambda_g(S_l)\nabla p_g \ \text{ weakly in } L^2(Q_T)^l. \tag{2.146}$$

Proof. If we apply Lemma 4.2 from [4] to the estimates (2.133), (2.129), and (2.127) we obtain

$$S^\eta \to S \text{ strongly in } L^2(Q_T) \text{ and a.e. in } Q_T.$$

In the same way the boundedness of r_g^η, the estimates (2.134) and (2.128) imply

$$r_g^\eta \to r_g \text{ strongly in } L^2(Q_T) \text{ and a.e. in } Q_T.$$

We can extract a subsequence such that $p_g^\eta \rightharpoonup p_g$ weakly in $L^2(Q_T)$ and then by using the monotonicity argument, as in Proposition 2.5.3, we find that $r_g = \hat{u}(p_g)S + \hat{\rho}_g(p_g)(1-S)$ and obtain the convergence

$$p_g^\eta \to p_g \text{ a.e. in } Q_T.$$

All other convergences follow immediately from the bounds (2.123)–(2.128) and (2.132). The limit liquid pressure p_l is defined from the limit global pressure p and the limit saturation S_l, by (1.31). □

By using the convergence results from the previous proposition combined with the boundedness of nonlinear coefficients, equality (1.34), and estimate (2.126) we can pass to the limit $\eta \to 0$ in (2.46) and (2.47) to obtain the variational equations (2.29) and (2.30). Passing to the limit $\eta \to 0$ in the inequality $p_g^\eta \geq 0$ we find $p_g \geq 0$ a.e. in Q_T. Using an integration by parts in the regularized η-problem and the limit problem, with the test function of the form $\psi(x)\varphi(t)$, $\psi \in V$, and $\varphi \in C^1([0,T])$ with $\varphi(0) = 1$, $\varphi(T) = 0$, we find in a standard way that the initial conditions (2.31), (2.32) are satisfied. This completes the proof of Theorem 2.2.1.

2.7 Conclusion

An existence result for the weak solution of the model describing flow of fluid composed of two phases, and which is mixture of two components: liquid component and slightly soluble gas component. The low solubility assumption is necessary for the compensation of the degeneracy of the diffusive terms and it is essential for the energy estimate derivation. This assumption allowed us to remove some nonphysical hypothesis on the diffusion terms that was used in some earlier works. Compared to the proof from [35] we have relaxed the assumption on function $\hat{u}$ regarding boundedness from below by some strictly positive constant obtaining a more physically appropriate assumption. The boundedness from above of functions $\hat{u}$ and $\hat{\rho}_g$ is assumed in this paper too, which means that the general cases of the Henry law and the ideal gas law remain an open problem.

After analyzing the existence of the solution to the two-phase, two-component flow model, the next step we want to address is the formulation and analysis of a numerical method for the proposed model. This part will be left for our future research, and we will use this thesis in order to lay the groundwork for this next step. Therefore, a slightly simpler immiscible two-phase flow model is considered first and the next chapter of this dissertation brings convergence analysis of a numerical method for the model in question.

Chapter 3

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

In this chapter we present a convergence proof for a cell-centered finite volume scheme for a model describing immiscible, compressible two-phase flow in porous media. We consider classical two-point flux discretization with "phase-by-phase" upwinding on an orthogonal mesh. The convergence of this scheme is already considered in [46] in the incompressible case, and in [76] for the compressible fluids. The proof presented here considers a compressible case and compared to the proof given in [76] it is based on a different technique. Namely, we use a fully equivalent global pressure formulation for the general case of immiscible compressible two-phase flow which was derived in [5]. The equations are rewritten by expressing the original equations in terms of the global pressure and the wetting saturation (see Chapter 1 Subsection 1.3.5). Here we prove the energy estimate, which is fundamental for the convergence proof, by using the global pressure based on the total flux (see [5]) and relaying on a discrete version of the relations between the phase pressure gradients and the global pressure gradient. With this technique we can also remove uncommon treatment of the mass densities by the harmonic mean, which is used in [76], by more commonly used upwind value. Unlike [76], where model with constant absolute permeability throughout the domain was studied, we consider isotropic model with a piecewise continuous function for absolute permeability with finitely many surfaces of discontinuity. We also give detailed explanation of the passage to limit in the discrete equations in order to fix some shortcomings in the proof given in [76].

The outline of this chapter is as follows. In Section 3.1 we give a brief description of the mathematical model for two-phase flow. More details on mathematical modeling can be found in Chapter 1. In Section 3.2 we present the cell-centered finite volume discretization and we define the finite volume scheme that will be studied. This approach leads to a fully coupled fully implicit scheme. In Section 3.3 we derive discrete relations connecting the phase pressures and the global pressure. Several auxiliary results are proven that will be used in the energy estimate for the scheme. The maximum principle for the water saturation is proved in Section 3.4. By applying suitable test functions and results from Section 3.3 the energy estimates are derived in Section 3.5. In Section 3.6 these estimates are used to prove the existence of a solution to the nonlinear discrete equations from Section 3.2. The compactness result for a sequence of the solutions is proved in Section 3.7. Finally, in 3.8 we pass to the limit in the discrete equations, when discretization parameters go to zero, and we find the weak solution to the continuous two-phase flow model, which completes the convergence proof.

3.1 Mathematical formulation

We consider general two-phase flow model given by the mass balance law for each phase,

$$\Phi\partial_t(\rho_n(p_n)S_n) - \operatorname{div}(\lambda_n(S_w)\rho_n(p_n)\mathbb{K}(\nabla p_n - \rho_n(p_n)\mathbf{g})) = F_n, \tag{3.1}$$

$$\Phi\partial_t(\rho_w(p_w)S_w) - \operatorname{div}(\lambda_w(S_w)\rho_w(p_w)\mathbb{K}(\nabla p_w - \rho_w(p_w)\mathbf{g})) = F_w, \tag{3.2}$$

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

We consider a fixed time $T > 0$, a polyhedral domain Ω and we set $Q_T = \Omega \times (0,T)$. The boundary is assumed to be Lipschitz continuous and divided in two parts $\partial\Omega = \Gamma_N \cup \Gamma_D$. On Γ_N homogeneous Neumann boundary condition is imposed

$$\begin{aligned} \lambda_n(S_w)\rho_n(p_n)\mathbb{K}(\nabla p_n - \rho_n(p_n)\mathbf{g}) \cdot \mathbf{n} = 0, \\ \lambda_w(S_w)\rho_w(p_w)\mathbb{K}(\nabla p_w - \rho_w(p_w)\mathbf{g}) \cdot \mathbf{n} = 0, \end{aligned} \quad \text{on } (0,T) \times \Gamma_N, \tag{3.3}$$

and on Γ_D the Dirichlet boundary condition is imposed in the following way

$$p_n(x,t) = 0, \quad p_w(x,t) = 0, \quad \text{on } (0,T) \times \Gamma_D. \tag{3.4}$$

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

$$F_w = \rho_w(p_w)(S_w^I F_I - S_w F_P), \quad F_n = \rho_n(p_n)(S_n^I F_I - S_n F_P), \tag{3.5}$$

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. The total source term imposed is

$$F_w + F_n = (\rho_w(p_w)S_w^I + \rho_n(p_n)S_n^I)F_I - (\rho_w(p_w)S_w + \rho_n(p_n)S_n)F_P.$$

Finally, the initial conditions are given by

$$p_n(0,x) = p_n^0(x), \quad p_w(0,x) = p_w^0(x), \quad x \in \Omega. \tag{3.6}$$

With this formulation we obtain a system of four equations with four unknowns p_w, p_n, S_w, and S_n that is usually reduced to a system of two differential equation with two unknowns, while other two unknowns are eliminated by algebraic relations.

It has been shown in Chapter 1 that the two-phase flow model can be rewritten in terms of the global pressure p and the water saturation S_w by the following equations:

$$\Phi\frac{\partial}{\partial t}\left(\rho_n S_n\right) - \operatorname{div}\left(\lambda_n \rho_n \mathbb{K}\left(\omega \nabla p - \rho \mathbf{g}\right) + b_g \mathbb{K}\mathbf{g} + \alpha \mathbb{K} \nabla p_c(S_w)\right) = F_n, \tag{3.7}$$

$$\Phi\frac{\partial}{\partial t}\left(\rho_w S_w\right) - \operatorname{div}\left(\lambda_w \rho_w \mathbb{K}\left(\omega \nabla p - \rho \mathbf{g}\right) - b_g \mathbb{K}\mathbf{g} - \alpha \mathbb{K} \nabla p_c(S_w)\right) = F_w. \tag{3.8}$$

The global pressure p is a pressure like unknown which is related to the phase pressures p_n and p_w by the following equations (see (1.47)),

$$p_w(S_w, p) = p - \int_1^{S_w} f_n(s,p) p_c'(s)\, ds, \tag{3.9}$$

$$p_n(S_w, p) = p_w(S_w, p) + p_c(S_w). \tag{3.10}$$

The fractional flow functions f_w and f_n and the rest of the coefficients from the system of equations (3.7)–(3.8) are given by (1.43) and the function $\omega(S_w, p)$ is given by (1.48).

It is also important to note the relation between the gradients of phase pressures and the gradient of the global pressure

$$\nabla p_n = \omega(S_w, p)\nabla p + f_w(S_w, p)\nabla p_c(S_w), \tag{3.11}$$

$$\nabla p_w = \omega(S_w, p)\nabla p - f_n(S_w, p)\nabla p_c(S_w). \tag{3.12}$$

As already noted in Chapter 1 degeneracy of the system (3.7)–(3.8) leads us to replace the saturation S_w with suitably defined saturation potential. Therefore, we define the function $\tilde{\alpha}(S_w, p)$ by

$$\tilde{\alpha}(S_w, p) = \frac{\rho_n(p_n(S_w, p))\rho_w(p_w(S_w, p))}{\lambda(S_w, p)}, \tag{3.13}$$

the saturation potential $\beta(S_w)$ by

$$\beta(S_w) = \int_0^{S_w} \lambda_w(s)\lambda_n(s)p_c'(s)\,ds, \tag{3.14}$$

and with these two functions we obtain the following form of the two-phase flow model:

$$\Phi\frac{\partial}{\partial t}(\rho_n S_n) - \operatorname{div}(\lambda_n\rho_n\mathbb{K}(\omega\nabla p - \rho\mathbf{g}) + b_g\mathbb{K}\mathbf{g} + \tilde{\alpha}\mathbb{K}\nabla\beta(S_w)) = F_n, \tag{3.15}$$

$$\Phi\frac{\partial}{\partial t}(\rho_w S_w) - \operatorname{div}(\lambda_w\rho_w\mathbb{K}(\omega\nabla p - \rho\mathbf{g}) - b_g\mathbb{K}\mathbf{g} - \tilde{\alpha}\mathbb{K}\nabla\beta(S_w)) = F_w, \tag{3.16}$$

which allow us to overcome degeneracy present in the diffusive part of the equations.

Note also that the relation between the gradients of phase pressures and the gradient of the global pressure (3.11), (3.12) can be written as

$$\lambda_n(S_w)\rho_n(p_n)\nabla p_n = \lambda_n(S_w)\rho_n(p_n)\omega(S_w, p)\nabla p + \tilde{\alpha}\nabla\beta(S_w), \tag{3.17}$$

$$\lambda_w(S_w)\rho_w(p_w)\nabla p_w = \lambda_w(S_w)\rho_w(p_w)\omega(S_w, p)\nabla p - \tilde{\alpha}\nabla\beta(S_w). \tag{3.18}$$

In the whole chapter the following assumptions are taken to be true.

(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.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 3.2.1, item vi). There are constants $k_M \geq k_m > 0$ such that $k_m \leq k(x) \leq k_M$ for $x \in \Omega$.

(A.3) 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 functions of S_α. Moreover, there exist constants $\lambda_M \geq \lambda_m > 0$ such that for all $S_w \in [0,1]$

$$0 < \lambda_m \leq \lambda_w(S_w) + \lambda_n(S_w) \leq \lambda_M. \tag{3.19}$$

(A.4) The capillary pressure function $p_c \in C^1([0,1])$ is a strictly monotone decreasing function.

(A.5) ρ_n and ρ_w are $C^1(\mathbb{R})$ increasing functions, and there exist constants $\rho_m, \rho_M, \rho_M^d > 0$ such that for all $p \in \mathbb{R}$ it holds

$$\rho_m \le \rho_\alpha(p) \le \rho_M, \quad \rho'_\alpha(p) \le \rho_M^d, \quad \alpha = w, n. \tag{3.20}$$

(A.6) $F_P, F_I \in L^2(Q_T)$, $p_w^0, S^0 \in L^2(\Omega)$ with $0 \le S^0 \le 1$ and $p_n^0 = p_w^0 + p_c(S^0)$.

(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 $C \ge 0$)

$$C \left| \int_{S_1}^{S_2} \lambda_w(s)\lambda_n(s)p'_c(s)\, ds \right|^\tau \ge |S_1 - S_2|. \tag{3.21}$$

In order to deal with the Dirichlet boundary condition, we define the space

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

We give below definition of a weak solution to (3.1)–(3.2) from [76]

Definition 3.1.1. *Let (A.1)–(A.7) hold true and assume* $(p_n^0, p_w^0) \in L^2(\Omega) \times L^2(\Omega)$, $0 \le S_w^0 \le 1$ *a.e.* $\in \Omega$. *Then the pair* (p_n, p_w) *is a weak solution to problem (3.1), (3.2), (3.3), (3.4), and (3.6) satisfying*

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

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

$$\begin{aligned}
&-\int_{Q_T} \Phi\rho_w(p_w)S_w\partial_t\varphi\, dx\, dt - \int_\Omega \Phi(x)\rho_w(p_w^0(x))S_w^0(x)\varphi(0,x)\, dx\\
&+\int_{Q_T} [\lambda_w(S_w)\rho_w(p_w)\mathbb{K}\nabla p_w - \lambda_w(S_w)\rho_w^2(p_w)\mathbb{K}\mathbf{g}]\cdot\nabla\varphi dxdt\\
&+\int_{Q_T} \rho_w(p_w)S_w F_P\varphi dxdt = \int_{Q_T} \rho_w(p_w)S_w^I F_P\varphi dxdt;
\end{aligned} \tag{3.22}$$

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

$$\begin{aligned}
&-\int_{Q_T} \Phi\rho_n(p_n)S_n\partial_t\psi\, dx\, dt - \int_\Omega \Phi(x)\rho_n(p_n^0(x))(1 - S_w^0(x))\psi(0,x)\, dx\\
&+\int_{Q_T} [\lambda_n(S_w)\rho_n(p_n)\mathbb{K}\nabla p_n - \lambda_n(S_w)\rho_n^2(p_n)\mathbb{K}\mathbf{g}]\cdot\nabla\psi dxdt\\
&+\int_{Q_T} \rho_n(p_n)S_n F_P\psi dxdt = \int_{Q_T} \rho_n(p_n)S_n^I F_P\psi dxdt.
\end{aligned} \tag{3.23}$$

3.2 Finite volume scheme

Before the description of the finite volume scheme, we give the definition of a finite volume mesh on $\Omega \times (0,T)$ from [45].

Definition 3.2.1. *(Admissible mesh of Ω) Let Ω be an open bounded connected polyhedral subset of $\mathbb{R}^l$, $l = 2$, or 3. An admissible finite volume 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 of Ω denoted by $\mathcal{P}$ satisfying the following properties:*

- *i) The closure of the union of all control volumes is $\overline{\Omega}$.*
- *ii) For any $K \in \mathcal{T}$, there exists a subset $\mathcal{E}_K$ of $\mathcal{E}$ such that $\partial K = \cup_{\sigma \in \mathcal{E}_K} \overline{\sigma}$. Furthermore, $\mathcal{E} = \cup_{K \in \mathcal{T}} \mathcal{E}_K$.*
- *iii) For any $(K,L) \in \mathcal{T}^2$ with $K \neq L$, either the $(l-1)$–dimensional Lebesgue measure of $\overline{K} \cap \overline{L}$ is 0 or $\overline{K} \cap \overline{L} = \overline{\sigma}$ for some $\sigma \in \mathcal{E}$, which will then be denoted by $\sigma_{K|L}$.*
- *iv) There are disjoint subsets $\mathcal{E}_D \subset \mathcal{E}$ and $\mathcal{E}_N \subset \mathcal{E}$ such that $\Gamma_D = \cup_{\sigma \in \mathcal{E}_D} \sigma$ and $\Gamma_N = \cup_{\sigma \in \mathcal{E}_N} \sigma$. We denote the set of all interior sides by $\mathcal{E}_I = \mathcal{E} \setminus (\mathcal{E}_D \cup \mathcal{E}_N)$.*
- *v) The family $\mathcal{P} = (x_K)_{K \in \mathcal{T}}$ is such that $x_K \in \overline{K}$ (for all $K \in \mathcal{T}$) and it is assumed that $x_K \neq x_L$, and that the straight line (x_K, x_L) is orthogonal to $\sigma_{K|L}$.*
- *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 $\mathcal{E}_{\text{disc}} \subset \mathcal{E}_I$.*

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. 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

$$\tau_{K|L} = |\sigma_{K|L}|/d_{K|L} \text{ and } \tau_{K,\sigma} = |\sigma|/d_{K,\sigma}.$$

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 $\sigma \in \mathscr{E}_D$. 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

$$\begin{aligned} &\exists \gamma > 0 \quad \forall h \quad \forall K \in \mathfrak{T} \quad \forall L \in N(K) \quad \operatorname{diam}(K) + \operatorname{diam}(L) \leq \gamma d_{K|L}, \\ &\exists \zeta > 0 \quad \forall K \in \mathfrak{T}, \forall \sigma \in \mathscr{E}_K \quad d_{K,\sigma} \geq \zeta d_\sigma, \end{aligned} \tag{3.24}$$

where

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

We denote by $H_h(\Omega)$ the space of functions from $L^2(\Omega)$ which are piecewise constants on each $K \in \mathfrak{T}$, 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 [76])

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

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 $K \in \mathfrak{T}$, with the inner product and the norm

$$(u_h, v_h)_{L_h} = \sum_{K \in \mathfrak{T}} |K| u_K v_K, \quad \|u_h\|^2_{L_h(\Omega)} = \sum_{K \in \mathfrak{T}} |K| |u_K|^2. \tag{3.25}$$

The discrete gradient $\nabla_h u_h$ of a function u_h is defined on the dual mesh (see [12]) in which the control volumes are attached to the sides $\sigma \in \mathscr{E}$. 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 $\sigma \in \mathscr{E}_K$, $\sigma \subset \partial\Omega$, 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

$$|T_{K|L}| = |\sigma_{K|L}| d_{K|L}/l \text{ and } |T_{K,\sigma}| = |\sigma| d_{K,\sigma}/l.$$

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

$$\nabla_h u_h(x) = \begin{cases} l\frac{u_L - u_K}{d_{K|L}}\eta_{K|L} \text{ if } x \in T_{K|L}, \\ l\frac{u_\sigma - u_K}{d_{K,\sigma}}\eta_{K|\sigma} \text{ if } x \in T_{K,\sigma},\ \sigma \subset \Gamma_D, \\ 0 \text{ if } x \in T_{K,\sigma},\ \sigma \subset \Gamma_N, \end{cases} \tag{3.26}$$

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.

For an arbitrary vector $\vec{F}_{K|L} \in \mathbb{R}^l$ associated with the interface $\sigma_{K|L} \in \mathscr{E} \setminus \mathscr{E}_N$, which satisfies $\vec{F}_{K|L} = -\vec{F}_{L|K}$ for $\sigma_{K|L} \notin \mathscr{E}_D$, one can define a piecewise constant vector function

$$\vec{F}_h = \sum_{\sigma \in \mathscr{E}} \vec{F}_{K|L}\mathbf{1}_{T_{K|L}}, \tag{3.27}$$

and corresponding discrete divergence of the field $\vec{F}_h$ as piecewise constant function

$$\mathrm{div}_K \vec{F}_h = \frac{1}{|K|} \sum_{L \in N_D(K)} |\sigma_{K|L}| \vec{F}_{K|L} \cdot \eta_{K|L}. \tag{3.28}$$

In sequel we will use discrete Poincaré inequality from [45]:

Lemma 3.2.2. *(Discrete Poincaré inequality) Let Ω be an open bounded polyhedral subset of $\mathbb{R}^l$, $l = 2$, or 3, $\mathcal{T}$ an admissible finite volume mesh in the sense of Definition 3.2.1, satisfying (3.24), 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 3.2.3. *The proof of the Lemma 3.2.2 is given in [45] for the case of the Dirichlet boundary conditions, meaning that $V = H_0^1(\Omega)$. It is also stated in [45] that in the case of the Dirichlet condition on a part of the boundary only, it is still possible to prove the discrete Poincaré inequality provided that the set Ω is connected. This particular case was considered in [23].*

Remark 3.2.4. *The first constraint on the family of meshes $(\mathcal{T}_h)_h$ in (3.24) is used in compactness proof (see [12]) 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 family of meshes $(\mathcal{T}_h)_h$ is used in the proof of the discrete Poincaré inequality (see [45, 23]).

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

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

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

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

The following lemma gives the discrete integration by parts formula (see [22]).

Lemma 3.2.5. *(Discrete integration by parts formula) Let Ω be an open bounded polygonal subset of $\mathbb{R}^l$, $\mathcal{T}$ an admissible finite volume mesh on Ω. 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 $\varphi(x) = \varphi_K,\ x\in K$. Then we have*

$$\sum_{K\in\mathcal{T}}\sum_{L\in N_D(K)}F_{K|L}\varphi_K = \frac{1}{2}\sum_{K\in\mathcal{T}}\sum_{L\in N(K)}F_{K|L}(\varphi_K-\varphi_L) + \sum_{K\in\mathcal{T}}\sum_{\sigma\in\partial K\cap\Gamma_D}F_{K,\sigma}\varphi_K.$$

The following lemma is an easy consequence of the discrete integration by parts formula.

Lemma 3.2.6. *Let $\varphi\in(C^1(\overline{Q}_T))^l$ be a function equal to zero on the Neumann boundary Γ_N. Then there is 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,*

$$E_h = \left|\int_0^T\int_\Omega\nabla_h p_h\cdot\varphi\,dxdt + \int_0^T\int_\Omega p_h div\varphi\,dxdt\right| \leq Ch\left(\|p_h\|^2_{L^2(0,T;H_h(\Omega))}+1\right). \tag{3.29}$$

Proof. For $t \in (t^k, t^{k+1}]$ we have

$$\int_\Omega p_h \mathrm{div}\varphi(x,t)\,dx = \sum_{K\in\mathfrak{T}_h}\int_K p_h \mathrm{div}\varphi(x,t)\,dx$$
$$= \sum_{K\in\mathfrak{T}_h}\sum_{L\in N_D(K)} p_K^{k+1}\int_{\sigma_{K|L}}\varphi(s,t)\cdot\eta_{K|L}\,ds$$
$$= \frac{1}{2}\sum_{K\in\mathfrak{T}_h}\sum_{L\in N(K)}(p_K^{k+1}-p_L^{k+1})\int_{\sigma_{K|L}}\varphi(s,t)\cdot\eta_{K|L}\,ds$$
$$+\sum_{K\in\mathfrak{T}_h}\sum_{\sigma\in\partial K\cap\Gamma_D}(p_K^{k+1}-p_\sigma^{k+1})\int_\sigma\varphi(s,t)\cdot\eta_{K|L}\,ds =: I,$$

where we have used the fact that $p_\sigma^{k+1}=0$ for $\sigma\in\partial K\cap\Gamma_D$. For the first term in (3.29) we obtain from the definition of the discrete gradient

$$\int_\Omega \nabla_h p_h\cdot\varphi(x,t)\,dx = \frac{1}{2}\sum_{K\in\mathfrak{T}_h}\sum_{L\in N(K)} l\frac{p_L^{k+1}-p_K^{k+1}}{d_{K|L}}\int_{T_{K|L}}\varphi(x,t)\cdot\eta_{K|L}\,dx$$
$$+\sum_{K\in\mathfrak{T}_h}\sum_{\sigma\in\partial K\cap\Gamma_D} l\frac{p_\sigma^{k+1}-p_K^{k+1}}{d_{K,\sigma}}\int_{T_{K,\sigma}}\varphi(x,t)\cdot\eta_{K,\sigma}\,dx =: II.$$

Now we have

$$I+II = \frac{1}{2}\sum_{K\in\mathfrak{T}_h}\sum_{L\in N(K)}|\sigma_{K|L}|(p_L^{k+1}-p_K^{k+1})\left(\frac{1}{|T_{K|L}|}\int_{T_{K|L}}\varphi(x,t)\cdot\eta_{K|L}\,dx - \frac{1}{|\sigma_{K|L}|}\int_{\sigma_{K|L}}\varphi(s,t)\cdot\eta_{K|L}\,ds\right)$$
$$+\sum_{K\in\mathfrak{T}_h}\sum_{\sigma\in\partial K\cap\Gamma_D}|\sigma|(p_\sigma^{k+1}-p_K^{k+1})\left(\frac{1}{|T_{K,\sigma}|}\int_{T_{K,\sigma}}\varphi(x,t)\cdot\eta_{K|L}\,dx - \frac{1}{|\sigma|}\int_\sigma\varphi(s,t)\cdot\eta_{K|L}\,ds\right).$$

Due to the smoothness of φ one obtain

$$\left|\frac{1}{|T_{K|L}|}\int_{T_{K|L}}\varphi(x,t)\cdot\eta_{K|L}\,dx - \frac{1}{|\sigma_{K|L}|}\int_{\sigma_{K|L}}\varphi(s,t)\cdot\eta_{K|L}\,ds\right| \le Ch,$$

and analogously for $\sigma\in\Gamma_D$, from where we conclude

$$E_h \le Ch\sum_{n=0}^{N-1}\delta t\left(\sum_{K\in\mathfrak{T}_h}\sum_{L\in N(K)}|\sigma_{K|L}||p_L^{k+1}-p_K^{k+1}| + \sum_{K\in\mathfrak{T}_h}\sum_{\sigma\in\partial K\cap\Gamma_D}|\sigma||p_\sigma^{k+1}-p_K^{k+1}|\right).$$

The previous expression can be written in the following way

$$E_h \leq Ch \sum_{n=0}^{N-1} \delta t \Bigg(\sum_{K \in \mathfrak{T}_h} \sum_{L \in N(K)} |\sigma_{K|L}| \frac{|p_L^{k+1} - p_K^{k+1}|}{\sqrt{d_{K|L}}} \sqrt{d_{K|L}} + \sum_{K \in \mathfrak{T}_h} \sum_{\sigma \in \partial K \cap \Gamma_D} |\sigma| \frac{|p_\sigma^{k+1} - p_K^{k+1}|}{\sqrt{d_{K,\sigma}}} \sqrt{d_{K,\sigma}} \Bigg),$$

which gives the estimate

$$|E_h| \leq Ch \sum_{n=0}^{N-1} \delta t \left(\sum_{K \in \mathfrak{T}_h} \sum_{L \in N(K)} \tau_{K|L} |p_L^{k+1} - p_K^{k+1}|^2 + \sum_{K \in \mathfrak{T}_h} \sum_{\sigma \in \partial K \cap \Gamma_D} \tau_{K,\sigma} |p_\sigma^{k+1} - p_K^{k+1}|^2 + |\Omega| \right),$$

which can be rewritten as (3.29). □

Remark 3.2.7. *In order to simplify notation when applying gathering by the edges we introduce the following notation. Let $F_{K|L} \in \mathbb{R}$ for $K \in \mathfrak{T}$, $L \in N_D(K)$ 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*

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

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 $|\tilde{T}_{K|L}| = |\tilde{\sigma}_{K|L}| d_{K|L}/l$. Then we can write

$$\sum_{K \in \mathfrak{T}} \sum_{L \in N_D(K)} \tau_{K|L} F_{K|L} \varphi_K = \frac{1}{2} \sum_{K \in \mathfrak{T}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} F_{K|L} (\varphi_K - \varphi_L),$$

and

$$\|u_h\|^2_{H_h(\Omega)} = \frac{l}{2} \sum_{K \in \mathfrak{T}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} |u_K - u_L|^2, \quad u_h \in H_h(\Omega),$$

$$\|u_h\|^2_{L^2(0,T;H_h(\Omega))} = \frac{l}{2} \sum_{k=0}^{N-1} \delta t \sum_{K \in \mathfrak{T}} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} |u_L^{k+1} - u_K^{k+1}|^2, \quad u_h \in X(\mathfrak{T}, \delta t).$$

We continue with a description of standard phase-by-phase upwind discretization of the two-phase flow equations which can be found in a book like [17]. The upwind discretization is also studied in [79, 29, 48, 67] and in many other publications.

The system (3.1)–(3.2) is discretized by the two-point cell-centered finite volume 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:

$$\lambda_{\alpha,K|L}^{up,k} = \begin{cases} \lambda_\alpha(S_{w,K}^k) & \text{if } p_{\alpha,K}^k - p_{\alpha,L}^k \geq 0 \\ \lambda_\alpha(S_{w,L}^k) & \text{if } p_{\alpha,K}^k - p_{\alpha,L}^k < 0 \end{cases} \quad \alpha = w, n. \tag{3.30}$$

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:

$$\rho_{\alpha,K|L}^{up,k} = \begin{cases} \rho_\alpha(p_{\alpha,K}^k) & \text{if } p_{\alpha,K}^k - p_{\alpha,L}^k \geq 0 \\ \rho_\alpha(p_{\alpha,L}^k) & \text{if } p_{\alpha,K}^k - p_{\alpha,L}^k < 0 \end{cases} \quad \alpha = w, n. \tag{3.31}$$

For the energy estimate presented in Section 3.5 we will also need harmonic mean approximation used in [76], and given by

$$\rho_{\alpha,K|L}^{k} = \begin{cases} (p_{\alpha,K}^k - p_{\alpha,L}^k) \Big/ \displaystyle\int_{p_{\alpha,L}^k}^{p_{\alpha,K}^k} \frac{d\sigma}{\rho_\alpha(\sigma)} & \text{if } p_{\alpha,K}^k \neq p_{\alpha,L}^k \\ \rho_\alpha(p_{\alpha,K}^k) & \text{if } p_{\alpha,K}^k = p_{\alpha,L}^k \end{cases} \quad \alpha = w, n. \tag{3.32}$$

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

$$\rho_{\alpha,K|L}^{G,k} = \frac{\rho_\alpha(p_{\alpha,K}^k) d_{K,\sigma} + \rho_\alpha(p_{\alpha,L}^k) d_{L,\sigma}}{d_{K|L}}, \tag{3.33}$$

where $g_{K|L} = \mathbf{g} \cdot \eta_{K|L}$ and $\eta_{K|L}$ 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:

$$\lambda_{\alpha,K|L}^{G,k} = \begin{cases} \lambda_\alpha(S_{w,K}^k) & \text{if } g_{K|L} \geq 0 \\ \lambda_\alpha(S_{w,L}^k) & \text{if } g_{K|L} < 0 \end{cases}. \tag{3.34}$$

The absolute permeability is approximated by a function k_h that is defined on the dual mesh as in [45]. Precisely, on the dual volume $T_{K|L}$ the function k_h is equal to the weighted harmonic mean

$$k_{K|L} = \frac{d_{K|L}}{d_{K,\sigma}/k_K + d_{L,\sigma}/k_L}, \tag{3.35}$$

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 3.2.8. *In a standard way one can proof $\|k - k^h\|_{L^2(\Omega)} \to 0$ as $h \to 0$. By using simple calculation we obtain*

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

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

The finite volume scheme for the discretization of equations (3.1)–(3.2) with boundary conditions (3.3), (3.4), and initial conditions (3.6) is given by the following set of equations with the unknowns $(p^{k+1}_{w,K})_{K\in\mathcal{T}}$, $(p^{k+1}_{n,K})_{K\in\mathcal{T}}$, $(S^{k+1}_{n,K})_{K\in\mathcal{T}}$, and $(S^{k+1}_{w,K})_{K\in\mathcal{T}}$, $k \in \{0,1,...,N-1\}$:

$$p^{k+1}_{n,K} - p^{k+1}_{w,K} = p_c(S^{k+1}_{w,K}), \quad S^{k+1}_{w,K} + S^{k+1}_{n,K} = 1, \tag{3.36}$$

$$\begin{aligned} |K|\Phi_K \frac{\rho^{k+1}_{n,K} S^{k+1}_{n,K} - \rho^k_{n,K} S^k_{n,K}}{\delta t} &+ \sum_{L\in N_D(K)} \tau_{K|L} k_{K|L} \lambda^{up,k+1}_{n,K|L} \rho^{up,k+1}_{n,K|L} (p^{k+1}_{n,K} - p^{k+1}_{n,L}) \\ &+ \sum_{L\in N_D(K)} |\sigma_{K|L}| k_{K|L} \lambda^{G,k+1}_{n,K|L} \left(\rho^{G,k+1}_{n,K|L}\right)^2 g_{K|L} = |K| F^{k+1}_{n,K}, \end{aligned} \tag{3.37}$$

$$\begin{aligned} |K|\Phi_K \frac{\rho^{k+1}_{w,K} S^{k+1}_{w,K} - \rho^k_{w,K} S^k_{w,K}}{\delta t} &+ \sum_{L\in N_D(K)} \tau_{K|L} k_{K|L} \lambda^{up,k+1}_{w,K|L} \rho^{up,k+1}_{w,K|L} (p^{k+1}_{w,K} - p^{k+1}_{w,L}) \\ &+ \sum_{L\in N_D(K)} |\sigma_{K|L}| k_{K|L} \lambda^{G,k+1}_{w,K|L} \left(\rho^{G,k+1}_{w,K|L}\right)^2 g_{K|L} = |K| F^{k+1}_{w,K}. \end{aligned} \tag{3.38}$$

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

$$\begin{aligned} \tau_{K|L}\lambda_{n,K|L}^{up,k+1}\rho_{n,K|L}^{up,k+1}(p_{n,K}^{k+1}-p_{n,L}^{k+1})+|\sigma_{K|L}|\lambda_{n,K|L}^{G,k+1}\left(\rho_{n,K|L}^{G,k+1}\right)^2 g_{K|L}=0 \\ \tau_{K|L}\lambda_{w,K|L}^{up,k+1}\rho_{w,K|L}^{up,k+1}(p_{w,K}^{k+1}-p_{w,L}^{k+1})+|\sigma_{K|L}|\lambda_{w,K|L}^{G,k+1}\left(\rho_{w,K|L}^{G,k+1}\right)^2 g_{K|L}=0. \end{aligned} \tag{3.39}$$

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

$$p_{n,L}^{k+1}=0, \quad p_{w,L}^{k+1}=0 \tag{3.40}$$

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

$$p_{w,K}^0=\frac{1}{|K|}\int_K p_w^0(x)\,dx, \quad p_{n,K}^0=\frac{1}{|K|}\int_K p_n^0(x)\,dx, \quad S_{w,K}^0=p_c^{-1}(p_{n,K}^0-p_{w,K}^0). \tag{3.41}$$

In this chapter we prove the following theorem.

Theorem 3.2.9. *Assume hypothesis (A.1)–(A.7) hold. Let $(D_h)_h$ be a sequence of discretization of $\Omega\times(0,T)$ such that $h\to 0$. Then there exists a subsequence of solutions to the discrete problem (3.36)–(3.41), which converges to a weak solution of the problem (3.1), (3.2), (3.3), (3.4), (3.6) in the sense of Definition 3.1.1.*

3.3 Preliminary results

In our approach to the convergence proof of the scheme (3.36)–(3.41) we use the global pressure p defined in (3.10) and we need to discretize the relations (3.11) and (3.12). In order to simplify notation we will denote S_w by S in this section.

The function ω is given by (1.48) and its approximation $\omega_{K|L}^k$ on edge $\sigma_{K|L}$ is given by

$$\omega_{K|L}^k=\begin{cases} \frac{p_w(S_{K|L}^k,p_K^k)-p_w(S_{K|L}^k,p_L^k)}{p_K^k-p_L^k} & \text{if } p_K^k\neq p_L^k \\ \frac{\partial p_w}{\partial p}(\overline{S}_{K|L}^k,p_K^k) & \text{if } p_K^k=p_L^k. \end{cases} \tag{3.42}$$

In (3.42) we have denoted $\overline{S}_{K|L}^k=\frac{S_K^k+S_L^k}{2}$ and $S_{K|L}^k$ will be defined as $S_{K|L}^{gup,k}$ later in (3.48).

Remark 3.3.1. *From Remark 1.3.4, smoothness of the functions $p_w(S,p)$, $p_n(S,p)$, and approximation (3.42) we conclude that*

$$0<\omega_m\le\omega_{K|L}^k\le\omega_M<+\infty. \tag{3.43}$$

We want the equations that relate the global pressure gradient to the phase pressure gradients (3.11) and (3.12), to stay valid in the discrete case too. Therefore we will use (3.11) and (3.12) to determine suitable approximation for the fractional flow functions f_n and f_w.

From (3.9) the wetting phase pressure p_w on the element K is defined as

$$p^k_{w,K} = p_w(S^k_K, p^k_K) = p^k_K - \int_1^{S^k_K} f_n(s, p^k_K) p'_c(s)\, ds. \tag{3.44}$$

The discretization (3.42) of the function ω on $\sigma_{K|L}$ is then given by

$$\begin{aligned}\omega^k_{K|L} &= \frac{p^k_K - p^k_L - \int_1^{S^k_{K|L}} f_n(s, p^k_K) p'_c(s)\, ds + \int_1^{S^k_{K|L}} f_n(s, p^k_L) p'_c(s)\, ds}{p^k_K - p^k_L} \\ &= 1 - \frac{1}{p^k_K - p^k_L} \int_1^{S^k_{K|L}} (f_n(s, p^k_K) - f_n(s, p^k_L)) p'_c(s)\, ds. \end{aligned} \tag{3.45}$$

Since we want the discrete equivalent of (3.12) we assume equality

$$p^k_{w,K} - p^k_{w,L} = \omega^k_{K|L}(p^k_K - p^k_L) - f^k_{n,K|L}(p_c(S^k_K) - p_c(S^k_L)), \tag{3.46}$$

to determine the approximation for the function f_n:

$$p^k_K - p^k_L - \int_1^{S^k_K} f_n(s, p^k_K) p'_c(s)\, ds + \int_1^{S^k_L} f_n(s, p^k_L) p'_c(s)\, ds = \omega^k_{K|L}(p^k_K - p^k_L) - f^k_{n,K|L}(u^k_K - u^k_L),$$

where we have denoted $u^k_K = p_c(S^k_K)$ and $u^k_L = p_c(S^k_L)$. By introducing (3.45) in the previous equation, we obtain

$$\begin{aligned} p^k_K - p^k_L &- \int_1^{S^k_K} f_n(s, p^k_K) p'_c(s)\, ds + \int_1^{S^k_L} f_n(s, p^k_L) p'_c(s)\, ds \\ &= p^k_K - p^k_L - \int_1^{S^k_{K|L}} (f_n(s, p^k_K) - f_n(s, p^k_L)) p'_c(s)\, ds - f^k_{n,K|L}(u^k_K - u^k_L). \end{aligned}$$

Now we have

$$f^k_{n,K|L}(u^k_K - u^k_L) = \int_{S^k_{K|L}}^{S^k_K} f_n(s, p^k_K) p'_c(s)\, ds - \int_{S^k_{K|L}}^{S^k_L} f_n(s, p^k_L) p'_c(s)\, ds, \tag{3.47}$$

Let us define the upwind value $S^{gup,k}_{K|L}$ with respect to the global pressure as

$$S^{gup,k}_{K|L} = \begin{cases} S^k_K & \text{if } p^k_K - p^k_L \geq 0 \\ S^k_L & \text{if } p^k_K - p^k_L < 0, \end{cases} \tag{3.48}$$

and corresponding upwind mobility as $\lambda_{\alpha,K|L}^{gup,k} = \lambda_\alpha\left(S_{K|L}^{gup,k}\right)$ for $\alpha = w,n$. We set $S_{K|L}^k = S_{K|L}^{gup,k}$ in (3.47) and we get

$$f_{n,K|L}^k = \frac{1}{u_K^k - u_L^k}\int_{S_L^k}^{S_K^k} f_n(s, p_{K|L}^k)p_c'(s)\,ds, \quad p_{K|L}^k = \min\{p_K^k, p_L^k\}. \tag{3.49}$$

In the limit $S_K^k = S_L^k = S$ we have $f_{n,K|L}^k = f_n(S, p_{K|L}^k)$.

The nonwetting phase pressure is defined by (3.10) which gives

$$p_{n,K}^k = p_n(S_K^k, p_K^k) = p_w(S_K^k, p_K^k) + p_c(S_K^k). \tag{3.50}$$

On the interface $\sigma_{K|L}$ we have

$$\begin{aligned} p_{n,K}^k - p_{n,L}^k &= p_{w,K}^k - p_{w,L}^k + u_K^k - u_L^k \\ &= \omega_{K|L}(p_K^k - p_L^k) - f_{n,K|L}^k(u_K^k - u_L^k) + u_K^k - u_L^k, \end{aligned}$$

which can be rewritten as

$$p_{n,K}^k - p_{n,L}^k = \omega_{K|L}^k(p_K^k - p_L^k) + f_{w,K|L}^k(u_K^k - u_L^k), \tag{3.51}$$

with $f_{w,K|L}^k = 1 - f_{n,K|L}^k$. The approximation $f_{w,K|L}^k$ for the wetting phase fractional flow function takes form

$$f_{w,K|L}^k = \frac{1}{u_K^k - u_L^k}\int_{S_L^k}^{S_K^k} f_w(s, p_{K|L}^k)p_c'(s)\,ds, \quad p_{K|L}^k = \min\{p_K^k, p_L^k\}. \tag{3.52}$$

In the case $S_K^k = S_L^k = S$ we have $f_{w,K|L}^k = f_w(S, p_{K|L}^k)$.

We have proved the following result.

Proposition 3.3.2. *Assume that p_K^k and p_L^k are two given values of the global pressure, $u_K^k = p_c(S_K^k)$ and $u_L^k = p_c(S_L^k)$ are two given values of the capillary pressure. We denote by $p_{n,K}^k$, $p_{n,L}^k$, $p_{w,K}^k$, and $p_{w,L}^k$ the corresponding values of the nonwetting and the wetting phase pressures defined by (3.10) and (3.9). Then we have*

$$p_{n,K}^k - p_{n,L}^k = \omega_{K|L}^k(p_K^k - p_L^k) + f_{w,K|L}^k(u_K^k - u_L^k), \tag{3.53}$$

$$p_{w,K}^k - p_{w,L}^k = \omega_{K|L}^k(p_K^k - p_L^k) - f_{n,K|L}^k(u_K^k - u_L^k), \tag{3.54}$$

where $\omega_{K|L}^k$ is defined by (3.42) with $S_{K|L}^k = S_{K|L}^{gup,k}$ (see (3.48)); $f_{n,K|L}^k$ is given by (3.49), and $f_{w,K|L}^k = 1 - f_{n,K|L}^k$ (see (3.52)).

Remark 3.3.3. *By the relations (3.53) and (3.54) one can define another finite volume scheme for the problem (3.1), (3.2), (3.3), (3.4), (3.6), where primary unknowns are the saturation* $(S_{w,K}^{k+1})_{K\in\mathcal{T}}$ *and the global pressure* $(p_K^{k+1})_{K\in\mathcal{T}}$ *,* $k\in\{0,1,...,N-1\}$*. The equations for this new scheme are given here:*

$$
\begin{aligned}
&|K|\Phi_K \frac{\rho_{n,K}^{k+1}S_{n,K}^{k+1}-\rho_{n,K}^{k}S_{n,K}^{k}}{\delta t} \\
&\quad + \sum_{L\in N_D(K)} \tau_{K|L}k_{K|L}\lambda_{n,K|L}^{up,k+1}\rho_{n,K|L}^{up,k+1}(\omega_{K|L}^{k+1}(p_K^{k+1}-p_L^{k+1})+f_{w,K|L}^{k+1}(u_K^{k+1}-u_L^{k+1})) \\
&\quad + \sum_{L\in N_D(K)} |\sigma_{K|L}|k_{K|L}\lambda_{n,K|L}^{G,k+1}\left(\rho_{n,K|L}^{G,k+1}\right)^2 g_{K|L} = |K|F_{n,K}^{k+1},
\end{aligned}
\tag{3.55}
$$

$$
\begin{aligned}
&|K|\Phi_K \frac{\rho_{w,K}^{k+1}S_{w,K}^{k+1}-\rho_{w,K}^{k}S_{w,K}^{k}}{\delta t} \\
&\quad + \sum_{L\in N_D(K)} \tau_{K|L}k_{K|L}\lambda_{w,K|L}^{up,k+1}\rho_{w,K|L}^{up,k+1}(\omega_{K|L}^{k+1}(p_K^{k+1}-p_L^{k+1})-f_{n,K|L}^{k+1}(u_K^{k+1}-u_L^{k+1})) \\
&\quad + \sum_{L\in N_D(K)} |\sigma_{K|L}|k_{K|L}\lambda_{w,K|L}^{G,k+1}\left(\rho_{w,K|L}^{G,k+1}\right)^2 g_{K|L} = |K|F_{w,K}^{k+1}.
\end{aligned}
\tag{3.56}
$$

Next we present three auxiliary lemmas.

Lemma 3.3.4. *For* $\alpha\in\{w,n\}$ *it holds* $\rho_{\alpha,K|L}^{up,k}\ge\rho_{\alpha,K|L}^{k}$*, where* $\rho_{\alpha,K|L}^{up,k}$ *is defined by (3.31) and* $\rho_{\alpha,K|L}^{k}$ *is defined by (3.32).*

Proof. In the case $p_{\alpha,K}^k-p_{\alpha,L}^k\ge 0$, the monotonicity of the function ρ_α leads to

$$
\rho_{\alpha,K|L}^{k}=\frac{p_{\alpha,K}^k-p_{\alpha,L}^k}{\displaystyle\int_{p_{\alpha,L}^k}^{p_{\alpha,K}^k}\frac{d\sigma}{\rho_\alpha(\sigma)}}\le\frac{p_{\alpha,K}^k-p_{\alpha,L}^k}{\frac{1}{\rho_\alpha(p_{\alpha,K}^k)}\left(p_{\alpha,K}^k-p_{\alpha,L}^k\right)}=\rho_\alpha(p_{\alpha,K}^k)=\rho_{\alpha,K|L}^{up,k}.
$$

In the same way we obtain in the case $p_{\alpha,K}^k-p_{\alpha,L}^k<0$

$$
\rho_{\alpha,K|L}^{k}=\frac{p_{\alpha,K}^k-p_{\alpha,L}^k}{\displaystyle\int_{p_{\alpha,L}^k}^{p_{\alpha,K}^k}\frac{d\sigma}{\rho_\alpha(\sigma)}}\le\frac{p_{\alpha,K}^k-p_{\alpha,L}^k}{\frac{1}{\rho_\alpha(p_{\alpha,L}^k)}\left(p_{\alpha,K}^k-p_{\alpha,L}^k\right)}=\rho_\alpha(p_{\alpha,L}^k)=\rho_{\alpha,K|L}^{up,k}.
$$

□

Lemma 3.3.5. *With the same notation as in Proposition 3.3.2, we have the following estimates:*

$$
f_{w,K|L}^k(u_K^k-u_L^k)(p_K^k-p_L^k)\ge f_w(S_{K|L}^{gup,k},p_{K|L})(u_K^k-u_L^k)(p_K^k-p_L^k), \tag{3.57}
$$

$$
f_{n,K|L}^k(u_K^k-u_L^k)(p_K^k-p_L^k)\le f_n(S_{K|L}^{gup,k},p_{K|L})(u_K^k-u_L^k)(p_K^k-p_L^k). \tag{3.58}
$$

Proof. First, we note that for $p \in \mathbb{R}$ and $s_K, s_L \in [0,1]$ it holds:

$$f_w(s_K, p)(u_K - u_L) \le \int_{s_L}^{s_K} f_w(s,p) p_c'(s) ds \le f_w(s_L, p)(u_K - u_L), \tag{3.59}$$

$$f_n(s_L, p)(u_K - u_L) \le \int_{s_L}^{s_K} f_n(s,p) p_c'(s) ds \le f_n(s_K, p)(u_K - u_L). \tag{3.60}$$

Indeed, in the case $s_K - s_L \ge 0$, since the capillary pressure p_c is a nonincreasing function of s we have $u_K - u_L \le 0$. Now (3.59) and (3.60) easily follow from the facts that f_w is a nondecreasing function of s, and f_n is a nonincreasing function of s. The case $s_K - s_L \le 0$ is treated in the same way.

Using (3.52), (3.59), (3.48), and the monotonicity of the function $S \mapsto f_w(S, p^k_{K|L})$, we get

$$\begin{aligned} f^k_{w,K|L}(u^k_K - u^k_L)(p^k_K - p^k_L) &= \int_{S^k_L}^{S^k_K} f_w(s, p^k_{K|L}) p_c'(s)\, ds (p^k_K - p^k_L) \\ &\ge f_w(S^{gup,k}_{K|L}, p^k_{K|L})(u^k_K - u^k_L)(p^k_K - p^k_L). \end{aligned}$$

The inequality (3.58) is proved in the same way. □

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

Lemma 3.3.6. *For $\alpha \in \{w, n\}$ it holds $\lambda^{up,k}_{\alpha,K|L} \ge \lambda^{gup,k}_{\alpha,K|L}$.*

Proof. Assume that $p^k_K - p^k_L \ge 0$ holds, which implies $\lambda^{gup,k}_{\alpha,K|L} = \lambda_\alpha(S^k_K)$, $\alpha = w, n$. Then it is not possible to have at the same time

$$p^k_{n,K} - p^k_{n,L} < 0 \text{ and } p^k_{w,K} - p^k_{w,L} < 0.$$

Indeed, this follows from the equations (3.46) and (3.51), which are repeated here,

$$\begin{aligned} p^k_{w,K} - p^k_{w,L} &= \omega^k_{K|L}(p^k_K - p^k_L) - f^k_{n,K|L}(p_c(S^k_K) - p_c(S^k_L)), \\ p^k_{n,K} - p^k_{n,L} &= \omega^k_{K|L}(p^k_K - p^k_L) + f^k_{w,K|L}(p_c(S^k_K) - p_c(S^k_L)), \end{aligned}$$

and the fact that $\omega^k_{K|L}(p^k_K - p^k_L) \ge 0$, $f^k_{n,K|L} \ge 0$, and $f^k_{w,K|L} \ge 0$. Therefore, we have three possibilities:

a) $p^k_{w,K} - p^k_{w,L} \ge 0$ and $p^k_{n,K} - p^k_{n,L} \ge 0$. In this case all the upwind values are the same.

b) $p^k_{w,K} - p^k_{w,L} \geq 0$ and $p^k_{n,K} - p^k_{n,L} < 0$. In this case we have $\lambda^{up,k}_{n,K|L} = \lambda_n(S^k_L)$ and $\lambda^{up,k}_{w,K|L} = \lambda_w(S^k_K)$, and also

$$f^k_{w,K|L}(p_c(S^k_K) - p_c(S^k_L)) < 0,$$

and consequently by using (A.4) we get $S^k_K > S^k_L$. Due to the monotonicity of the function λ_n one has

$$\lambda^{up,k}_{n,K|L} = \lambda_n(S^k_L) \geq \lambda_n(S^k_K) = \lambda^{gup,k}_{n,K|L}.$$

c) $p^k_{w,K} - p^k_{w,L} < 0$ and $p^k_{n,K} - p^k_{n,L} \geq 0$. In this case we have $\lambda^{up,k}_{n,K|L} = \lambda_n(S^k_K)$ and $\lambda^{up,k}_{w,K|L} = \lambda_w(S^k_L)$, and also

$$f^k_{n,K|L}(p_c(S^k_K) - p_c(S^k_L)) > 0,$$

and consequently by using (A.4) we get $S^k_K < S^k_L$. Due to the monotonicity of λ_w one has

$$\lambda^{up,k}_{w,K|L} = \lambda_w(S^k_L) \geq \lambda_w(S^k_K) = \lambda^{gup,k}_{w,K|L}.$$

This proves the statement in the case $p^k_K - p^k_L \geq 0$.

Let us now consider the case $p^k_K - p^k_L < 0$, meaning that $\lambda^{gup,k}_{\alpha,K|L} = \lambda_\alpha(S^k_L)$, $\alpha = w, n$. In this case, by the same reasoning as above, we can not have

$$p^k_{n,K} - p^k_{n,L} > 0 \text{ and } p^k_{w,K} - p^k_{w,L} > 0.$$

We again have three possibilities:

a) $p^k_{w,K} - p^k_{w,L} < 0$ and $p^k_{n,K} - p^k_{n,L} < 0$. In this case all the upwind values are the same.

b) $p^k_{w,K} - p^k_{w,L} \geq 0$ and $p^k_{n,K} - p^k_{n,L} \leq 0$. In this case we have

$$f^k_{n,K|L}(p_c(S^k_K) - p_c(S^k_L)) < 0,$$

which leads to $S^k_K > S^k_L$. For the nonwetting phase mobility we have $\lambda^{up,k}_{n,K|L} = \lambda_n(S^k_L) = \lambda^{gup,k}_{n,K|L}$ and for the wetting phase mobility, which is an increasing function of the wetting phase saturation, we have

$$\lambda^{up,k}_{w,K|L} = \lambda_w(S^k_K) \geq \lambda_w(S^k_L) = \lambda^{gup,k}_{w,K|L}.$$

c) $p^k_{w,K} - p^k_{w,L} \leq 0$ and $p^k_{n,K} - p^k_{n,L} \geq 0$. In this case we have

$$f^k_{w,K|L}(p_c(S^k_K) - p_c(S^k_L)) > 0,$$

meaning $S_K^k < S_L^k$. Now we have for the wetting phase mobility $\lambda_{w,K|L}^{up,k} = \lambda_w(S_L^k) = \lambda_{w,K|L}^{gup,k}$, and since the nonwetting phase mobility is a decreasing function of the wetting phase saturation, we have

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

□

Lemma 3.3.7. *Let D_h be a finite volume discretization of $\Omega \times (0,T)$ and let assumptions (A.1)–(A.7) hold. Then the following inequality holds:*

$$\begin{aligned} \lambda_{w,K|L}^{gup,k}\overline{\rho}_{w,K|L}^{k}(p_{w,K}^k - p_{w,L}^k)^2 + \lambda_{n,K|L}^{gup,k}\overline{\rho}_{n,K|L}^{k}(p_{n,K}^k - p_{n,L}^k)^2 \\ \geq (\rho\lambda)_{K|L}^k \left(\omega_{K|L}^k\right)^2 (p_K^k - p_L^k)^2 + \alpha_{K|L}^k (u_K^k - u_L^k)^2, \end{aligned} \tag{3.61}$$

where we have denoted

$$\begin{aligned} \overline{\rho}_{\alpha,K|L}^k &= \rho_\alpha(p_\alpha(S_{K|L}^{gup,k}, p_{K|L}^k)), \quad \alpha = w,n, \\ (\rho\lambda)_{K|L}^k &= \lambda_{n,K|L}^{gup,k}\overline{\rho}_{n,K|L}^k + \lambda_{w,K|L}^{gup,k}\overline{\rho}_{w,K|L}^k, \\ \alpha_{K|L}^k &= \lambda_{w,K|L}^{gup,k}\overline{\rho}_{w,K|L}^k \left(f_{n,K|L}^k\right)^2 + \lambda_{n,K|L}^{gup,k}\overline{\rho}_{n,K|L}^k \left(f_{w,K|L}^k\right)^2, \end{aligned} \tag{3.62}$$

for all $K \in \mathcal{T}$, $L \in N(K)$, and $k \in \{1,\dots,N\}$. Moreover,

$$\alpha_{K|L}^k (u_K^k - u_L^k)^2 \geq C_\beta (\beta(S_K^k) - \beta(S_L^k))^2, \tag{3.63}$$

where 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. From (3.54) we have

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

and from (3.53)

$$\lambda_{n,K|L}^{gup,k}\overline{\rho}_{n,K|L}^{k}(p_{n,K}^k - p_{n,L}^k)^2 = \lambda_{n,K|L}^{gup,k}\overline{\rho}_{n,K|L}^{k}(\omega_{K|L}^k(p_K^k - p_L^k) + f_{w,K|L}^k(u_K^k - u_L^k))^2$$

$$
\begin{aligned}
&= \lambda^{gup,k}_{n,K|L}\overline{\rho}^k_{n,K|L}\left(\omega^k_{K|L}\right)^2(p^k_K - p^k_L)^2 \\
&+ 2\lambda^{gup,k}_{n,K|L}\overline{\rho}^k_{n,K|L} f^k_{w,K|L}\omega^k_{K|L}(p^k_K - p^k_L)(u^k_K - u^k_L) \\
&+ \lambda^{gup,k}_{n,K|L}\overline{\rho}^k_{n,K|L}\left(f^k_{w,K|L}\right)^2(u^k_K - u^k_L)^2.
\end{aligned}
$$

After summing these two equations we obtain

$$
\begin{aligned}
\lambda^{gup,k}_{w,K|L}\overline{\rho}^k_{w,K|L}&(p^k_{w,K} - p^k_{w,L})^2 + \lambda^{gup,k}_{n,K|L}\overline{\rho}^k_{n,K|L}(p^k_{n,K} - p^k_{n,L})^2 \\
&= (\rho\lambda)^k_{K|L}\left(\omega^k_{K|L}\right)^2(p^k_K - p^k_L)^2 \\
&+ 2\omega^k_{K|L}\left(\lambda^{gup,k}_{n,K|L}\overline{\rho}^k_{n,K|L} f^k_{w,K|L} - \lambda^{gup,k}_{w,K|L}\overline{\rho}^k_{w,K|L} f^k_{n,K|L}\right)(p^k_K - p^k_L)(u^k_K - u^k_L) \\
&+ \left(\lambda^{gup,k}_{w,K|L}\overline{\rho}^k_{w,K|L}\left(f^k_{n,K|L}\right)^2 + \lambda^{gup,k}_{n,K|L}\overline{\rho}^k_{n,K|L}\left(f^k_{w,K|L}\right)^2\right)(u^k_K - u^k_L)^2.
\end{aligned}
$$

From Lemma 3.3.5 we get

$$
\begin{aligned}
&2\omega^n_{K|L}\left(\lambda^{gup,k}_{n,K|L}\overline{\rho}^k_{n,K|L} f^k_{w,K|L} - \lambda^{gup,k}_{w,K|L}\overline{\rho}^k_{w,K|L} f^k_{n,K|L}\right)(p^k_K - p^k_L)(u^k_K - u^k_L) \\
&\geq 2\omega^k_{K|L}\left(\lambda^{gup,k}_{n,K|L}\overline{\rho}^k_{n,K|L} f_w(S^{gup,k}_{K|L}, p^k_{K|L}) - \lambda^{gup,k}_{w,K|L}\overline{\rho}^k_{w,K|L} f_n(S^{gup,k}_{K|L}, p^k_{K|L})\right)(p^k_K - p^k_L)(u^k_K - u^k_L) = 0,
\end{aligned}
$$

which gives the estimate (3.61).

On the interface $\sigma_{K|L}$ we have

$$
\beta(S^k_K) - \beta(S^k_L) = \int_{S^k_L}^{S^k_K} \lambda_w(s)\lambda_n(s)p'_c(s)\,ds. \tag{3.64}
$$

In order to prove (3.63) let us first consider the case $p^k_K - p^k_L \geq 0$ and $S^k_K - S^k_L \geq 0$. In this case we have $\lambda^{gup,k}_{w,K|L} = \lambda_w(S^k_K)$ and $\lambda^{gup,k}_{n,K|L} = \lambda_n(S^k_K)$, and

$$
\left(\beta(S^k_K) - \beta(S^k_L)\right)^2 \leq \lambda^2_w(S^k_K)\left(\int_{S^k_L}^{S^k_K} \lambda_n(s)p'_c(s)\,ds\right)^2 \leq \frac{1}{\mu_w}\lambda_w(S^k_K)\left(\int_{S^k_L}^{S^k_K} \lambda_n(s)p'_c(s)\,ds\right)^2.
$$

In the same way for all the other cases from the monotonicity of the mobilities and using $S^{gup,k}_{K|L} \in \{S^k_K, S^k_L\}$ we get

$$
\begin{aligned}
\left(\beta(S^k_K) - \beta(S^k_L)\right)^2 &\leq \lambda^2_w(S^{gup,k}_{K|L})\left(\int_{S^k_L}^{S^k_K} \lambda_n(s)p'_c(s)\,ds\right)^2 + \lambda^2_n(S^{gup,k}_{K|L})\left(\int_{S^k_L}^{S^k_K} \lambda_w(s)p'_c(s)\,ds\right)^2 \\
&\leq \frac{\lambda_w(S^{gup,k}_{K|L})}{\mu_w}\left(\int_{S^k_L}^{S^k_K} \lambda_n(s)p'_c(s)\,ds\right)^2 + \frac{\lambda_n(S^{gup,k}_{K|L})}{\mu_n}\left(\int_{S^k_L}^{S^k_K} \lambda_w(s)p'_c(s)\,ds\right)^2.
\end{aligned}
$$

The boundedness of the mass densities and the relative mobilities gives us for $\alpha \in \{w,n\}$,

$$\frac{\rho_\alpha(s,p^k_{K|L})}{\rho_w(s,p^k_{K|L})\lambda_w(s)+\rho_g(s,p^k_{K|L})\lambda_g(s)} \geq \frac{\rho_m}{\rho_M(1/\mu_w+1/\mu_n)},$$

giving the estimate

$$\begin{aligned}\left(\beta(S^k_K)-\beta(S^k_L)\right)^2 \leq (1/C_\beta)\Bigg\{&\overline{\rho}^k_{w,K|L}\lambda_w(S^{gup,k}_{K|L})\left(\int_{S^k_L}^{S^k_K} f_n(s,p^k_{K|L})p_c'(s)\,ds\right)^2\\ &+\overline{\rho}^k_{n,K|L}\lambda_n(S^{gup,k}_{K|L})\left(\int_{S^k_L}^{S^k_K} f_w(s,p^k_{K|L})p_c'(s)\,ds\right)^2\Bigg\}.\end{aligned}$$

This proves (3.63).

□

3.4 The maximum principle

Lemma 3.4.1. ***(Maximum principle)*** *Let D_h be a finite volume discretization of $\Omega\times(0,T)$ and let $(p_{n,h},p_{w,h})$ be a solution to the finite volume scheme (3.36)–(3.41). Assume that $(S^0_{w,K})_{K\in\mathcal{T}}\in[0,1]$. Then we have*

$$0\leq S^k_{w,K}\leq 1,\quad \forall K\in\mathcal{T},\ \forall k\in\{0,\dots,N\}.$$

Proof. The maximum principle is proved by mathematical induction in the same way as in [76] and is given here again for the completeness of the convergence proof. We use notation $x^+=\max(x,0)$ and $x^-=\max(-x,0)$ such that $x=x^+-x^-$ and $|x|=x^++x^-$.

We assume that at the preceding time level k it holds $0\leq S^k_{w,K}\leq 1$. In order to show $S^{k+1}_w\geq 0$ we chose the element K such that $S^{k+1}_{w,K}\leq S^{k+1}_{w,L}$ for all elements L and we multiply (3.38) for the element K by $(S^{k+1}_{w,K})^-$ which gives

$$\begin{aligned}|K|\Phi_K\frac{\rho^{k+1}_{w,K}S^{k+1}_{w,K}-\rho^k_{w,K}S^k_{w,K}}{\delta t}(S^{k+1}_{w,K})^- + \sum_{L\in N_D(K)}|\sigma_{K|L}|\lambda^{up,k+1}_{w,K|L}\rho^{up,k+1}_{w,K|L}Q^{k+1}_{w,K|L}(S^{k+1}_{w,K})^-\\ +\sum_{L\in N_D(K)}|\sigma_{K|L}|k_{K|L}\lambda^{G,k+1}_{w,K|L}\left(\rho^{G,k+1}_{w,K|L}\right)^2 g_{K|L}(S^{k+1}_{w,K})^- = |K|F^{k+1}_{w,K}(S^{k+1}_{w,K})^-,\end{aligned}$$

where we have denoted $Q^{k+1}_{w,K|L} = \frac{1}{d_{K|L}} k_{K|L}(p^{k+1}_{w,K} - p^{k+1}_{w,L})$. By neglecting $-\rho^k_{w,K} S^k_{w,K} (S^{k+1}_{w,K})^- \leq 0$ we get

$$
\begin{aligned}
&\frac{|K|\Phi_K}{\delta t} \rho^{k+1}_{w,K} S^{k+1}_{w,K} (S^{k+1}_{w,K})^- + \sum_{L \in N_D(K)} |\sigma_{K|L}| \lambda^{up,k+1}_{w,K|L} \rho^{up,k+1}_{w,K|L} Q^{k+1}_{w,K|L} (S^{k+1}_{w,K})^- \\
&+ \sum_{L \in N_D(K)} |\sigma_{K|L}| k_{K|L} \lambda^{G,k+1}_{w,K|L} \left(\rho^{G,k+1}_{w,K|L}\right)^2 g_{K|L} (S^{k+1}_{w,K})^- \geq |K| F^{k+1}_{w,K} (S^{k+1}_{w,K})^-.
\end{aligned}
$$

Note that $(S^{k+1}_{w,K})^- > 0$ if and only if $S^{k+1}_{w,K} < 0$. We have then $S^{k+1}_{w,K}(S^{k+1}_{w,K})^- = -[(S^{k+1}_{w,K})^-]^2$. This gives

$$
\begin{aligned}
&\frac{|K|\Phi_K}{\delta t} \rho^{k+1}_{w,K} [(S^{k+1}_{w,K})^-]^2 \leq \sum_{L \in N_D(K)} |\sigma_{K|L}| \lambda^{up,k+1}_{w,K|L} \rho^{up,k+1}_{w,K|L} Q^{k+1}_{w,K|L} (S^{k+1}_{w,K})^- \\
&+ \sum_{L \in N_D(K)} |\sigma_{K|L}| k_{K|L} \lambda^{G,k+1}_{w,K|L} \left(\rho^{G,k+1}_{w,K|L}\right)^2 g_{K|L} (S^{k+1}_{w,K})^- - |K| F^{k+1}_{w,K} (S^{k+1}_{w,K})^-.
\end{aligned}
$$

If $Q^{k+1}_{w,K|L} \geq 0$ then $\lambda^{up,k+1}_{w,K|L} = \lambda_w(S^{k+1}_{w,K})$ and

$$
\lambda^{up,k+1}_{w,K|L} (S^{k+1}_{w,K})^- = 0,
$$

since the mobility function $\lambda_w(S_w)$ is equal to zero at $S_w = 0$ and is naturally extended as zero for negative saturation values. On the other hand, for $Q^{k+1}_{w,K|L} \leq 0$ we conclude that the term $|\sigma| \lambda^{up,k+1}_{w,K|L} \rho^{up,k+1}_{w,K|L} Q^{k+1}_{w,K|L} (S^{k+1}_{w,K})^-$ is nonpositive and can be neglected.

For the gravity term note that

$$
\sum_{L \in N_D(K)} |\sigma_{K|L}| k_{K|L} \lambda^{G,k+1}_{w,K|L} \left(\rho^{G,k+1}_{w,K|L}\right)^2 g_{K|L} (S^{k+1}_{w,K})^- \leq 0
$$

if $g_{K|L} \leq 0$ and the whole term can be neglected. If $g_{K|L} > 0$ then again $\lambda^{G,k+1}_{w,K|L} = \lambda_w(S^{k+1}_{w,K})$ and

$$
\lambda^{G,k+1}_{w,K|L} (S^{k+1}_{w,K})^- = 0.
$$

In that way we get

$$
\begin{aligned}
\frac{|K|\Phi_K}{\delta t} \rho^{k+1}_{w,K} [(S^{k+1}_{w,K})^-]^2 &\leq -|K| F^{k+1}_{w,K} (S^{k+1}_{w,K})^- \\
&= -|K| \rho_w(p^{k+1}_{w,K}) (S^{I,k+1}_{w,K} F^{k+1}_{I,K} - S^{k+1}_{w,K} F^{k+1}_{P,K}) (S^{k+1}_{w,K})^- \\
&\leq |K| \rho_w(p^{k+1}_{w,K}) S^{k+1}_{w,K} F^{k+1}_{P,K} (S^{k+1}_{w,K})^-
\end{aligned}
$$

$$= -|K|\rho_w(p_{w,K}^{k+1})F_{P,K}^{k+1}[(S_{w,K}^{k+1})^-]^2,$$

where we have used $S_{w,K}^{I,k+1} \geq 0$ and $F_{I,K}^{k+1} \geq 0$. This finally gives

$$\rho_{w,K}^{k+1}\left(\frac{|K|\Phi_K}{\delta t} + |K|F_{P,K}^{k+1}\right)[(S_{w,K}^{k+1})^-]^2 \leq 0,$$

and therefore, due to $F_{P,K}^{k+1} \geq 0$ we get $S_{w,K}^{k+1} \geq 0$.

To show $S_w \leq 1$ we use the equation (3.37) for the element K such that $S_{w,K}^{k+1} \geq S_{w,L}^{k+1}$ for all L in the grid. By multiplying by $(S_{n,K}^{k+1})^-$ we get

$$|K|\Phi_K\frac{\rho_{n,K}^{k+1}S_{n,K}^{k+1} - \rho_{n,K}^{k}S_{n,K}^{k}}{\delta t}(S_{n,K}^{k+1})^- + \sum_{L\in N_D(K)}|\sigma_{K|L}|\lambda_{n,K|L}^{up,k+1}\rho_{n,K|L}^{up,k+1}Q_{n,K|L}^{k+1}(S_{n,K}^{k+1})^-$$
$$+\sum_{L\in N_D(K)}|\sigma_{K|L}|k_{K|L}\lambda_{n,K|L}^{G,k+1}\left(\rho_{n,K|L}^{G,k+1}\right)^2 g_{K|L}(S_{n,K}^{k+1})^- = |K|F_{n,K}^{k+1}(S_{n,K}^{k+1})^-,$$

where we have denoted $Q_{n,K|L}^{k+1} = \frac{1}{d_{K|L}}k_{K|L}(p_{n,K}^{k+1} - p_{n,L}^{k+1})$. By the same procedure used in the proof of $S_w^{k+1} \geq 0$ we get,

$$\frac{|K|\Phi_K\rho_{n,K}^{k+1}}{\delta t}[(S_{n,K}^{k+1})^-]^2 \leq \sum_{L\in N_D(K)}|\sigma_{K|L}|\lambda_{n,K|L}^{up,k+1}\rho_{n,K|L}^{up,k+1}Q_{n,K|L}^{k+1}(S_{n,K}^{k+1})^-$$
$$+\sum_{L\in N_D(K)}|\sigma_{K|L}|k_{K|L}\lambda_{n,K|L}^{G,k+1}\left(\rho_{n,K|L}^{G,k+1}\right)^2 g_{K|L}(S_{n,K}^{k+1})^- - |K|F_{n,K}^{k+1}(S_{n,K}^{k+1})^-.$$

By using the upwind discretization we find out that for $Q_{n,K|L}^{k+1} \geq 0$ it holds $\lambda_{n,K|L}^{up,k+1} = \lambda_n(S_{w,K}^{k+1})$ and

$$\lambda_{n,K|L}^{up,k+1}(1 - S_{w,K}^{k+1})^- = 0,$$

since the mobility function $\lambda_n(S_w)$ is zero at $S_w = 1$ and it is naturally extended as zero for the values of saturation S_w greater than one. For the gravity term we again have

$$\sum_{L\in N_D(K)}|\sigma_{K|L}|k_{K|L}\lambda_{n,K|L}^{G,k+1}\left(\rho_{n,K|L}^{G,k+1}\right)^2 g_{K|L}(S_{n,K}^{k+1})^- \leq 0$$

if $g_{K|L} \leq 0$ and the whole term can be neglected. If $g_{K|L} > 0$ then again $\lambda_{n,K|L}^{G,k+1} = \lambda_n(S_{w,K}^{k+1})$ and

$$\lambda_{n,K|L}^{G,k+1}(1 - S_{w,K}^{k+1})^- = 0.$$

Thus, we find

$$\frac{|K|\Phi_K\rho_{n,K}^{k+1}}{\delta t}[(S_{n,K}^{k+1})^-]^2+|K|F_{n,K}^{k+1}(S_{n,K}^{k+1})^-\leq 0.$$

From here we conclude

$$\frac{|K|\Phi_K\rho_{n,K}^{k+1}}{\delta t}[(S_{n,K}^{k+1})^-]^2+|K|\rho_{n,K}^{k+1}(S_{n,K}^{I,k+1}F_{I,K}^{k+1}-S_{n,K}^{k+1}F_{P,K}^{k+1})(S_{n,K}^{k+1})^-\leq 0,$$

or

$$\frac{|K|\Phi_K\rho_{n,K}^{k+1}}{\delta t}[(S_{n,K}^{k+1})^-]^2+|K|\rho_{n,K}^{k+1}(S_{n,K}^{I,k+1}F_{I,K}^{k+1}(S_{n,K}^{k+1})^-+S_{n,K}^{k+1}F_{P,K}^{k+1}[(S_{n,K}^{k+1})^-]^2)\leq 0.$$

It follows that $(S_{n,K}^{k+1})^-=0$, meaning $S_{n,K}^{k+1}\geq 0$, or $S_{w,K}^{k+1}\leq 1$.

In that way we have proved for all $K\in\mathfrak{T}$

$$0\leq S_{w,K}^{k+1}\leq 1.$$

□

3.5 Energy estimate

Theorem 3.5.1. *Let D_h be a finite volume discretization of $\Omega\times(0,T)$ and let $(p_{n,h},p_{w,h})$ be a solution to the finite volume scheme (3.36)–(3.41). Then, there is 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*

$$\begin{aligned}\sum_{K\in\mathfrak{T}}|K|\Phi_K\mathscr{H}(p_{n,K}^N,p_{w,K}^N)-\sum_{K\in\mathfrak{T}}|K|\Phi_K\mathscr{H}(p_{n,K}^0,p_{w,K}^0)&\\+\frac{\lambda_m}{\rho_M}\frac{\rho_m\omega_m^2k_m}{4}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}\tilde{\tau}_{K|L}|p_K^{k+1}-p_L^{k+1}|^2&\\+\frac{C_\beta k_m}{4\rho_M}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}\tilde{\tau}_{K|L}|\beta(S_K^{k+1})-\beta(S_L^{k+1})|^2\leq C,&\end{aligned}\tag{3.65}$$

and

$$\begin{aligned}\sum_{K\in\mathfrak{T}}|K|\Phi_K\mathscr{H}(p_{n,K}^N,p_{w,K}^N)-\sum_{K\in\mathfrak{T}}|K|\Phi_K\mathscr{H}(p_{n,K}^0,p_{w,K}^0)&\\+\frac{\rho_mk_m}{4\rho_M}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}\tilde{\tau}_{K|L}\lambda_{w,K|L}^{up,k+1}(p_{w,K}^{k+1}-p_{w,L}^{k+1})^2&\end{aligned}\tag{3.66}$$

$$+\frac{\rho_m k_m}{4\rho_M}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}\tilde{\tau}_{K|L}\lambda_{n,K|L}^{up,k+1}(p_{n,K}^{k+1}-p_{n,L}^{k+1})^2\leq C,$$

where we have denoted

$$\mathscr{H}(p_n,p_w)=S_w(\rho_w(p_w)g(p_w)-p_w)+S_n(\rho_n(p_n)h(p_n)-p_n)-\int_0^{S_w}p_c(s)\,ds \tag{3.67}$$

with C_β given in Lemma 3.3.7. The functions $g(p_w)$ and $h(p_n)$ are given by

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

Proof. We use the functions $g(p_w)$ and $h(p_n)$ as the test functions in (3.37) and (3.38) to obtain

$$|K|\Phi_K\frac{\rho_{w,K}^{k+1}S_{w,K}^{k+1}-\rho_{w,K}^kS_{w,K}^k}{\delta t}g(p_{w,K}^{k+1})+\sum_{L\in N_D(K)}\tau_{K|L}k_{K|L}\lambda_{w,K|L}^{up,k+1}\rho_{w,K|L}^{up,k+1}(p_{w,K}^{k+1}-p_{w,L}^{k+1})g(p_{w,K}^{k+1})$$
$$+\sum_{L\in N_D(K)}|\sigma_{K|L}|k_{K|L}\lambda_{w,K|L}^{G,k+1}\left(\rho_{w,K|L}^{G,k+1}\right)^2g_{K|L}g(p_{w,K}^{k+1})=|K|F_{w,K}^{k+1}g(p_{w,K}^{k+1})$$

and

$$|K|\Phi_K\frac{\rho_{n,K}^{k+1}S_{n,K}^{k+1}-\rho_{n,K}^kS_{n,K}^k}{\delta t}h(p_{n,K}^{k+1})+\sum_{L\in N_D(K)}\tau_{K|L}k_{K|L}\lambda_{n,K|L}^{up,k+1}\rho_{n,K|L}^{up,k+1}(p_{n,K}^{k+1}-p_{n,L}^{k+1})h(p_{n,K}^{k+1})$$
$$+\sum_{L\in N_D(K)}|\sigma_{K|L}|k_{K|L}\lambda_{n,K|L}^{G,k+1}\left(\rho_{n,K|L}^{G,k+1}\right)^2g_{K|L}h(p_{n,K}^{k+1})=|K|F_{n,K}^{k+1}h(p_{n,K}^{k+1}).$$

By summing these two equations, multiplying by δt and summing over all elements and all time levels we get:

$$\sum_{k=0}^{N-1}\sum_{K\in\mathfrak{T}}|K|\Phi_K\left\{(\rho_{w,K}^{k+1}S_{w,K}^{k+1}-\rho_{w,K}^kS_{w,K}^k)g(p_{w,K}^{k+1})+(\rho_{n,K}^{k+1}S_{n,K}^{k+1}-\rho_{n,K}^kS_{n,K}^k)h(p_{n,K}^{k+1})\right\}$$
$$+\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}\tau_{K|L}k_{K|L}\lambda_{w,K|L}^{up,k+1}\rho_{w,K|L}^{up,k+1}(p_{w,K}^{k+1}-p_{w,L}^{k+1})g(p_{w,K}^{k+1})$$
$$+\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}\tau_{K|L}k_{K|L}\lambda_{n,K|L}^{up,k+1}\rho_{n,K|L}^{up,k+1}(p_{n,K}^{k+1}-p_{n,L}^{k+1})h(p_{n,K}^{k+1})$$
$$=-\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}|\sigma_{K|L}|k_{K|L}\lambda_{w,K|L}^{G,k+1}\left(\rho_{w,K|L}^{G,k+1}\right)^2g_{K|L}g(p_{w,K}^{k+1}) \tag{3.68}$$

$$
\begin{aligned}
&-\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}|\sigma_{K|L}|k_{K|L}\lambda_{n,K|L}^{G,k+1}\left(\rho_{n,K|L}^{G,k+1}\right)^2 g_{K|L}h(p_{n,K}^{k+1})\\
&+\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}|K|(\rho_w(p_{w,K}^{k+1})S_{w,K}^{I,k+1}F_{I,K}^{k+1}g(p_{w,K}^{k+1})+\rho_n(p_{n,K}^{k+1})S_{n,K}^{I,k+1}F_{I,K}^{k+1}h(p_{n,K}^{k+1}))\\
&-\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}|K|(\rho_w(p_{w,K}^{k+1})S_{w,K}^{k+1}F_{P,K}^{k+1}g(p_{w,K}^{k+1})+\rho_n(p_{n,K}^{k+1})S_{n,K}^{k+1}F_{P,K}^{k+1}h(p_{n,K}^{k+1})).
\end{aligned}
$$

In order to simplify notation we will write equation (3.68) as

$$A^1+A^2+A^3=A^4+A^5+A^6+A^7$$

where A^i are the successive terms in equation (3.68).

1. The accumulation term A^1 can be written as

$$A^1=\sum_{k=0}^{N-1}\sum_{K\in\mathfrak{T}}|K|\Phi_K A_K^1,$$

where

$$
\begin{aligned}
A_K^1 &= (\rho_{w,K}^{k+1}S_{w,K}^{k+1}-\rho_{w,K}^{k}S_{w,K}^{k})g(p_{w,K}^{k+1})+(\rho_{n,K}^{k+1}S_{n,K}^{k+1}-\rho_{n,K}^{k}S_{n,K}^{k})h(p_{n,K}^{k+1})\\
&=\rho_{w,K}^{k+1}S_{w,K}^{k+1}g(p_{w,K}^{k+1})-\rho_{w,K}^{k}S_{w,K}^{k}g(p_{w,K}^{k})+\rho_{n,K}^{k+1}S_{n,K}^{k+1}h(p_{n,K}^{k+1})-\rho_{n,K}^{k}S_{n,K}^{k}h(p_{n,K}^{k})\\
&+\rho_{w,K}^{k}S_{w,K}^{k}(g(p_{w,K}^{k})-g(p_{w,K}^{k+1}))+\rho_{n,K}^{k}S_{n,K}^{k}(h(p_{n,K}^{k})-h(p_{n,K}^{k+1})).
\end{aligned}
$$

From the monotonicity of the mass densities we get

$$\rho_{n,K}^{k}[h(p_{n,K}^{k})-h(p_{n,K}^{k+1})]\ge p_{n,K}^{k}-p_{n,K}^{k+1},\quad \rho_{w,K}^{k}[g(p_{w,K}^{k})-g(p_{w,K}^{k+1})]\ge p_{w,K}^{k}-p_{w,K}^{k+1},$$

and therefore,

$$
\begin{aligned}
A_K^1 &\ge \rho_{w,K}^{k+1}S_{w,K}^{k+1}g(p_{w,K}^{k+1})-\rho_{w,K}^{k}S_{w,K}^{k}g(p_{w,K}^{k})+\rho_{n,K}^{k+1}S_{n,K}^{k+1}h(p_{n,K}^{k+1})-\rho_{n,K}^{k}S_{n,K}^{k}h(p_{n,K}^{k})\\
&+S_{w,K}^{k}(p_{w,K}^{k}-p_{w,K}^{k+1})+S_{n,K}^{k}(p_{n,K}^{k}-p_{n,K}^{k+1})\\
&=\rho_{w,K}^{k+1}S_{w,K}^{k+1}g(p_{w,K}^{k+1})-\rho_{w,K}^{k}S_{w,K}^{k}g(p_{w,K}^{k})+\rho_{n,K}^{k+1}S_{n,K}^{k+1}h(p_{n,K}^{k+1})-\rho_{n,K}^{k}S_{n,K}^{k}h(p_{n,K}^{k})\\
&-S_{w,K}^{k+1}p_{w,K}^{k+1}-S_{n,K}^{k+1}p_{n,K}^{k+1}+S_{w,K}^{k}p_{w,K}^{k}+S_{n,K}^{k}p_{n,K}^{k}+(S_{w,K}^{k+1}-S_{w,K}^{k})p_{w,K}^{k+1}+(S_{n,K}^{k+1}-S_{n,K}^{k})p_{n,K}^{k+1}.
\end{aligned}
$$

The last two terms can be estimated as follows:

$$
\begin{aligned}
(S_{w,K}^{k+1}-S_{w,K}^{k})p_{w,K}^{k+1}+(S_{n,K}^{k+1}-S_{n,K}^{k})p_{n,K}^{k+1} &= (S_{w,K}^{k+1}-S_{w,K}^{k})(p_{w,K}^{k+1}-p_{n,K}^{k+1})\\
&=-(S_{w,K}^{k+1}-S_{w,K}^{k})p_c(S_{w,K}^{k+1})\ge-\int_{S_{w,K}^{k}}^{S_{w,K}^{k+1}}p_c(s)\,ds,
\end{aligned}
$$

where in the last step we have used the monotonicity of the capillary pressure function. By using $\mathscr{H}$ defined in (3.67) we can write

$$A^1 \geq \sum_{k=0}^{N-1} \sum_{K\in\mathfrak{T}} |K|\Phi_K \Big(\mathscr{H}(p_{n,K}^{k+1}, p_{w,K}^{k+1}) - \mathscr{H}(p_{n,K}^{k}, p_{w,K}^{k}) \Big). \tag{3.69}$$

2. Gradient estimate. The terms A^2 and A^3 can be written as sums over all interior and Dirichlet's sides:

$$A^2 = \frac{1}{2}\sum_{k=0}^{N-1} \delta t \sum_{K\in\mathfrak{T}} \sum_{L\in N_D(K)} \tilde{\tau}_{K|L} \lambda_{w,K|L}^{up,k+1} \rho_{w,K|L}^{up,k+1} k_{K|L} \left(p_{w,K}^{k+1} - p_{w,L}^{k+1} \right) \left(g(p_{w,K}^{k+1}) - g(p_{w,L}^{k+1}) \right),$$
$$A^3 = \frac{1}{2}\sum_{k=0}^{N-1} \delta t \sum_{K\in\mathfrak{T}} \sum_{L\in N_D(K)} \tilde{\tau}_{K|L} \lambda_{n,K|L}^{up,k+1} \rho_{n,K|L}^{up,k+1} k_{K|L} \left(p_{n,K}^{k+1} - p_{n,L}^{k+1} \right) \left(h(p_{n,K}^{k+1}) - h(p_{n,L}^{k+1}) \right),$$

where we have used notation from Remark 3.2.7.

Due to the Lemma 3.3.4 and the fact that

$$\begin{aligned} &\left(p_{w,K}^{k+1} - p_{w,L}^{k+1} \right) \left(g(p_{w,K}^{k+1}) - g(p_{w,L}^{k+1}) \right) \geq 0, \\ &\left(p_{n,K}^{k+1} - p_{n,L}^{k+1} \right) \left(h(p_{n,K}^{k+1}) - h(p_{n,L}^{k+1}) \right) \geq 0, \end{aligned} \tag{3.70}$$

we conclude

$$A^2 \geq \frac{1}{2}\sum_{k=0}^{N-1} \delta t \sum_{K\in\mathfrak{T}} \sum_{L\in N_D(K)} \tilde{\tau}_{K|L} \lambda_{w,K|L}^{up,k+1} \rho_{w,K|L}^{k+1} k_{K|L} \left(p_{w,K}^{k+1} - p_{w,L}^{k+1} \right) \left(g(p_{w,K}^{k+1}) - g(p_{w,L}^{k+1}) \right),$$
$$A^3 \geq \frac{1}{2}\sum_{k=0}^{N-1} \delta t \sum_{K\in\mathfrak{T}} \sum_{L\in N_D(K)} \tilde{\tau}_{K|L} \lambda_{n,K|L}^{up,k+1} \rho_{n,K|L}^{k+1} k_{K|L} \left(p_{n,K}^{k+1} - p_{n,L}^{k+1} \right) \left(h(p_{n,K}^{k+1}) - h(p_{n,L}^{k+1}) \right).$$

From the definition of the mass densities on the interface (3.32) one concludes

$$\rho_{n,K|L}^{k+1}(h(p_{n,K}^{k+1}) - h(p_{n,L}^{k+1})) = p_{n,K}^{k+1} - p_{n,L}^{k+1},$$
$$\rho_{w,K|L}^{k+1}(g(p_{w,K}^{k+1}) - g(p_{w,L}^{k+1})) = p_{w,K}^{k+1} - p_{w,L}^{k+1},$$

which leads to

$$\begin{aligned} A^2 + A^3 \geq &\frac{1}{2}\sum_{k=0}^{N-1} \delta t \sum_{K\in\mathfrak{T}} \sum_{L\in N_D(K)} \tilde{\tau}_{K|L} k_{K|L} \lambda_{w,K|L}^{up,k+1} (p_{w,K}^{k+1} - p_{w,L}^{k+1})^2 \\ &+ \frac{1}{2}\sum_{k=0}^{N-1} \delta t \sum_{K\in\mathfrak{T}} \sum_{L\in N_D(K)} \tilde{\tau}_{K|L} k_{K|L} \lambda_{n,K|L}^{up,k+1} (p_{n,K}^{k+1} - p_{n,L}^{k+1})^2. \end{aligned} \tag{3.71}$$

From Lemma 3.3.6 we can replace the phase upwind mobilities $\lambda_{\alpha,K|L}^{up,k+1}$ by the global upwind mobilities $\lambda_{\alpha,K|L}^{gup,k+1}$, and then using the boundedness of the functions ρ_n and ρ_w we obtain,

$$\begin{aligned}A^2+A^3 \geq \frac{1}{2\rho_M}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}\tilde{\tau}_{K|L}k_{K|L}\lambda_{w,K|L}^{gup,k+1}\overline{\rho}_{w,K|L}^{k+1}(p_{w,K}^{k+1}-p_{w,L}^{k+1})^2\\+\frac{1}{2\rho_M}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}\tilde{\tau}_{K|L}k_{K|L}\lambda_{n,K|L}^{gup,k+1}\overline{\rho}_{n,K|L}^{k+1}(p_{n,K}^{k+1}-p_{n,L}^{k+1})^2.\end{aligned}$$

Finally, by using Lemma 3.3.7 we derive estimates for the global pressure discrete gradient and the saturation potential discrete gradient

$$\begin{aligned}A^2+A^3 \geq \frac{\rho_m\lambda_m\omega_m^2k_m}{2\rho_M}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}\tilde{\tau}_{K|L}(p_K^{k+1}-p_L^{k+1})^2\\+\frac{C_\beta k_m}{2\rho_M}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}\tilde{\tau}_{K|L}(\beta(S_{w,K}^{k+1})-\beta(S_{w,L}^{k+1}))^2.\end{aligned}\tag{3.72}$$

3. Here we estimate the terms A^4 and A^5. Using Remark 3.2.7 and Proposition 3.3.2 for A^4 we get

$$\begin{aligned}A^4 &= \frac{1}{2}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}|\tilde{\sigma}_{K|L}|k_{K|L}\lambda_{w,K|L}^{G,k+1}\left(\rho_{w,K|L}^{G,k+1}\right)^2 g_{K|L}G_{w,K|L}^{k+1}(p_{w,L}^{k+1}-p_{w,K}^{k+1})\\&= \frac{1}{2}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}|\tilde{\sigma}_{K|L}|k_{K|L}\lambda_{w,K|L}^{G,k+1}\left(\rho_{w,K|L}^{G,k+1}\right)^2 g_{K|L}G_{w,K|L}^{k+1}\omega_{K|L}(p_L^{k+1}-p_K^{k+1})\\&-\frac{1}{2}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}|\tilde{\sigma}_{K|L}|k_{K|L}\lambda_{w,K|L}^{G,k+1}\left(\rho_{w,K|L}^{G,k+1}\right)^2 g_{K|L}G_{w,K|L}^{k+1}f_{n,K|L}^{k+1}(u_L^{k+1}-u_K^{k+1})\\&= A_I^4+A_{II}^4,\end{aligned}$$

where

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

In order to estimate the term A_I^4 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

$$A_I^4\leq CT|\Omega|+\frac{\varepsilon}{2}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}\tilde{\tau}_{K|L}|p_L^{k+1}-p_K^{k+1}|^2,$$

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 $f_{n,K|L}^{k+1}$ into the term A_{II}^4 we obtain

$$A_{II}^4 = \frac{1}{2}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)} |\tilde{\sigma}_{K|L}| k_{K|L} \lambda_{w,K|L}^{G,k+1}\left(\rho_{w,K|L}^{G,k+1}\right)^2 g_{K|L} G_{w,K|L}^{k+1}\int_{S_{w,L}^{k+1}}^{S_{w,K}^{k+1}} f_n(s, p_{K|L}^{k+1}) p_c'(s)\, ds.$$

In the case $g_{K|L} \geq 0$ we have $\lambda_{w,K|L}^{G,k+1} = \lambda_w(S_{w,K}^{k+1})$. If $S_{w,K}^{k+1} \geq S_{w,L}^{k+1}$ the term A_{II}^4 is nonpositive, so it can be neglected. If we have $S_{w,K}^{k+1} < S_{w,L}^{k+1}$, due to the monotonicity of the wetting phase mobility, we can estimate

$$\begin{aligned}
A_{II}^4 &\leq \frac{1}{2}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)} |\tilde{\sigma}_{K|L}| k_{K|L}\left(\rho_{w,K|L}^{G,k+1}\right)^2 g_{K|L} G_{w,K|L}^{k+1}\int_{S_{w,L}^{k+1}}^{S_{w,K}^{k+1}} \lambda_w(s) f_n(s, p_{K|L}^{k+1}) p_c'(s)\, ds \\
&\leq \frac{\rho_M^3 |g| k_M}{2\lambda_m \rho_m^2}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)} |\tilde{\sigma}_{K|L}| \left|\int_{S_{w,L}^{k+1}}^{S_{w,K}^{k+1}} \lambda_w(s)\lambda_n(s) p_c'(s)\, ds\right|.
\end{aligned}$$

In the case $g_{K|L} < 0$ we have $\lambda_{w,K|L}^{G,k+1} = \lambda_w(S_{w,L}^{k+1})$. If $S_{w,K}^{k+1} < S_{w,L}^{k+1}$ the term A_{II}^4 is negative and it can be neglected. If $S_{w,K}^{k+1} \geq S_{w,L}^{k+1}$ we obtain again

$$\begin{aligned}
A_{II}^4 &\leq \frac{1}{2}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)} |\tilde{\sigma}_{K|L}| k_{K|L}\left(\rho_{w,K|L}^{G,k+1}\right)^2 g_{K|L} G_{w,K|L}^{k+1}\int_{S_{w,L}^{k+1}}^{S_{w,K}^{k+1}} \lambda_w(s) f_n(s, p_{K|L}^{k+1}) p_c'(s)\, ds \\
&\leq \frac{\rho_M^3 |g| k_M}{2\lambda_m \rho_m^2}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)} |\tilde{\sigma}_{K|L}| \left|\int_{S_{w,L}^{k+1}}^{S_{w,K}^{k+1}} \lambda_w(s)\lambda_n(s) p_c'(s)\, ds\right|.
\end{aligned}$$

By using the same arguments as in term A_I^4 we obtain for arbitrary $\tilde{\varepsilon} > 0$

$$A_{II}^4 \leq CT|\Omega| + \frac{\tilde{\varepsilon}}{2}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)} \tilde{\tau}_{K|L} |\beta(S_{w,L}^{k+1}) - \beta(S_{w,K}^{k+1})|^2$$

with $C = C(\rho_M, \rho_m, \lambda_m, k_m, g, \tilde{\varepsilon})$, which leads to the estimate

$$\begin{aligned}
A^4 \leq CT|\Omega| &+ \frac{\varepsilon}{2}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)} \tilde{\tau}_{K|L} |p_L^{k+1} - p_K^{k+1}|^2 \\
&+ \frac{\tilde{\varepsilon}}{2}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)} \tilde{\tau}_{K|L} |\beta(S_{w,L}^{k+1}) - \beta(S_{w,K}^{k+1})|^2.
\end{aligned} \tag{3.73}$$

We now estimate the term A^5,

$$A^5 = -\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)} |\tilde{\sigma}_{K|L}| k_{K|L} \lambda_{n,K|L}^{G,k+1}\left(\rho_{n,K|L}^{G,k+1}\right)^2 g_{K|L} h(p_{n,K}^{k+1})$$

$$
\begin{aligned}
&= \frac{1}{2}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}|\tilde{\sigma}_{K|L}|k_{K|L}\lambda_{n,K|L}^{G,k+1}\left(\rho_{n,K|L}^{G,k+1}\right)^2 g_{K|L}(h(p_{n,L}^{k+1})-h(p_{n,K}^{k+1}))\\
&= \frac{1}{2}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}|\tilde{\sigma}_{K|L}|k_{K|L}\lambda_{n,K|L}^{G,k+1}\left(\rho_{n,K|L}^{G,k+1}\right)^2 g_{K|L}G_{n,K|L}^{k+1}(p_{n,L}^{k+1}-p_{n,K}^{k+1}),
\end{aligned}
$$

where we have again denoted

$$
G_{n,K|L}^{k+1} = \frac{h(p_{n,L}^{k+1})-h(p_{n,K}^{k+1})}{p_{n,L}^{k+1}-p_{n,K}^{k+1}}, \quad 0 < \frac{1}{\rho_M} \le G_{n,K|L}^{k+1} \le \frac{1}{\rho_m}.
$$

After introducing (3.53) we can write

$$
\begin{aligned}
A^5 &= \frac{1}{2}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}|\tilde{\sigma}_{K|L}|k_{K|L}\lambda_{n,K|L}^{G,k+1}\left(\rho_{n,K|L}^{G,k+1}\right)^2 g_{K|L}G_{n,K|L}^{k+1}\omega_{K|L}(p_L^{k+1}-p_K^{k+1})\\
&\quad + \frac{1}{2}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}|\tilde{\sigma}_{K|L}|k_{K|L}\lambda_{n,K|L}^{G,k+1}\left(\rho_{n,K|L}^{G,k+1}\right)^2 g_{K|L}G_{n,K|L}^{k+1}f_{w,K|L}^{k+1}(u_L^{k+1}-u_K^{k+1})\\
&= A_I^5 + A_{II}^5.
\end{aligned}
$$

The term A_I^5 is bounded as the term A_I^4, giving

$$
A_I^5 \le CT|\Omega| + \frac{\varepsilon}{2}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}\tilde{\tau}_{K|L}|p_L^{k+1}-p_K^{k+1}|^2,
$$

where $C = C(\lambda_M, \rho_M, \rho_m, |g|, \omega_M, k_M, \varepsilon)$. After introducing the definition of $f_{w,K|L}^{k+1}$ into the term A_{II}^5 we obtain

$$
A_{II}^5 = \frac{1}{2}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}|\tilde{\sigma}_{K|L}|k_{K|L}\lambda_{n,K|L}^{G,k+1}\left(\rho_{n,K|L}^{G,k+1}\right)^2 g_{K|L}G_{n,K|L}^{k+1}\int_{S_{w,K}^{k+1}}^{S_{w,L}^{k+1}} f_w(s,p_{K|L}^{k+1})p_c'(s)\,ds.
$$

In the case $g_{K|L} \ge 0$ we have $\lambda_{n,K|L}^{G,k+1} = \lambda_n(S_{w,K}^{k+1})$. If $S_{w,K}^{k+1} < S_{w,L}^{k+1}$ the term A_{II}^5 is nonpositive and it can be neglected. If $S_{w,K}^{k+1} \ge S_{w,L}^{k+1}$ we have, due to monotonicity of the nonwetting phase mobility,

$$
A_{II}^5 \le \frac{1}{2}\sum_{k=0}^{N-1}\delta t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}|\tilde{\sigma}_{K|L}|k_{K|L}\left(\rho_{n,K|L}^{G,k+1}\right)^2 g_{K|L}G_{n,K|L}^{k+1}\int_{S_{w,K}^{k+1}}^{S_{w,L}^{k+1}} \lambda_n(s)f_w(s,p_{K|L}^{k+1})p_c'(s)\,ds.
$$

In the case $g_{K|L} < 0$ we have $\lambda_{n,K|L}^{G,k+1} = \lambda_n(S_{w,L}^{k+1})$. In the case $S_{w,K}^{k+1} \ge S_{w,L}^{k+1}$ the term A_{II}^5 is nonpositive and it can be neglected. If $S_{w,K}^{k+1} < S_{w,L}^{k+1}$ we have, due to monotonicity of the nonwetting phase mobility

$$A_{II}^5 \le \frac{1}{2}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)} |\tilde{\sigma}_{K|L}| k_{K|L} \left(\rho_{n,K|L}^{G,k+1}\right)^2 g_{K|L} G_{n,K|L}^{k+1} \int_{S_{w,K}^{k+1}}^{S_{w,L}^{k+1}} \lambda_n(s) f_w(s, p_{K|L}^{k+1}) p_c'(s)\, ds.$$

Therefore, we conclude

$$A_{II}^5 \le \frac{\rho_M^3 |g| k_M}{2\lambda_m \rho_m^2}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)} |\tilde{\sigma}_{K|L}| \left| \int_{S_{w,L}^{k+1}}^{S_{w,K}^{k+1}} \lambda_w(s)\lambda_n(s) p_c'(s)\, ds \right|,$$

which leads to

$$A_{II}^5 \le CT|\Omega| + \frac{\tilde{\varepsilon}}{2}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)} \tilde{\tau}_{K|L} |\beta(S_{w,L}^{k+1}) - \beta(S_{w,K}^{k+1})|^2,$$

for any $\tilde{\varepsilon} > 0$ and $C = C(\rho_M, \rho_m, \lambda_m, k_m, g, \tilde{\varepsilon})$. Consequently

$$\begin{aligned} A^5 \le CT|\Omega| &+ \frac{\varepsilon}{2}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)} \tilde{\tau}_{K|L} |p_L^{k+1} - p_K^{k+1}|^2 \\ &+ \frac{\tilde{\varepsilon}}{2}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)} \tilde{\tau}_{K|L} |\beta(S_{w,L}^{k+1}) - \beta(S_{w,K}^{k+1})|^2. \end{aligned} \tag{3.74}$$

4. Finally we estimate A^6 and A^7.

Using the estimates $|\rho_w(p_w) g(p_w)| \le \frac{\rho_M}{\rho_m}|p_w|$ and $|\rho_n(p_n) h(p_n)| \le \frac{\rho_M}{\rho_m}|p_n|$ we get

$$A^7 \le C\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}} |K||F_{P,K}^{k+1}|(|S_{w,K}^{k+1} p_{w,K}^{k+1}| + |S_{n,K}^{k+1} p_{n,K}^{k+1}|).$$

By using Remark 1.3.3 and the fact that $F_P \in L^2(Q_T)$ we get

$$A^7 \le C\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}} |K||F_{P,K}^{k+1}|(|p_K^{k+1}| + M) \le C_1 + \frac{\varepsilon_1}{2}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}} |K||p_K^{k+1}|^2,$$

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

$$A^7 \le C_1 + \frac{\varepsilon_1 C_\Omega}{2}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)} \tilde{\tau}_{K|L} |p_K^{k+1} - p_L^{k+1}|^2. \tag{3.75}$$

We note that the wetting phase term in A^6 is nonpositive for $p_{w,K}^{k+1} \le 0$ and then it can be neglected. From the definition of the global pressure (3.10), (3.9) we have $p_w \le p \le |p|$. This fact, combined with $g(p_w) \le \frac{1}{\rho_m} p_w$ and $|h(p_n)| \le \frac{1}{\rho_m}|p_n|$, leads to

$$A^6 \le \frac{\rho_M}{\rho_m}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}} |K||F_{I,K}^{k+1}| \left(|p_K^{k+1}| + M\right) \le C_2 + \frac{\varepsilon_1}{2}\sum_{k=0}^{N-1}\delta t \sum_{K\in\mathfrak{T}} |K||p_K^{k+1}|^2,$$

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

$$A^6 \leq C_2 + \frac{\varepsilon_1 C_\Omega}{2} \sum_{k=0}^{N-1} \delta t \sum_{K\in\mathfrak{T}} \sum_{L\in N_D(K)} \tilde{\tau}_{K|L} |p_K^{k+1} - p_L^{k+1}|^2. \tag{3.76}$$

Finally, using (3.69), (3.72), (3.73), (3.74), (3.75), and (3.76)

$$\begin{aligned}
&\sum_{k=0}^{N-1} \sum_{K\in\mathfrak{T}} |K| \Phi_K \Big(\mathscr{H}(p_{n,K}^{k+1}, p_{w,K}^{k+1}) - \mathscr{H}(p_{n,K}^{k}, p_{w,K}^{k}) \Big) \\
&+ \frac{\rho_m \lambda_m \omega_m^2 k_m}{2\rho_M} \sum_{k=0}^{N-1} \delta t \sum_{K\in\mathfrak{T}} \sum_{L\in N_D(K)} \tilde{\tau}_{K|L} |p_K^{k+1} - p_L^{k+1}|^2 \\
&+ \frac{C_\beta k_m}{2\rho_M} \sum_{k=0}^{N-1} \delta t \sum_{K\in\mathfrak{T}} \sum_{L\in N_D(K)} \tilde{\tau}_{K|L} |\beta(S_K^{k+1}) - \beta(S_L^{k+1})|^2 \\
&\leq 2CT|\Omega| + \varepsilon \sum_{k=0}^{N-1} \delta t \sum_{K\in\mathfrak{T}} \sum_{L\in N_D(K)} \tilde{\tau}_{K|L} |p_L^{k+1} - p_K^{k+1}|^2 \\
&+ \tilde{\varepsilon} \sum_{k=0}^{N-1} \delta t \sum_{K\in\mathfrak{T}} \sum_{L\in N_D(K)} \tilde{\tau}_{K|L} |\beta(S_L^{k+1}) - \beta(S_K^{k+1})|^2 \\
&+ C_1 + C_2 + \varepsilon_1 C_\Omega \sum_{k=0}^{N-1} \delta t \sum_{K\in\mathfrak{T}} \sum_{L\in N_D(K)} \tilde{\tau}_{K|L} |p_K^{k+1} - p_L^{k+1}|^2.
\end{aligned}$$

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 (3.65).

The estimate (3.66) is obtained from (3.69), (3.71), (3.73), (3.74), (3.75), (3.76), and an application of the estimate (3.65).

□

Lemma 3.5.2. *There is a constant $C > 0$ such that $\mathscr{H}(p_n, p_w) \geq -C$, for all $p_w, p_n \in \mathbb{R}$.*

Proof. From the monotonicity of the phase pressures one can obtain $\rho_w(p_w)g(p_w) - p_w \geq 0$ and $\rho_n(p_n)h(p_n) - p_n \geq 0$. By Lemma 3.4.1 and the assumption (A.4) we get

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

□

Let us note that Theorem 3.5.1 and Lemma 3.5.2 proves the following corollary.

Corollary 3.5.3. *Let D_h be a finite volume discretization of $\Omega \times (0,T)$ and let $(p_{n,h}, p_{w,h})$ be a solution to the finite volume scheme (3.36)–(3.41). Then, there exists a constant $C > 0$, independent of h, such that the following estimates hold:*

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

3.6 Existence of a solution to the finite volume scheme

In this section we prove the existence of a solution of the finite volume scheme (3.36)–(3.41). The proof follows [76]. First we recall classical lemma that characterizes the zeros of a vector field (see [44]).

Lemma 3.6.1. *Assume the continuous function $v : \mathbb{R}^l \to \mathbb{R}^l$ satisfies*

$$v(x) \cdot x \geq 0, \quad \text{if } \|x\|_{\mathbb{R}^l} = r,$$

for some $r > 0$. Then there exists $x \in B(0,r)$ such that

$$v(x) = 0.$$

Proposition 3.6.2. *The finite volume scheme (3.36)–(3.41) admits at least one solution $(p_{n,K}^{k+1}, p_{w,K}^{k+1})_{K\in\mathcal{T}}$, $k \in \{0, \cdots, N-1\}$.*

Proof. First we introduce the following notation $\mathcal{M} = Card(\mathcal{T})$, $p_{n,\mathcal{M}} = \{p_{n,K}^{k+1}\}_{K\in\mathcal{T}} \in \mathbb{R}^{\mathcal{M}}$, $p_{w,\mathcal{M}} = \{p_{w,K}^{k+1}\}_{K\in\mathcal{T}} \in \mathbb{R}^{\mathcal{M}}$. We define the mapping $\mathcal{B}_h : \mathbb{R}^{\mathcal{M}} \times \mathbb{R}^{\mathcal{M}} \to \mathbb{R}^{\mathcal{M}} \times \mathbb{R}^{\mathcal{M}}$ as

$$\mathcal{B}_h(p_{n,\mathcal{M}}, p_{w,\mathcal{M}}) = \left(\{\mathcal{B}_{n,K}^{k+1}\}_{K\in\mathcal{T}}, \{\mathcal{B}_{w,K}^{k+1}\}_{K\in\mathcal{T}}\right),$$

where we have denoted

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

$$\mathcal{B}_{w,K}^{k+1} = |K|\Phi_K \frac{\rho_{w,K}^{k+1} S_{w,K}^{k+1} - \rho_{w,K}^{k} S_{w,K}^{k}}{\delta t} + \sum_{L\in N_D(K)} \tau_{K|L} k_{K|L} \lambda_{w,K|L}^{up,k+1} \rho_{w,K|L}^{up,k+1} \left(p_{w,K}^{k+1} - p_{w,L}^{k+1}\right)$$

$$+\sum_{L\in N_D(K)}|\sigma_{K|L}|k_{K|L}\lambda_{w,K|L}^{G,k+1}\left(\rho_{w,K|L}^{G,k+1}\right)^2 g_{K|L}-|K|\rho_{w,K}^{k+1}(S_{w,K}^{I,k+1}F_{I,K}^{k+1}-S_{w,K}^{k+1}F_{P,K}^{k+1}).$$

The function $\mathcal{B}_h$ is well defined and continuous. Let us introduce new vectors

$$v_{n,\mathcal{M}}=\{h(p_{n,K}^{k+1})\}_{K\in\mathcal{T}}\in\mathbb{R}^{\mathcal{M}},\quad v_{w,\mathcal{M}}=\{g(p_{w,K}^{k+1})\}_{K\in\mathcal{T}}\in\mathbb{R}^{\mathcal{M}}$$

and a mapping $\mathcal{F}(p_{n,\mathcal{M}},p_{w,\mathcal{M}})=(v_{n,\mathcal{M}},v_{w,\mathcal{M}})$ which is evidently bijective. The equation $\mathcal{B}_h(p_{n,\mathcal{M}},p_{w,\mathcal{M}})=0$ is equivalent to $\mathcal{P}_h(v_{n,\mathcal{M}},v_{w,\mathcal{M}})=\mathcal{B}_h\circ\mathcal{F}^{-1}(v_{n,\mathcal{M}},v_{w,\mathcal{M}})=0$ and we need only to show

$$\mathcal{P}_h(v_{n,\mathcal{M}},v_{w,\mathcal{M}})\cdot(v_{n,\mathcal{M}},v_{w,\mathcal{M}})\geq 0,\text{ for some }||(v_{n,\mathcal{M}},v_{w,\mathcal{M}})||_{\mathbb{R}^{2\mathcal{M}}}=r>0,$$

in order to apply Lemma 3.6.1. By the same reasoning as in proof of Theorem 3.5.1 we obtain

$$\mathcal{P}_h(v_{n,\mathcal{M}},v_{w,\mathcal{M}})\cdot(v_{n,\mathcal{M}},v_{w,\mathcal{M}})\geq\frac{1}{\delta t}\sum_{K\in\mathcal{T}}\Phi_K|K|\left(\mathscr{H}(p_{n,K}^{k+1},p_{w,K}^{k+1})-\mathscr{H}(p_{n,K}^{k},p_{w,K}^{k})\right)$$
$$+C\left(\|p_h^{k+1}\|_{H_h(\Omega)}^2+\|\beta(S_{w,h}^{k+1})\|_{H_h(\Omega)}^2\right)-C',$$

for some constants $C,C'>0$. After applying Lemma 3.5.2, we obtain

$$\mathcal{P}_h(v_{n,\mathcal{M}},v_{w,\mathcal{M}})\cdot(v_{n,\mathcal{M}},v_{w,\mathcal{M}})\geq-\frac{1}{\delta t}\sum_{K\in\mathcal{T}}\Phi_K|K|\mathscr{H}(p_{n,K}^{k},p_{w,K}^{k})+C\|p_h^{k+1}\|_{H_h(\Omega)}^2-C'',\quad(3.77)$$

where $C''>0$. Since the functions ρ_n,ρ_w are bounded from below we have $|h(p_n)|\leq 1/\rho_m|p_n|$ and $|g(p_w)|\leq 1/\rho_m|p_w|$, which leads to

$$||(v_{n,\mathcal{M}},v_{w,\mathcal{M}})||_{\mathbb{R}^{2\mathcal{M}}}^2=||(h(p_{n,\mathcal{M}}),g(p_{w,\mathcal{M}}))||_{\mathbb{R}^{2\mathcal{M}}}^2\leq C_1\left(\|p_{n,h}^{k+1}\|_{L^2(\Omega)}^2+\|p_{w,h}^{k+1}\|_{L^2(\Omega)}^2\right)$$
$$\leq 2C_1\left(\|p_h^{k+1}\|_{L^2(\Omega)}^2+C_2\right)\leq 2C_3\left(\|p_h^{k+1}\|_{H_h(\Omega)}^2+C_2\right),$$

since, due to (A.4) and (3.10), (3.9), $|p_w|$ and $|p_n|$ can be bounded by $|p|+M$, for some constant M. With this inequality (3.77) becomes

$$\mathcal{P}_h(v_{n,\mathcal{M}},v_{w,\mathcal{M}})\cdot(v_{n,\mathcal{M}},v_{w,\mathcal{M}})\geq-\frac{1}{\delta t}\sum_{K\in\mathcal{T}}\Phi_K|K|\mathscr{H}(p_{n,K}^{k},p_{w,K}^{k})+C_4||(v_{n,\mathcal{M}},v_{w,\mathcal{M}})||_{\mathbb{R}^{2\mathcal{M}}}^2-C_5,$$

for some $C_4,C_5>0$. Note that the first term on the right-hand side in this inequality is independent of $||(v_{n,\mathcal{M}},v_{w,\mathcal{M}})||_{\mathbb{R}^{2\mathcal{M}}}$, and therefore we conclude

$$\mathcal{P}_h(v_{n,\mathcal{M}},v_{w,\mathcal{M}})\cdot(v_{n,\mathcal{M}},v_{w,\mathcal{M}})\geq 0,$$

for some $r=||(v_{n,\mathcal{M}},v_{w,\mathcal{M}})||_{\mathbb{R}^{2\mathcal{M}}}>0$ large enough. The existence of a solution to (3.36)–(3.41) follows from Lemma 3.6.1. □

3.7 Compactness result

In this section we prove a strong convergence of the finite volume approximation by applying the compactness theorem of Kolmogorov, M. Riesz and Fréchet. This is an often used technique that can be found in [45] and [76]. For convenience we recall the version of the theorem that will be used.

We set $(\tau_h f)(x) = f(x+h)$, $x \in \mathbb{R}^l$ and $h \in \mathbb{R}^l$. We will also use notation $\Omega' \Subset \Omega$ for Ω' compactly contained in Ω.

Theorem 3.7.1. *([31]). Let Ω be an open set in $\mathbb{R}^l$ and let $\mathscr{F}$ be a bounded set in $L^p(\Omega)$ with $1 \le p < \infty$. Assume that*

1. *For all $\varepsilon > 0$ and for all $\Omega' \Subset \Omega$ there exists $\delta < d(\Omega', \partial\Omega)$ such that*

$$\forall h \in \mathbb{R}^l,\ |h| < \delta,\ \forall f \in \mathscr{F}, \quad \|\tau_h f - f\|_{L^p(\Omega')} < \varepsilon. \tag{3.78}$$

2. *For all $\varepsilon > 0$ there exists $\Omega' \Subset \Omega$ such that*

$$\forall f \in \mathscr{F}, \quad \|f\|_{L^p(\Omega \setminus \Omega')} < \varepsilon. \tag{3.79}$$

Then $\mathscr{F}$ is relatively compact in $L^p(\Omega)$.

Since we will apply Theorem 3.7.1 to a family of bounded functions, depending on x and t, it will be convenient to use the following specialization of Theorem 3.7.1 which is sufficient for our goals.

Corollary 3.7.2. *Let Ω be an open set in $\mathbb{R}^l$ and $0 < T < \infty$. Let $\mathscr{F}$ be a bounded set in $L^1(\Omega \times (0,T))$. Assume that*

1. *For all $\varepsilon > 0$ and for all $\Omega' \Subset \Omega$ there exists $\delta < d(\Omega', \partial\Omega)$ such that*

$$\forall h \in \mathbb{R}^l,\ |h| < \delta,\ \forall f \in \mathscr{F}, \quad \int_0^T \int_{\Omega'} |f(x+h,t) - f(x,t)|\, dxdt < \varepsilon; \tag{3.80}$$

2. *For all $\varepsilon > 0$ and for all $\Omega' \Subset \Omega$ there exists $0 < \Delta < T$ such that*

$$\forall 0 < \tau < \Delta,\ \forall f \in \mathscr{F}, \quad \int_0^{T-\tau} \int_{\Omega'} |f(x,t+\tau) - f(x,t)|\, dxdt < \varepsilon; \tag{3.81}$$

3. For all $\varepsilon > 0$ *there exists* $\Omega' \Subset \Omega$ *such that*

$$\forall f \in \mathscr{F}, \quad \int_0^T \int_{\Omega \setminus \Omega'} |f(x,t)|\, dxdt < \varepsilon. \tag{3.82}$$

Then $\mathscr{F}$ *is relatively compact in* $L^1(\Omega \times (0,T))$.

Proof. Choose $\varepsilon > 0$ and $Q' \Subset Q = \Omega \times (0,T)$. Then one can find $\Omega' \Subset \Omega$ and $\eta_0, \eta_1 > 0$ such that $Q' \subset \Omega' \times (\eta_0, T - \eta_1)$. Let us choose δ in (3.80) which corresponds to $\varepsilon/2$ and Δ in (3.81), $\Delta < \min(\eta_0, \eta_1)$ which corresponds to $\varepsilon/2$. Then for $\mathbf{H} = (h, \tau)$ which satisfies $|h| < \delta$ and $|\tau| < \Delta$ we have

$$\begin{aligned} \int_{\eta_0}^{T-\eta_1} \int_{\Omega'} |f(x+h,t+\tau) - f(x,t)|\, dxdt &\le \int_0^T \int_{\Omega'} |f(x+h,t+\tau) - f(x,t+\tau)|\, dxdt \\ &+ \int_{\eta_0}^{T-\eta_1} \int_{\Omega'} |f(x,t+\tau) - f(x,t)|\, dxdt < \varepsilon. \end{aligned}$$

From (3.82) follows (3.79) which completes the proof. □

In the proof of Theorem 3.7.9 we need the following technical result (see [45], Lemma 9.3).

Lemma 3.7.3. *Let* D_h *be a finite volume discretization on* $\Omega \times (0,T)$. *Then there are constants* $\delta > 0$ *and* $C > 0$, *independent of discretization parameter h, such that for any* $u_h \in X(\mathcal{T}, \delta t)$ *and any* $y \in \mathbb{R}^l$, $|y| < \delta$ *it holds*

$$\int_{\Omega' \times (0,T)} |u_h(x+y,t) - u_h(x,t)|^2\, dxdt \le C|y|(|y| + h) \sum_{k=0}^{N_h - 1} \delta t \sum_{\sigma \in \mathscr{E}_I} \tau_\sigma |u_L^{k+1} - u_K^{k+1}|^2. \tag{3.83}$$

where $\Omega' = \{x \in \Omega, [x, x+y] \subset \Omega\}$.

Proof. Here we give for completeness a brief version of a proof of the Lemma 9.3 from [45]. First one defines, for $\sigma \in \mathscr{E}_I$, the indicator function $\chi_\sigma : \Omega' \times \mathbb{R}^l \to \{0,1\}$ by

$$\chi_\sigma(x,y) = \begin{cases} 1 & \text{if } [x,y] \cap \sigma \neq \emptyset \\ 0 & \text{if } [x,y] \cap \sigma = \emptyset. \end{cases}$$

For $y \in \mathbb{R}^l$, $y \neq 0$, one has

$$|u_h(x+y,t) - u_h(x,t)| \le \sum_{\sigma \in \mathscr{E}_I} \chi_\sigma(x, x+y) |u_L^{k+1} - u_K^{k+1}|, \quad \text{for a.e. } x \in \Omega,$$

where L and K are such that $\sigma = \sigma_{K|L}$ and $k \in \{0, 1, \ldots, N_h - 1\}$ such that $t^k < t \le t^{k+1}$. By using the Cauchy-Schwarz inequality, one obtains

$$|u_h(x+y,t) - u_h(x,t)|^2 \le \sum_{\sigma \in \mathscr{E}_I} \chi_\sigma(x, x+y) \frac{|u_L^{k+1} - u_K^{k+1}|^2}{d_{K|L} c_\sigma} \sum_{\sigma \in \mathscr{E}_I} \chi_\sigma(x, x+y) d_{K|L} c_\sigma, \tag{3.84}$$

where $c_\sigma = \left| \mathbf{n}_\sigma \cdot \frac{y}{|y|} \right|$, and $\mathbf{n}_\sigma$ denotes the unit outer normal vector to $\sigma = \sigma_{K|L}$. In [45] it has been shown that there is $C > 0, C = C(\Omega)$, such that

$$\sum_{\sigma \in \mathscr{E}_I} \chi_\sigma(x, x+y) d_{K|L} c_\sigma \le |y| + C \text{size}(\mathcal{T}_h), \qquad \int_{\Omega'} \chi_\sigma(x, x+y)\, dx \le |\sigma| c_\sigma |y|,$$

for a.e. $x \in \Omega$. Integrating (3.84) over Ω' and applying the last two estimates we get (3.83). □

Let us define functions

$$U_h = \rho_w(p_{w,h}) S_{w,h}, \quad V_h = \rho_n(p_{n,h}) S_{n,h}. \tag{3.85}$$

Proposition 3.7.4. *Let D_h be a finite volume discretization on $\Omega \times (0,T)$ and let $(p_{n,h}, p_{w,h})$ be a solution to (3.37)–(3.38). Then we have*

$$\int_{\Omega' \times (0,T)} |U_h(x+y,t) - U_h(x,t)|\, dxdt \le \omega(|y|), \tag{3.86}$$

$$\int_{\Omega' \times (0,T)} |V_h(x+y,t) - V_h(x,t)|\, dxdt \le \omega(|y|), \tag{3.87}$$

for all $y \in \mathbb{R}^l$ and $\Omega' = \{x \in \Omega, [x, x+y] \subset \Omega\}$ and $\omega(|y|) \to 0$ when $|y| \to 0$.

Proof. Let us denote $S_1 = S_w(x+y,t)$, $S_2 = S_w(x,t)$, $p_1 = p(x+y,t)$, and $p_2 = p(x,t)$. From the definition of the function V and (A.5) we have (for simplicity we also omit writing dependence on h)

$$\begin{aligned}
|V(x+y,t) - V(x,t)| &\le |(\rho_n(p_n(S_1,p_1)) - \rho_n(p_n(S_1,p_2)))(1-S_1)| \\
&\quad + |(\rho_n(p_n(S_1,p_2)) - \rho_n(p_n(S_2,p_2)))(1-S_1)| \\
&\quad + |\rho_n(p_n(S_2,p_2))[(1-S_1) - (1-S_2)]| \\
&\le \rho_M^d |p_n(S_1,p_1) - p_n(S_1,p_2)| \\
&\quad + \rho_M^d |p_n(S_1,p_2) - p_n(S_2,p_2)| + \rho_M |S_2 - S_1| \\
&\le \rho_M^d \omega_M |p_1 - p_2| + \rho_M^d \left| \int_{S_1}^{S_2} f_w(s,p_2) p_c'(s)\, ds \right| + \rho_M |S_2 - S_1|.
\end{aligned}$$

Using (A.5) we can conclude that there exists a constant $C > 0$ such that

$$\begin{aligned}
&\int_{\Omega' \times (0,T)} |V(x+y,t) - V(x,t)|\, dxdt \\
&\qquad \le C \left(\int_{\Omega' \times (0,T)} |S_w(x+y,t) - S_w(x,t)|\, dxdt + \int_{\Omega' \times (0,T)} |p(x+y,t) - p(x,t)|\, dxdt \right) \\
&\qquad = E_1 + E_2.
\end{aligned}$$

The term E_1 can be estimated due to (A.7) as ($\tau < 1$)

$$\begin{aligned}
E_1 &\le C \int_{\Omega' \times (0,T)} |\beta(S_w(x+y,t)) - \beta(S_w(x,t))|^{\tau}\, dxdt \\
&\le C \left(\int_{\Omega' \times (0,T)} |\beta(S_w(x+y,t)) - \beta(S_w(x,t))|\, dxdt \right)^{\tau}.
\end{aligned}$$

From Lemma 3.7.3 and the a priori estimate (3.65) we get

$$E_1 \le C \left(|y|(y + |h|) \sum_{k=0}^{N_h - 1} \delta t \sum_{\sigma \in \mathscr{E}_I} \tau_\sigma |\beta(S_{w,L}^{k+1}) - \beta(S_{w,K}^{k+1})|^2 \right)^{\tau} \le C\,(|y|(y + |h|))^{\tau}.$$

In the same way we have

$$E_2 \le C|y|(|y| + |h|) \sum_{k=0}^{N_h - 1} \delta t \sum_{\sigma \in \mathscr{E}_I} \tau_\sigma |p_L^{k+1} - p_K^{k+1}|^2 \le C|y|(|y| + |h|),$$

leading to

$$\int_{\Omega' \times (0,T)} |V_h(x+y,t) - V_h(x,t)|\, dxdt \le C((|y|(y + |h|))^{\tau} + |y|(y + |h|)).$$

The proof of (3.86) is similar to that of (3.87) and thus omitted. □

We define piecewise linear in time representations of U_h and V_h as,

$$\overline{U}_h(x,t) = \sum_{k=0}^{N_h - 1} \sum_{K \in \mathfrak{T}_h} \left(\frac{t - t^k}{\delta t} U_K^{k+1} + \frac{t^{k+1} - t}{\delta t} U_K^k \right) \mathbf{1}_{Q_K^k}(x,t), \tag{3.88}$$

$$\overline{V}_h(x,t) = \sum_{k=0}^{N_h - 1} \sum_{K \in \mathfrak{T}_h} \left(\frac{t - t^k}{\delta t} V_K^{k+1} + \frac{t^{k+1} - t}{\delta t} V_K^k \right) \mathbf{1}_{Q_K^k}(x,t), \tag{3.89}$$

where we have denoted $Q_K^k = K \times (t^k, t^{k+1}]$.

Remark 3.7.5. *By simple calculation for any $\Omega' \subset \Omega$ one get*

$$\begin{aligned}\int_0^T \int_{\Omega'} |\overline{V}_h(x+y,t) - \overline{V}_h(x,t)|\, dxdt \le & \int_0^T \int_{\Omega'} |V_h(x+y,t) - V_h(x,t)|\, dxdt \\ & + \frac{\delta t}{2} \int_{\Omega'} |V_h(x+y,0) - V_h(x,0)|\, dx,\end{aligned} \tag{3.90}$$

$$\begin{aligned}\int_0^T \int_{\Omega'} |V_h(x,t) - \overline{V}_h(x,t)|\, dx dt = & \frac{\delta t}{2} \sum_{k=0}^{N_h-1} \int_{\Omega'} |V^{k+1} - V^k|\, dx \\ & \le 2 \int_0^{T-\delta t} \int_{\Omega'} |\overline{V}_h(x,t+\delta t) - \overline{V}_h(x,t)|\, dx dt,\end{aligned} \tag{3.91}$$

and the same inequalities hold for $\overline{U}_h$.

Corollary 3.7.6. *Let D_h be a finite volume discretization on $\Omega \times (0,T)$ and let $(p_{n,h}, p_{w,h})$ be a solution to (3.36)–(3.41). Then we have*

$$\int_{\Omega' \times (0,T)} |\overline{U}_h(x+y,t) - \overline{U}_h(x,t)|\, dxdt \le \omega(|y|), \tag{3.92}$$

$$\int_{\Omega' \times (0,T)} |\overline{V}_h(x+y,t) - \overline{V}_h(x,t)|\, dxdt \le \omega(|y|), \tag{3.93}$$

for all $y \in \mathbb{R}^l$ and $\Omega' = \{x \in \Omega, [x, x+y] \subset \Omega\}$ and $\omega(|y|) \to 0$ when $|y| \to 0$.

Proof. To the first term on the right-hand side in (3.90) we can apply (3.87), to obtain

$$\int_{\Omega' \times (0,T)} |\overline{V}_h(x+y,t) - \overline{V}_h(x,t)|\, dxdt \le \omega(|y|) + \frac{\delta t}{2} \int_{\Omega'} |V_h(x+y,0) - V_h(x,0)|\, dx. \tag{3.94}$$

In the second term on the right-hand side in (3.94) we note that $V_h(x,0) = \rho_n(p^0_{n,h}) S^0_{n,h}$ and therefore it can be bounded as follows:

$$\begin{aligned}& \int_{\Omega'} |V_h(x+y,0) - V_h(x,0)|\, dx \\ & \qquad \le C \left(\int_{\Omega'} |p^0_{n,h}(x+y) - p^0_{n,h}(x)|\, dx + \int_{\Omega'} |S^0_{n,h}(x+y) - S^0_{n,h}(x)|\, dx \right),\end{aligned} \tag{3.95}$$

where the constant C depends only on ρ_M and ρ_M^d (see (A.5)). The functions $p^0_{n,h}$, $p^0_{w,h}$ and $S^0_{n,h}$ are given by (3.41) and from the properties of the mean value operator it follows, for $\alpha \in \{w, n\}$,

$$\int_{\Omega'} |p^0_{\alpha,h}(x+y) - p^0_{\alpha,h}(x)|\, dx \le \int_{\Omega} |p^0_{\alpha}(x+y) - p^0_{\alpha}(x)|\, dx. \tag{3.96}$$

The boundedness of the capillary pressure derivative will give

$$\int_{\Omega'} |S^0_{\alpha,h}(x+y) - S^0_{\alpha,h}(x)|\,dx \le C \int_{\Omega} |p^0_c(x+y) - p^0_c(x)|\,dx, \tag{3.97}$$

therefore we obtain

$$\int_{\Omega'} |V_h(x+y,0) - V_h(x,0)|\,dx \le C \left(\int_{\Omega} |p^0_\alpha(x+y) - p^0_\alpha(x)|\,dx + \int_{\Omega} |p^0_c(x+y) - p^0_c(x)|\,dx \right).$$

By using the continuity of the translations in $L^1(\Omega)$ (see [42]) it follows that the second integral in (3.94) goes to zero as $|y| \to 0$ uniformly in size($\mathcal{T}$). This proves (3.93), and (3.92) is proved in the same way.

□

Proposition 3.7.7. *Let D_h be a finite volume discretization on $\Omega \times (0,T)$ and let $(p_{n,h}, p_{w,h})$ be a solution to (3.36)–(3.41). For fixed $\Omega' \Subset \Omega$ we have*

$$\int_{\Omega' \times (0,T-\tau)} |\overline{U}_h(x,t+\tau) - \overline{U}_h(x,t)|\,dxdt \le \omega(\tau), \tag{3.98}$$

$$\int_{\Omega' \times (0,T-\tau)} |\overline{V}_h(x,t+\tau) - \overline{V}_h(x,t)|\,dxdt \le \omega(\tau), \tag{3.99}$$

for all $\tau \in (0,T)$ and $\omega(\tau) \to 0$ when $\tau \to 0$.

Proof. By following the proof of Proposition 5.1. from [12], we first write (3.37) in the following form

$$\Phi_K \frac{\rho^{k+1}_{n,K} S^{k+1}_{n,K} - \rho^k_{n,K} S^k_{n,K}}{\delta t} = \frac{1}{|K|} \sum_{L \in N_D(K)} |\sigma_{K|L}| \vec{\mathscr{F}}^{k+1}_{K|L} \cdot \eta_{K|L} + F^{k+1}_{n,K}, \tag{3.100}$$

where we have introduced

$$\vec{\mathscr{F}}^{k+1}_{K|L} = -k_{K|L} \left(\lambda^{up,k+1}_{n,K|L} \rho^{up,k+1}_{n,K|L} \frac{p^{k+1}_{n,K} - p^{k+1}_{n,L}}{d_{K|L}} + \lambda^{G,k+1}_{n,K|L} \left(\rho^{G,k+1}_{n,K|L}\right)^2 g_{K|L} \right) \eta_{K|L}.$$

Additionally, we use the following notation

$$\vec{\mathscr{F}}_h := \sum_{k=0}^{N_h-1} \sum_{\sigma=K|L} \vec{\mathscr{F}}^{k+1}_{K|L} \mathbf{1}_{(t^k,t^{k+1}] \times T_{K|L}}, \quad f_h = \sum_{k=0}^{N_h-1} \sum_{K \in \mathcal{T}_h} F^{k+1}_{n,K} \mathbf{1}_{(t^k,t^{k+1}] \times K}.$$

If we extend $\overline{U}_h$ by the $U^{N_h+1}_h$ for $t > \delta t N_h$ and $\vec{\mathscr{F}}_h$ and f_h by zero for $t > \delta t N_h$ and by using discrete divergence definition (3.28) we can rewrite equations (3.100) in the following form

$$\Phi_h \partial_t \overline{U}_h = \mathrm{div}_h \vec{\mathscr{F}}_h + f_h. \tag{3.101}$$

The rest of the proof is the same as the proof of Lemma 4.6. from [62] with slight modification regarding the definition of the function U_h and is based on the construction of the function $\omega(\tau)$ which satisfies (3.98). First, we fix $h > 0$ and set

$$I_h(\tau) = \int_0^{+\infty} \int_{\Omega'} |\overline{U}_h(x,t+\tau) - \overline{U}_h(x,t)|\, dxdt = \int_0^{+\infty} \int_{\Omega'} |W_h(\cdot,t)|\, dxdt, \qquad (3.102)$$

where the function $W_h(\cdot,t)$ is defined by

$$W_h(\cdot,t) = \overline{U}_h(\cdot,t+\tau) - \overline{U}_h(\cdot,t), \quad t > 0.$$

For t large enough $W_h(\cdot,t) = 0$ due to the extension of the function $\overline{U}_h(\cdot,t)$ by $U_h^{N_h+1}$ for $t > \delta t N_h$. The next step in the proof is the usage of mollifiers $(\rho_\delta)_\delta$ on $\mathbb{R}^l$ which are defined by

$$\rho_\delta(x) = \delta^{-l}\rho(x/\delta) \;\text{ with }\; \rho \in C_c^\infty(\mathbb{R}^l),\ \operatorname{supp}\rho \subset \overline{B(0,1)},\ \rho \geq 0, \;\text{ and }\; \int_{\mathbb{R}^l} \rho(x)\, dx = 1.$$

Obviously ρ_δ satisfies $|\nabla\rho_\delta| \leq C/\delta^{l+1}$, where C does not depend on h and δ. One then defines the function $\varphi(\cdot,t) : \mathbb{R}^l \to \mathbb{R}$ by

$$\varphi(t) := \rho_\delta \star (\operatorname{sign} W_h(t) \mathbf{1}_{\Omega'}),$$

and the corresponding discrete function by $\varphi_K(t) = \frac{1}{|K|}\int_K \varphi(x,t)\, dx$. From the definition of the function $\varphi(\cdot,t)$ one can conclude that $\varphi_h(t)$ is null on the set $\{x \in \Omega : d(x,\overline{\Omega'}) \geq \delta + \operatorname{size}(\mathfrak{T}_h)\}$, for all t, which means that for all sufficiently small h and δ, $\operatorname{supp}\varphi_h(t) \subset \Omega'' \Subset \Omega$.

The next step of the proof is multiplication of the equation (3.101) by the $|K|\varphi_K(s)$, integration in t over $[s, s+\tau]$, summation over all K, and integration in s over $\langle 0, +\infty\rangle$ to obtain

$$\int_0^{+\infty} \sum_{K\in\mathfrak{T}_h} \Phi_K |K| \varphi_K(s) W_K(s)\, ds = \int_0^{+\infty} \int_s^{s+\tau} \sum_{K\in\mathfrak{T}_h} |K|\varphi_K(s) \left(\operatorname{div}_K \vec{\mathscr{F}}_h(t) + (f_h(t))_K\right) dtds. \qquad (3.103)$$

Like in [62] we define $Q'' = (0, N_h\delta t) \times \Omega''$ and introduce

$$I_h^\delta(\tau) = \int_0^{+\infty} \int_{\Omega'} \varphi_h(x,s) W_h(x,s)\, dxds \leq \frac{1}{\Phi_m} \int_0^{+\infty} \sum_{K\in\mathfrak{T}_h} \Phi_K |K| \varphi_K(s) W_K(s)\, ds.$$

Now we have

$$\Phi_m I_h^\delta(\tau) \leq \int_0^{+\infty} \int_s^{s+\tau} \sum_{K\in\mathfrak{T}_h} \sum_{L\in N_D(K)} |\sigma_{K|L}| \varphi_K(s) k_{K|L} \lambda_{n,K|L}^{up}(t) \rho_{n,K|L}^{up}(t) \frac{p_{n,L}(t) - p_{n,K}(t)}{d_{K|L}}\, dtds$$

$$
\begin{aligned}
&- \int_0^{+\infty}\int_s^{s+\tau} \sum_{K\in\mathfrak{T}_h}\sum_{L\in N_D(K)} |\sigma_{K|L}|\varphi_K(s)k_{K|L}\lambda^G_{n,K|L}(t)\left(\rho^G_{n,K|L}(t)\right)^2 g_{K|L}\,dtds \\
&+ \int_0^{+\infty}\int_s^{s+\tau} \sum_{K\in\mathfrak{T}_h} \varphi_K(s)F_{n,K}(t)\,dtds.
\end{aligned}
$$

If we gather by the edges we get

$$
\begin{aligned}
&\Phi_m I_h^\delta(\tau) \le \\
&\frac{1}{2}\int_0^{+\infty}\int_s^{s+\tau} \sum_{K\in\mathfrak{T}_h}\sum_{L\in N_D(K)} \tilde{\tau}_{K|L}k_{K|L}\lambda^{up}_{n,K|L}(t)\rho^{up}_{n,K|L}(t)\left(\varphi_K(s)-\varphi_L(s)\right)\left(p_{n,L}(t)-p_{n,K}(t)\right)dtds \\
&+\frac{1}{2}\int_0^{+\infty}\int_s^{s+\tau} \sum_{K\in\mathfrak{T}_h}\sum_{L\in N_D(K)} |\tilde{\sigma}_{K|L}|k_{K|L}\lambda^G_{n,K|L}(t)\left(\rho^G_{n,K|L}(t)\right)^2 \frac{\varphi_L(s)-\varphi_K(s)}{d_{K|L}} d_{K|L}g_{K|L}\,dtds \\
&+\int_0^{+\infty}\int_s^{s+\tau} \sum_{K\in\mathfrak{T}_h} \varphi_K(s)F_{n,K}(t)\,dtds = I+II+III.
\end{aligned}
$$

The term I can be estimated as follows,

$$
\begin{aligned}
I \le \frac{1}{2}\int_0^{+\infty}\int_s^{s+\tau} &\sum_{K\in\mathfrak{T}_h}\sum_{L\in N_D(K)} \tilde{\tau}_{K|L}k_{K|L}\lambda^{up}_{n,K|L}(t)\rho^{up}_{n,K|L}(t)|\varphi_K(s)-\varphi_L(s)|^2\,dtds \\
+\frac{1}{2}\int_0^{+\infty}\int_s^{s+\tau} &\sum_{K\in\mathfrak{T}_h}\sum_{L\in N_D(K)} \tilde{\tau}_{K|L}k_{K|L}\lambda^{up}_{n,K|L}(t)\rho^{up}_{n,K|L}(t)|p_{n,K}(t)-p_{n,L}(t)|^2\,dtds.
\end{aligned}
$$

By using the boundedness of the functions λ_n and ρ_n, this can be further estimated as

$$
\begin{aligned}
I \le \frac{1}{2}k_M\lambda_M\rho_M\tau\int_0^{+\infty} &\sum_{K\in\mathfrak{T}_h}\sum_{L\in N_D(K)} \tilde{\tau}_{K|L}|\varphi_K(s)-\varphi_L(s)|^2\,ds \\
+\frac{1}{2}k_M\rho_M\int_0^{+\infty}\int_s^{s+\tau} &\sum_{K\in\mathfrak{T}_h}\sum_{L\in N_D(K)} \tilde{\tau}_{K|L}\lambda^{up}_{n,K|L}(t)|p_{n,K}(t)-p_{n,L}(t)|^2\,dtds.
\end{aligned}
\tag{3.104}
$$

In the second term on the right-hand side of (3.104), we apply the Fubini theorem

$$
\begin{aligned}
\int_0^{+\infty}\int_s^{s+\tau} &\lambda^{up}_{n,K|L}(t)|p_{n,K}(t)-p_{n,L}(t)|^2\,dtds \\
&= \int_0^{+\infty}\int_{\max(0,t-\tau)}^{t} \lambda^{up}_{n,K|L}(t)|p_{n,K}(t)-p_{n,L}(t)|^2\,dsdt \\
&\le \tau\int_0^{+\infty} \lambda^{up}_{n,K|L}(t)|p_{n,K}(t)-p_{n,L}(t)|^2\,dt,
\end{aligned}
$$

and by the energy estimate (3.66), we obtain

$$
I \le C\tau\left(\|\varphi_h\|^2_{L^2(0,T;H_h(\Omega))}+1\right) \le C\tau\left(\|\nabla\varphi_h\|^2_{L^2(Q'')}+1\right) \le C\tau(1+\delta^{-2l-2}). \tag{3.105}
$$

In the second term, from the boundedness of the functions λ_n and ρ_n we conclude

$$II \leq \frac{C}{2}\int_0^{+\infty}\int_s^{s+\tau}\sum_{K\in\mathfrak{T}_h}\sum_{L\in N_D(K)}|\tilde{T}_{K|L}|\frac{|\varphi_L(s)-\varphi_K(s)|}{d_{K|L}}dtds \leq C\tau\|\nabla\varphi_h\|_{L^1(Q'')} \leq C\tau\delta^{-l-1}. \tag{3.106}$$

The third term can be estimated as

$$III \leq \frac{1}{2}\int_0^{+\infty}\int_s^{s+\tau}\sum_{K\in\mathfrak{T}_h}|\varphi_K(s)|^2\,dtds + \frac{1}{2}\int_0^{+\infty}\int_s^{s+\tau}\sum_{K\in\mathfrak{T}_h}|F_{n,K}(t)|^2\,dtds. \tag{3.107}$$

After applying the Fubini theorem to the second integral in (3.107) we have

$$III \leq C\tau(1+\|f_h\|^2_{L^2(Q'')}). \tag{3.108}$$

By combining (3.105), (3.106), and (3.108) we obtain

$$I_h^\delta(\tau) \leq C\tau(1+\delta^{-2l-2}), \tag{3.109}$$

for all h and δ small enough, uniformly in h.

We want to estimate (3.102) by estimating the difference

$$I_h(\tau)-I_h^\delta(\tau) = \int_0^{+\infty}\int_{\Omega'}(|W_h(x,t)|-W_h(x,t)\varphi(x,t))\,dxdt. \tag{3.110}$$

Let us denote $U'_\delta := \{x\in\mathbb{R}^l : d(x,\partial\Omega') < \delta\}$ such that $U'_\delta \subset \Omega'' \subset \Omega$ for all δ small enough. Without loss of generality, one can assume that the boundary of Ω' can be chosen regular enough so that $|U'_\delta| \to 0$ as $\delta \to 0$. Corollary 3.7.6 and the Frechet-Kolomogorov theorem give relative compactness in $L^1_{loc}(\Omega)$ of the family $\left(\int_0^{+\infty}|W_h(\cdot,t)|\,dt\right)_h$, which leads to equi-integrability of these functions on Ω'', see [47], meaning that

$$\int_0^{+\infty}\int_{U'_\delta}|W_h(x,t)|\,dxdt \leq \hat{\omega}(\delta), \quad \text{uniformly in } h \text{ with } \lim_{\delta\to 0}\hat{\omega}(\delta)=0.$$

By using the definition of φ one concludes

$$\begin{aligned}\left|I_h(\tau)-I_h^\delta(\tau)\right| &\leq 2\hat{\omega}(\delta)+\int_0^{+\infty}\int_{\Omega'\setminus U'_\delta}||W_h(x,t)|-W_h(x,t)(\rho_\delta\star\operatorname{sign}W_h(t))(x)|\,dxdt\\ &\leq 2\hat{\omega}(\delta)+\int_0^{+\infty}\int_{\Omega'\setminus U'_\delta}\int_{\mathbb{R}^l}\rho_\delta(x-y)\,||W_h(x,t)|-W_h(x,t)\operatorname{sign}W_h(y,t)|\,dydxdt.\end{aligned}$$

By using the inequality $||a| - a\,\mathrm{sign}\,b| \leq 2|a-b|$ we obtain

$$\begin{aligned}&\left|I_h(\tau) - I_h^\delta(\tau)\right| \\ &\qquad \leq 2\hat{\omega}(\delta) + 2\int_0^{+\infty}\int_{\Omega'\setminus U'_\delta}\int_{\mathbb{R}^l} \rho_\delta(x-y)\,|W_h(x,t) - W_h(y,t)|\,dydxdt\end{aligned} \tag{3.111}$$

and by setting $\sigma := (x-y)/\delta$ we obtain

$$\begin{aligned}&\left|I_h(\tau) - I_h^\delta(\tau)\right| \\ &\qquad \leq 2\hat{\omega}(\delta) + 2\int_{\mathbb{R}^l}\rho(\sigma)\int_0^{+\infty}\int_{\Omega'\setminus U'_\delta}\left|\overline{U}_h(x,t) - \overline{U}_h(x-\delta\sigma,t)\right|\,dxdtd\sigma.\end{aligned} \tag{3.112}$$

Corollary 3.7.6 gives existence of a continuity module $\overline{\omega}(\delta)$ such that

$$\left|I_h(\tau) - I_h^\delta(\tau)\right| \leq 2\hat{\omega}(\delta) + 2\overline{\omega}(\delta). \tag{3.113}$$

By combining the estimates (3.109) and (3.113) we obtain $I_h \leq \omega(\tau)$, where

$$\omega(\tau) := \inf_{\delta>0} C\left(\tau(1+\delta^{-2l-2}) + 2\hat{\omega}(\delta) + 2\overline{\omega}(\delta)\right).$$

Since $\tilde{\omega}(\tau) \to 0$ as $\tau \to 0$, we obtain (3.98). In the same way one can prove (3.99). □

Corollary 3.7.8. *Let $(D_h)_h$ be a sequence of finite volume discretizations of $\Omega \times (0,T)$ such that $\lim_{h\to 0} size(D_h) = 0$. Then,*

$$\|U_h - \overline{U}_h\|_{L^1(\Omega)} \to 0, \quad \|V_h - \overline{V}_h\|_{L^1(\Omega)} \to 0. \tag{3.114}$$

Proof. For every $\Omega' \Subset \Omega$ the convergence

$$\|U_h - \overline{U}_h\|_{L^1(\Omega')} \to 0, \quad \|V_h - \overline{V}_h\|_{L^1(\Omega')} \to 0,$$

is a consequence of Proposition 3.7.7 and Remark 3.7.5. Since $\Omega \setminus \Omega'$ can have arbitrary small measure, and the functions $U_h - \overline{U}_h$ and $V_h - \overline{V}_h$ are uniformly bounded we find (3.114). □

Theorem 3.7.9. *Let $(D_h)_h$ be a sequence of finite volume discretizations of $\Omega \times (0,T)$ such that $\lim_{h\to 0} size(D_h) = 0$. Then there exist subsequences $(p_{\alpha,h})_h$, $\alpha \in \{w,n\}$, $(S_{w,h})_h$, and $(p_h)_h$ such that*

$$U_h \to U \quad \textit{strongly in } L^p(Q_T),\ 1 \leq p < \infty, \textit{ and a.e. in } Q_T, \tag{3.115}$$

$$V_h \to V \quad \textit{strongly in } L^p(Q_T),\ 1 \leq p < \infty, \textit{ and a.e. in } Q_T, \tag{3.116}$$

$$S_{w,h} \to S_w \quad \textit{a.e. in } Q_T, \tag{3.117}$$

$$p_h \to p \quad \textit{a.e. in } Q_T, \tag{3.118}$$

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

Proof. From Corollary 3.7.6, Proposition 3.7.7 and the boundedness of the sequences $(\overline{U}_h)$ and $(\overline{V}_h)$ we can apply the Riesz-Frechet-Kolomogorov compactness theorem and conclude that the sequences $(\overline{U}_h)$ and $(\overline{V}_h)$ are relatively compact in $L^1(\Omega \times (0,T))$ (see Corollary 3.7.2). Therefore, we can find a subsequence and functions $U, V \in L^1(\Omega \times (0,T))$ such that

$$\begin{aligned} \overline{U}_h \to U &\quad \text{strongly in } L^1(Q_T) \text{ and a.e. in } Q_T, \\ \overline{V}_h \to V &\quad \text{strongly in } L^1(Q_T) \text{ and a.e. in } Q_T. \end{aligned}$$

Due to Corollary 3.7.8 we find (3.115) and (3.116) for $p = 1$. The limit functions U and V are obviously in $L^\infty(Q_T)$ and the convergence holds in any $L^p(Q_T)$ for all $1 \le p < \infty$.

In [6] it has been proved 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 and therefore $(S_{w,h}, p_h) = G^{-1}(U_h, V_h)$ converge a.e. in Q_T to some functions S_w and p. In the limit it holds $G(S_w, p) = (U, V)$. This proves the theorem. □

3.8 Proof of the Theorem 3.2.9

In order to prove Theorem 3.2.9 we follow the approach from [76] and [12]. First we prove some auxiliary lemmas.

From a priori estimates (3.65) we have the following convergences.

Lemma 3.8.1. *Let $(D_h)_h$ be a sequence of finite volume discretizations of $\Omega \times (0,T)$ such that* $\lim_{h\to 0} size(D_h) = 0$. *Then there exists subsequences $(S_{w,h})_h$ and $(p_h)_h$ such that*

$$p, \beta(S_w) - \beta(1) \in L^2(0,T;V), \quad 0 \le S_w \le 1, \tag{3.119}$$

$$\nabla_h \beta(S_{w,h}) \to \nabla \beta(S_w) \quad \textit{weakly in } (L^2(Q_T))^l, \tag{3.120}$$

$$\nabla_h p_h \to \nabla p \quad \textit{weakly in } (L^2(Q_T))^l, \tag{3.121}$$

where p and S_w are the limits from Theorem 3.7.9.

Proof. From Corollary 3.5.3 it follows that the sequence $(\nabla_h p_h)_h$ is bounded in $\left(L^2(Q_T)\right)^l$, and therefore there exists $\xi \in \left(L^2(Q_T)\right)^l$ such that

$$\nabla_h p_h \to \xi \quad \text{weakly in } (L^2(Q_T))^l. \tag{3.122}$$

By the discrete Poincaré inequality, Lemma 3.2.2, the sequence $(p_h)_h$ is also bounded in $L^2(Q_T)$, and therefore by Lemma 3.2.6 we conclude that $\xi = \nabla p$ and $p \in L^2(0,T;V)$. This weak limit is equal to the limit in (3.118).

The same reasoning can be applied to the sequence $(\beta(S_{\alpha,h}))_h$. From the estimate (3.65) we can find $\xi \in \left(L^2(Q_T)\right)^l$ such that

$$\nabla_h \beta(S_{\alpha,h}) \to \xi \quad \text{weakly in } (L^2(Q_T))^l. \tag{3.123}$$

By the discrete Poincaré's inequality, since $\beta(S_{\alpha,h}) = \beta(1)$ on Γ_D, the sequence $(\beta(S_{\alpha,h}))_h$ is also bounded in $L^2(Q_T)$, and therefore by Lemma 3.2.6 we conclude that $\xi = \nabla\beta(S_w)$ and $\beta(S_w) - \beta(1) \in L^2(0,T;V)$. This weak limit is equal to the limit in (3.117). This completes the proof. □

Lemma 3.8.2. *Functions $\rho_\alpha(p_\alpha(S_w,p))$ and $\rho_\alpha(p_\alpha(S_w,p))/\lambda(S_w,p)$ are Lipschitz continuous.*

Proof. *i*) From

$$\frac{\partial \rho_n(p_n(S_w,p))}{\partial S_w} = \rho_n'(p_n) f_w(S_w,p) p_c'(S_w), \quad \frac{\partial \rho_w(p_w(S_w,p))}{\partial S_w} = -\rho_w'(p_w) f_n(S_w,p) p_c'(S_w),$$

and

$$\frac{\partial \rho_\alpha(p_\alpha(S_w,p))}{\partial p} = \rho_\alpha'(p_\alpha)\omega(S_w,p),$$

by (A.4) and (A.5) all derivatives of $\rho_\alpha(p_\alpha(S_\alpha,p))$ are bounded. *ii*) Due to i), (A.3), and (A.5), $\lambda(S_w,p)$ is Lipschitz continuous and $\lambda(S_w,p) \geq \rho_m \lambda_m$. Therefore, $\rho_\alpha(p_\alpha(S_w,p))/\lambda(S_w,p)$ is also Lipschitz continuous. □

Lemma 3.8.3. *Let $S_{w,h}$ and p_h be convergent subsequences from Theorem 3.7.9, and define the functions $\overline{S}_h$, $\underline{S}_h$, $\overline{p}_h$, and $\underline{p}_h$ on the dual mesh composed of elements $T_{K|L}$, $K \in \mathcal{T}_h$, $L \in N_D(K)$, defined as*

$$\overline{S}_h|_{\langle t^k,t^{k+1}]\times T_{K|L}} := \max\{S_{w,K}^{k+1}, S_{w,L}^{k+1}\}, \quad \underline{S}_h|_{\langle t^k,t^{k+1}]\times T_{K|L}} := \min\{S_{w,K}^{k+1}, S_{w,L}^{k+1}\},$$
$$\overline{p}_h|_{\langle t^k,t^{k+1}]\times T_{K|L}} := \max\{p_K^{k+1}, p_L^{k+1}\}, \quad \underline{p}_h|_{\langle t^k,t^{k+1}]\times T_{K|L}} := \min\{p_K^{k+1}, p_L^{k+1}\}.$$

Then there is a constant C independent of discretization such that

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

If $\tilde{S}_h$ and $\tilde{p}_h$ are any other dual mesh functions satisfying

$$\underline{S}_h \le \tilde{S}_h \le \overline{S}_h, \quad \underline{p}_h \le \tilde{p}_h \le \overline{p}_h$$

then for any continuous function $\mathscr{A} : [0,1] \times \mathbb{R} \to \mathbb{R}$ we have

$$\mathscr{A}(\tilde{S}_h, \tilde{p}_h) \to \mathscr{A}(S_w, p) \text{ a.e. in } Q_T, \tag{3.124}$$

where S_w and p are given limits in Theorem 3.7.9.

Proof. In order to simplify notation we will denote S_w by S. Since the function β is monotone we conclude

$$\begin{aligned}\int_{Q_T} |\beta(\overline{S}_h) - \beta(\underline{S}_h)|^2 \, dxdt &= \frac{1}{2} \sum_{k=0}^{N_h-1} \delta t \sum_{K\in\mathfrak{T}} \sum_{L\in N(K)} \int_{T_{K|L}} |\beta(\overline{S}_h) - \beta(\underline{S}_h)|^2 \, dx \\ &+ \sum_{k=0}^{N_h-1} \delta t \sum_{K\in\mathfrak{T}} \sum_{\sigma\in\partial K\cap\Gamma_D} \int_{T_{K,\sigma}} |\beta(\overline{S}_h) - \beta(\underline{S}_h)|^2 \, dx \\ &\le \frac{1}{2} \sum_{k=0}^{N_h-1} \delta t \sum_{K\in\mathfrak{T}} \sum_{L\in N_D(K)} |\tilde{T}_{K|L}| |\beta(S_L^{k+1}) - \beta(S_K^{k+1})|^2.\end{aligned}$$

From Corollary 3.5.3 we get

$$\int_{Q_T} |\beta(\overline{S}_h) - \beta(\underline{S}_h)|^2 \, dxdt \le C\text{size}(\mathfrak{T})^2,$$

which leads to

$$|\overline{S}_h - \underline{S}_h| \to 0 \text{ a.e. in } Q_T, \tag{3.125}$$

on a subsequence when $h \to 0$. In the same way we get

$$\int_{Q_T} |\overline{p}_h - \underline{p}_h|^2 \, dxdt \le C \sum_{k=0}^{N_h-1} \delta t \sum_{K\in\mathfrak{T}} \sum_{L\in N_D(K)} |\tilde{T}_{K|L}| |p_L^{k+1} - p_K^{k+1}|^2 \le C\text{size}(\mathfrak{T})^2, \tag{3.126}$$

and

$$|\overline{p}_h - \underline{p}_h| \to 0 \text{ a.e. in } Q_T. \tag{3.127}$$

Since $\underline{S}_h \le S_h \le \overline{S}_h$, $\underline{p}_h \le p_h \le \overline{p}_h$ and $\mathscr{A}$ is a continuous function we obtain

$$\mathscr{A}(\underline{S}_h, \underline{p}_h) \to \mathscr{A}(S_w, p) \text{ a.e. in } Q_T, \quad \mathscr{A}(\overline{S}_h, \overline{p}_h) \to \mathscr{A}(S_w, p) \text{ a.e. in } Q_T,$$

on a subsequence when $h \to 0$, and (3.124) follows. □

Lemma 3.8.4. *Let $\tilde{\alpha}(S_w, p)$ be given by (3.13). Then following equality holds*

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

where

$$\begin{aligned}|\Delta_{K|L}^{k+1}| \le\; & C\left|\beta(S_{w,K}^{k+1})-\beta(S_{w,L}^{k+1})\right|^{2\tau} \\ & +C\left(\left|\overline{S}_{w,K|L}^{k+1}-\underline{S}_{w,K|L}^{k+1}\right|+\left|\overline{p}_{K|L}^{k+1}-\underline{p}_{K|L}^{k+1}\right|\right)\left|\beta(S_{w,K}^{k+1})-\beta(S_{w,L}^{k+1})\right|,\end{aligned} \tag{3.128}$$

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 $k+1$ since all the quantities are given on the same time level.

First we recall the definition of $f_{w,K|L}$

$$f_{w,K|L} = \frac{1}{u_K-u_L}\int_{S_L}^{S_K} f_w(s,p_{K|L})p_c'(s)\,ds.$$

There exist $\overline{a} \in \left[\underline{S}_{K|L}, \overline{S}_{K|L}\right]$ such that

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

Since

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

we can estimate

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

First we estimate c_1:

$$\begin{aligned}|c_1| &\le \frac{\rho_M^2}{\lambda_m}\left|\lambda_n(S_{K|L})\lambda_w(\overline{a})\,(u_K-u_L)-(\beta(S_K)-\beta(S_L))\right| \\ &= \frac{\rho_M^2}{\lambda_m}\left|\lambda_n(S_{K|L})\lambda_w(\overline{a})-\lambda_n(a_1)\lambda_w(a_1)\right|\left|u_K-u_L\right|,\end{aligned}$$

for some $a_1 \in \left[\underline{S}_{K|L}, \overline{S}_{K|L}\right]$. If we apply (A.4) and (A.7) we obtain

$$\begin{aligned}|c_1| &\le C\left|\lambda_n(S_{K|L})\lambda_w(\overline{a}) - \lambda_n(a_1)\lambda_w(a_1)\right| |S_K - S_L| \\ &\le C\left|\lambda_n(S_{K|L})\lambda_w(\overline{a}) - \lambda_n(a_1)\lambda_w(a_1)\right| |\beta(S_K) - \beta(S_L)|^\tau .\end{aligned}$$

From (A.3) we obtain

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

In order to bound the term c_2 we need to estimate the difference

$$\begin{aligned}&\left|\frac{\rho_n(p^{up}_{n,K|L})\rho_w(p_w(\overline{a}, p_{K|L}))}{\lambda(\overline{a}, p_{K|L})} - \tilde{\alpha}(\underline{S}_{K|L}, \underline{p}_{K|L})\right| \\ &= \left|\frac{\rho_n(p^{up}_{n,K|L})\rho_w(p_w(\overline{a}, p_{K|L}))}{\lambda(\overline{a}, p_{K|L})} - \frac{\rho_n(p_n(\underline{S}_{K|L}, \underline{p}_{K|L}))\rho_w(p_w(\underline{S}_{K|L}, \underline{p}_{K|L}))}{\lambda(\underline{S}_{K|L}, \underline{p}_{K|L})}\right| \\ &\le \left|\rho_n(p^{up}_{n,K|L})\right| \left|\frac{\rho_w(p_w(\overline{a}, p_{K|L}))}{\lambda(\overline{a}, p_{K|L})} - \frac{\rho_w(p_w(\underline{S}_{K|L}, \underline{p}_{K|L}))}{\lambda(\underline{S}_{K|L}, \underline{p}_{K|L})}\right| \\ &+ \left|\rho_n(p^{up}_{n,K|L}) - \rho_n(p_n(\underline{S}_{K|L}, \underline{p}_{K|L}))\right| \left|\frac{\rho_w(p_w(\underline{S}_{K|L}, \underline{p}_{K|L}))}{\lambda(\underline{S}_{K|L}, \underline{p}_{K|L})}\right| \\ &\le C\left(\left|\overline{S}_{K|L} - \underline{S}_{K|L}\right| + \left|\overline{p}_{K|L} - \underline{p}_{K|L}\right|\right),\end{aligned}$$

where we have applied Lemma 3.8.2, (A.3), and (A.5). Therefore, we conclude

$$c_2 \le C\left(\left|\overline{S}_{K|L} - \underline{S}_{K|L}\right| + \left|\overline{p}_{K|L} - \underline{p}_{K|L}\right|\right) |\beta(S_K) - \beta(S_L)| ,$$

which concludes the proof. □

We now pass to the proof of Theorem 3.2.9. Let $\varphi \in D([0,T) \times \overline{\Omega})$ and set $\varphi^k_K := \varphi(x_K, t^k)$ for all $K \in \mathcal{T}_h$ and $k \in \{0, 1, \dots, N_h\}$. In order to pass to the limit in (3.37) we multiply (3.37) by $\delta t \varphi^{k+1}_K$, introduce the global pressure variable by (3.53), (3.54), and sum over $K \in \mathcal{T}_h$ and $k \in \{0, 1, \dots, N_h - 1\}$ to obtain

$$S^h_1 + S^h_2 + S^h_3 + S^h_4 + S^h_5 = 0,$$

where we have denoted

$$S^h_1 = \sum_{k=0}^{N_h-1} \sum_{K\in\mathcal{T}_h} |K|\Phi_K \left(\rho^{k+1}_{n,K} S^{k+1}_{n,K} - \rho^k_{n,K} S^k_{n,K}\right) \varphi^{k+1}_K \tag{3.129}$$

$$S_2^h = \sum_{k=0}^{N_h-1} \delta t \sum_{K\in\mathfrak{T}_h} \sum_{L\in N_D(K)} \tau_{K|L} k_{K|L} \lambda_{n,K|L}^{up,k+1} \rho_{n,K|L}^{up,k+1} \omega_{K|L}^{k+1} (p_K^{k+1} - p_L^{k+1}) \varphi_K^{k+1} \tag{3.130}$$

$$S_3^h = \sum_{k=0}^{N_h-1} \delta t \sum_{K\in\mathfrak{T}_h} \sum_{L\in N_D(K)} \tau_{K|L} k_{K|L} \lambda_{n,K|L}^{up,k+1} \rho_{n,K|L}^{up,k+1} f_{w,K|L}^{k+1} \left(u_K^{k+1} - u_L^{k+1}\right) \varphi_K^{k+1} \tag{3.131}$$

$$S_4^h = \sum_{k=0}^{N_h-1} \delta t \sum_{K\in\mathfrak{T}_h} |K| \left(\rho_{n,K}^{k+1} S_{n,K}^{k+1} F_{p,K}^{k+1} \varphi_K^{k+1} - \rho_{n,K}^{k+1} S_{n,K}^{I,k+1} F_{I,K}^{k+1} \varphi_K^{k+1}\right) \tag{3.132}$$

$$S_5^h = \sum_{k=0}^{N_h-1} \delta t \sum_{K\in\mathfrak{T}_h} \sum_{L\in N_D(K)} |\sigma_{K|L}| k_{K|L} \lambda_{n,K|L}^{G,k+1} \left(\rho_{n,K|L}^{G,k+1}\right)^2 g_{K|L} \varphi_K^{k+1} \tag{3.133}$$

By making summation by parts in time and by using the fact $\varphi_K^{N_h} = 0$ for all $K \in \mathfrak{T}_h$ we obtain

$$\begin{aligned}
S_1^h &= -\sum_{k=0}^{N_h-1} \sum_{K\in\mathfrak{T}_h} |K| \Phi_K \rho_{n,K}^{k+1} S_{n,K}^{k+1} \left(\varphi_K^{k+1} - \varphi_K^k\right) - \sum_{K\in\mathfrak{T}_h} |K| \Phi_K \rho_{n,K}^0 S_{n,K}^0 \varphi_K^0 \\
&= -\sum_{k=0}^{N_h-1} \sum_{K\in\mathfrak{T}_h} \int_{t^k}^{t^{k+1}} \int_K \Phi_K \rho_{n,K}^{k+1} S_{n,K}^{k+1} \partial_t \varphi(x_K,t)\, dx\, dt - \sum_{K\in\mathfrak{T}_h} \int_K \Phi(x) \rho_n^{0,h}(x) S_n^{0,h}(x) \varphi(x_K,0)\, dx.
\end{aligned}$$

If we denote by $\varphi_h \in C^1([0,T], H_h(\Omega))$ the function defined by $\varphi_K(t) := \varphi(x_K,t)$ for all $K \in \mathfrak{T}_h$, then we can write

$$S_1^h = -\int_{Q_T} \Phi^h(x) \rho_n^h(x,t) S_{n,h}(x,t) \partial_t \varphi_h(x,t)\, dx\, dt - \int_\Omega \Phi(x) \rho_n^{0,h}(x) S_{n,h}^0(x) \varphi_h(x,0)\, dx.$$

By smoothness of the function φ there is a constant C independent of h such that

$$\sup_{(x,t)\in\Omega\times(0,T)} |\varphi_h(x,0) - \varphi(x,0)| + |\partial_t \varphi_h(x,t) - \partial_t \varphi(x,t)| \leq Ch. \tag{3.134}$$

By Theorem 3.7.9, definition of the initial conditions and (3.134) we get

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

For term S_2^h we obtain after gathering by edges

$$\begin{aligned}
S_2^h &= -\frac{1}{2} \sum_{k=0}^{N_h-1} \delta t \sum_{K\in\mathfrak{T}_h} \sum_{L\in N_D(K)} \tilde{\tau}_{K|L} k_{K|L} \lambda_{n,K|L}^{up,k+1} \rho_{n,K|L}^{up,k+1} \omega_{K|L}^{k+1} (p_K^{k+1} - p_L^{k+1})(\varphi_L^{k+1} - \varphi_K^{k+1}) \\
&= \frac{1}{2} \sum_{k=0}^{N_h-1} \delta t \sum_{K\in\mathfrak{T}_h} \sum_{L\in N_D(K)} \frac{1}{l} |\tilde{\sigma}_{K|L}| d_{K|L} k_{K|L} \lambda_{n,K|L}^{up,k+1} \rho_{n,K|L}^{up,k+1} \omega_{K|L}^{k+1} l \frac{p_L^{k+1} - p_K^{k+1}}{d_{K|L}} \frac{\varphi_L^{k+1} - \varphi_K^{k+1}}{d_{K|L}} \\
&= \frac{1}{2} \sum_{k=0}^{N_h-1} \delta t \sum_{K\in\mathfrak{T}_h} \sum_{L\in N_D(K)} |\tilde{T}_{K|L}| k_{K|L} \lambda_{n,K|L}^{up,k+1} \rho_{n,K|L}^{up,k+1} \omega_{K|L}^{k+1} \left(\nabla_{K|L} p_h^{k+1} \cdot \eta_{K|L}\right)
\end{aligned}$$

$$\times \left(\nabla \varphi(\overline{x_{K|L}}, t^{k+1}) \cdot \eta_{K|L} \right),$$

where $\overline{x_{K|L}}$ is some point on the segment with the endpoints x_K and x_L. Using the fact

$$\left(\nabla_{K|L} p_h^{k+1} \cdot \eta_{K|L} \right) \left(\nabla \varphi(\overline{x_{K|L}}, t^{k+1}) \cdot \eta_{K|L} \right) = \nabla_{K|L} p_h^{k+1} \cdot \nabla \varphi(\overline{x_{K|L}}, t^{k+1}),$$

we obtain

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

If we introduce the piecewise constant functions $S_{w,h}^{up}$, $\overline{\overline{S}}_{w,h}$, $\overline{\overline{p}}_h$, $\tilde{S}_{w,h}$, and $\tilde{p}_h$ defined on dual mesh as

$$S_{w,h}^{up}|_{\langle t^k, t^{k+1}] \times T_{K|L}} := S_{w,K|L}^{k+1},$$

$$\overline{\overline{S}}_{w,h}|_{\langle t^k, t^{k+1}] \times T_{K|L}} := \overline{\overline{S}}_{w,K|L}^{k+1}, \quad \overline{\overline{p}}_h|_{\langle t^k, t^{k+1}] \times T_{K|L}} := \overline{\overline{p}}_{K|L}^{k+1} \text{ where } p_{n,K|L}^{up,k+1} = p_n(\overline{\overline{S}}_{w,K|L}^{k+1}, \overline{\overline{p}}_{K|L}^{k+1}),$$

and

$$\tilde{S}_{w,h}|_{\langle t^k, t^{k+1}] \times T_{K|L}} := \tilde{S}_{w,K|L}^{k+1}, \quad \tilde{p}_h|_{\langle t^k, t^{k+1}] \times T_{K|L}} := \tilde{p}_{K|L}^{k+1} \text{ where } \omega_{K|L}^{k+1} = \omega(\tilde{S}_{w,K|L}^{k+1}, \tilde{p}_{K|L}^{k+1}),$$

then we can write

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

From the regularity of the test function φ we have $(\nabla \varphi)_h \to \nabla \varphi$ in $L^\infty(Q_T)$. By Lemma 3.8.1 we also have weak convergence of $\nabla_h p_h$ to ∇p. Since the functions λ_n, $\rho_n \circ p_n$, and ω are bounded and continuous, from Theorem 3.7.9 and Lemma 3.8.3 it follows

$$\lambda_n(S_{w,h}^{up}) \rho_n(p_n(\overline{\overline{S}}_{w,h}, \overline{\overline{p}}_h)) \omega(\tilde{S}_{w,h}, \tilde{p}_h) \to \lambda_n(S_w) \rho_n(p_n(S_w, p)) \omega(S_w, p) \text{ a.e. in } Q_T.$$

Finally, the convergence $\|k - k_h\|_{L^2(\Omega)} \to 0$ (see Remark 3.2.8) gives

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

Using the same technique as in term S_2^h, first we write the term S_3^h in the following form

$$S_3^h = \frac{1}{2} \sum_{k=0}^{N_h-1} \delta t \sum_{K \in \mathfrak{T}_h} \sum_{L \in N_D(K)} \tilde{\tau}_{K|L} k_{K|L} \lambda_{n,K|L}^{up,k+1} \rho_{n,K|L}^{up,k+1} f_{w,K|L}^{k+1} (u_K^{k+1} - u_L^{k+1})(\varphi_K^{k+1} - \varphi_L^{k+1}).$$

By Lemma 3.8.4 we have

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

Using (3.128) we get

$$
\begin{aligned}
|c_{II}| \le C&\sum_{k=0}^{N_h-1}\delta_t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}\tilde{\tau}_{K|L}^{\tau}\tilde{\tau}_{K|L}^{1-\tau}\left|\beta(S_{w,K}^{k+1})-\beta(S_{w,L}^{k+1})\right|^{2\tau}|\varphi_K^{k+1}-\varphi_L^{k+1}|\\
&+C\sum_{k=0}^{N_h-1}\delta t\sum_{K\in\mathfrak{T}_h}\sum_{L\in N_D(K)}|\tilde{T}_{K|L}|\left(\left|\overline{S}_{w,K|L}^{k+1}-\underline{S}_{w,K|L}^{k+1}\right|+\left|\overline{p}_{K|L}^{k+1}-\underline{p}_{K|L}^{k+1}\right|\right)\\
&\times\left|l\frac{\beta(S_{w,K}^{k+1})-\beta(S_{w,L}^{k+1})}{d_{K|L}}\right|\left|\frac{\varphi_K^{k+1}-\varphi_L^{k+1}}{d_{K|L}}\right|,
\end{aligned}
$$

and by Cauchy-Schwarz's and Hölder's inequalities we get the following estimate:

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

We can estimate

$$
\left(\sum_{k=0}^{N_h-1}\delta_t\sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)}\tilde{\tau}_{K|L}|\varphi_L^{k+1}-\varphi_K^{k+1}|^{\frac{1}{1-\tau}}\right)^{1-\tau}
$$

$$\leq \|\nabla\varphi\|_\infty \left(\sum_{k=0}^{N_h-1}\delta_t \sum_{K\in\mathfrak{T}}\sum_{L\in N_D(K)} l|\tilde{T}_{K|L}||d_{K|L}|^{\frac{1}{1-\tau}-2}\right)^{1-\tau}$$
$$\leq C\|\nabla\varphi\|_\infty h^{1-2(1-\tau)},$$

which gives us

$$|c_{II}| \leq C(h^{2\tau-1}+h)$$

and due to (A.7) the term c_{II} tends to zero when $h\to 0$. Therefore, we get

$$\lim_{h\to 0} S_3^h = \lim_{h\to 0}\int_{Q_T} k_h(x)\tilde{\alpha}(\underline{S}_{w,h},\underline{p}_h)\nabla_h\beta(S_{w,h})\cdot(\nabla\varphi)_h\, dxdt.$$

Using the same reasoning as in the term S_2^h we can pass to the limit and we get

$$\lim_{h\to 0} S_3^h = \int_{Q_T} k(x)\tilde{\alpha}(S_w,p)\nabla\beta(S_w)\cdot\nabla\varphi\, dxdt. \tag{3.135}$$

The term S_4^h can be written in the following way

$$S_4^h = \int_0^T\int_\Omega \left(\rho_n^h S_n^h F_P^h\varphi_h - \rho_n^h S_n^{I,h}F_I^h\varphi_h\right) dx\,dt.$$

Using (3.117) and (3.118) we can pass to the limit in this term to obtain

$$\lim_{h\to 0} S_4^h = \int_0^T\int_\Omega \left(\rho_n S_n F_P\varphi - \rho_n S_n^I F_I\varphi\right) dx\,dt. \tag{3.136}$$

In the same way as for the terms S_2^h and S_3^h we obtain for the term S_5^h,

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

Again by introducing the piecewise constant functions $S_{w,h}^{G,up}$, $S_{w,h}^G$, and p_h^G such that $\underline{S}_{w,h} \leq S_{w,h}^{G,up}, S_{w,h}^G \leq \overline{S}_{w,h}$ and $\underline{p}_h \leq p_h^G \leq \overline{p}_h$ we can rewrite the term S_5^h as

$$S_5^h = -\int_0^T\int_\Omega k_h(x)\lambda_n(S_{w,h}^{G,up})\rho_n^2(p_n(S_{w,h}^G,p_h^G))\mathbf{g}\cdot\nabla_h\varphi\, dx\,dt.$$

We note that for smooth test function φ, by Lemma 3.2.6, $\nabla_h\varphi\to\nabla\varphi$ weakly in $L^2(Q_T)$. Then the same arguments as in S_2^h and S_3^h ensure

$$\lim_{h\to 0} S_5^h = -\int_0^T\int_\Omega k(x)\lambda_n(S_w)\rho_n^2(p_n)\mathbf{g}\cdot\nabla\varphi\, dx\,dt. \tag{3.137}$$

We can perform similar calculations and reasoning in all terms of the equation (3.38) and after passing to the limit as $h \to 0$ we obtain the following variational formulation

$$
\begin{aligned}
&-\int_{Q_T} \Phi\rho_w(p_w)S_w\partial_t\varphi\,dx\,dt - \int_\Omega \Phi(x)\rho_w(p_w^0(x))S_w^0(x)\varphi(0,x)\,dx \\
&+\int_{Q_T} [\mathbb{K}(\lambda_w(S_w)\rho_w(p_w)\omega(S_w,p)\nabla p - \tilde{\alpha}(S_w,p)\nabla\beta(S_w)) - \lambda_w(S_w)\rho_w^2(p_w)\mathbb{K}\mathbf{g}]\cdot\nabla\varphi dxdt \\
&+\int_{Q_T} \rho_w(p_w)S_wF_P\varphi dxdt = \int_{Q_T} \rho_w(p_w)S_w^IF_P\varphi dxdt;
\end{aligned} \tag{3.138}
$$

$$
\begin{aligned}
&-\int_{Q_T} \Phi\rho_n(p_n)S_n\partial_t\psi\,dx\,dt - \int_\Omega \Phi(x)\rho_n(p_n^0(x))(1-S_w^0(x))\psi(0,x)\,dx \\
&+\int_{Q_T} [\mathbb{K}(\lambda_n(S_w)\rho_n(p_n)\omega(S_w,p)\nabla p + \tilde{\alpha}(S_w,p)\nabla\beta(S_w)) - \lambda_n(S_w)\rho_n^2(p_n)\mathbb{K}\mathbf{g}]\cdot\nabla\psi dxdt \\
&+\int_{Q_T} \rho_n(p_n)S_nF_P\psi dxdt = \int_{Q_T} \rho_n(p_n)S_n^IF_P\psi dxdt,
\end{aligned} \tag{3.139}
$$

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 (3.10) and (3.9). From (3.17) and (3.18) we can reintroduce the gradients of the phase pressures into the previous variational formulation which then reduces to the variational problem from Definition 3.1.1. Theorem 3.2.9 is proved.

3.9 Numerical simulation

This test case is taken from [56]. The spatial domain $\Omega = (0,1)^2$ is homogeneous with porosity $\Phi = 0.206$ and absolute permeability $k = 0.15\cdot 10^{-10}$ m^2. The relative permeability laws are taken as

$$kr_n(S_w) = (1-S_w)^2, \quad kr_w(S_w) = S_w^2.$$

The capillary pressure law is set to $p_c(S_w) = P_{max}(1-S_w)$, where $P_{max} = 10^5$ Pa. The following properties are used for the fluid system: $\mu_w = 10^{-3}$ Pa·s, $\mu_n = 9\cdot 10^{-5}$ Pa·s, $\rho_w = 1000$ kg/m^3, $\rho_n(p_n) = \rho_r(1 + c_r(p_n - p_r))$, where $\rho_r = 400$ kg/m^3, $c_r = 10^{-6}$ Pa, and $p_r = 1.013\cdot 10^5$ Pa. The initial conditions are imposed as follows

$$S_n(x,0) = 0.9, \quad p_n(x,0) = 1.013\cdot 10^5 \text{ Pa}, \quad x \in \Omega.$$

On the injection part of the boundary, which is $\{0\} \times [0.8, 1]$, Dirichlet boundary conditions are imposed $S_n = 0.1$, $p_n = 4.6732 \cdot 10^5$ Pa. On the extraction part of the boundary, which is $\{1\} \times [0, 0.2]$, we have set the capillary pressure gradient to zero and $p_n = 1.013 \times 10^5$ Pa. The remaining parts of the boundary are assumed to be impervious. Time of simulation is 40 s.

The obtained results are given in Figures 3.1 - 3.4, where one can see typical displacement of the nonwetting phase by the wetting phase. We observe that the front is not symmetric since the injection part of the boundary is set at the left part of the boundary. The presented results correspond to the one presented in [56] and to the one obtained by DuMu^x 2p module. They also correspond to the results obtained by the numerical method based on fractional flow formulation and global pressure presented in Chapter 4.

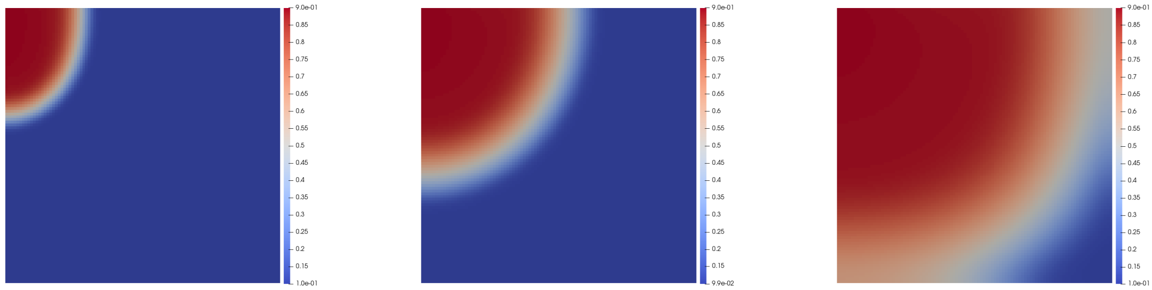

Figure 3.1: Water saturation at $t = 2$ s, 10 s, 40 s

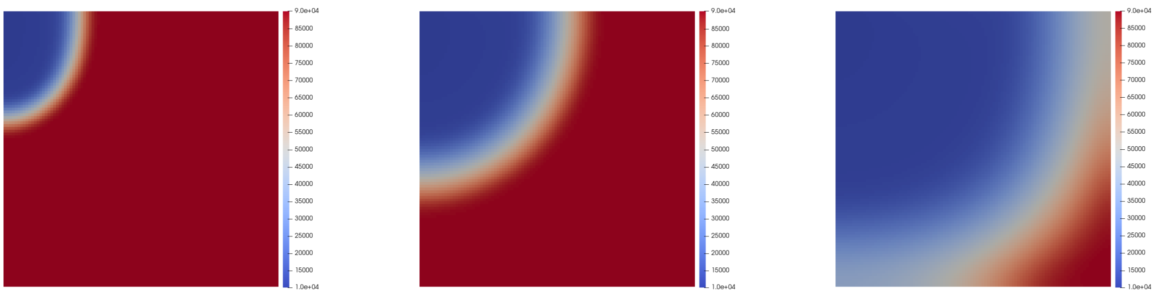

Figure 3.2: Capillary pressure at $t = 2$ s, 10 s, 40 s

3.10 Conclusion

In this chapter we have proved the convergence of the cell-centered finite volume method for immiscible, compressible, two-phase flow. In contrast to similar result given in [76] we use in our

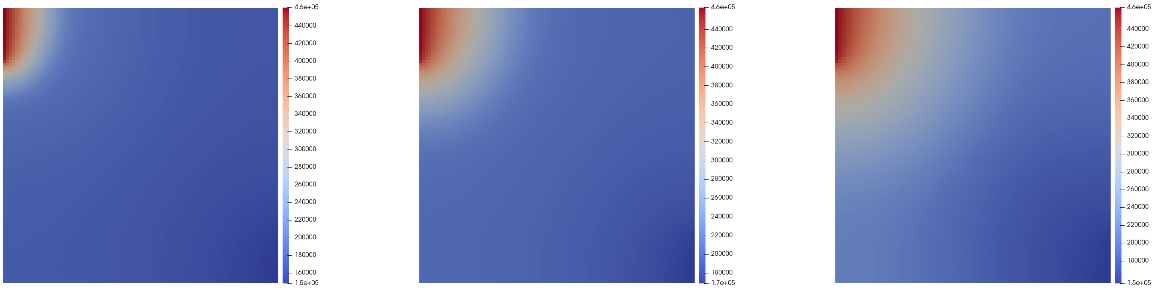

Figure 3.3: Gas phase pressure at $t = 2$ s, 10 s, 40 s

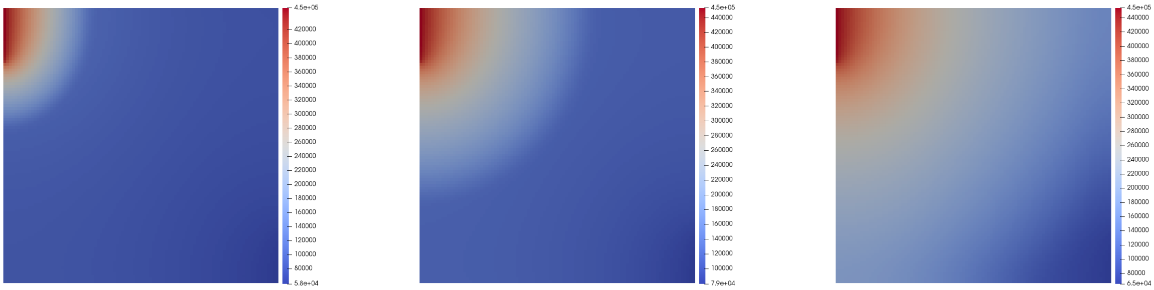

Figure 3.4: Liquid phase pressure at $t = 2$ s, 10 s, 40 s

proof a technique based on total flux global pressure defined in [5] for derivation of the energy estimate. In comparison to the scheme studied in [76], our discretization uses more common treatment of the mass densities.

Chapter 4

Cell-centerd finite volume discretization of compressible two-phase flow in porous media by the concept of global pressure

In this chapter we give discretization of the compressible two-phase flow model based on the fractional flow formulation and the concept of the global pressure based on the total flux, which was described in detail in Chapter 1. Aside from this dissertation, this model was only considered in [7] in one-dimensional case with numerical method based on vertex centered finite volume discretization. The special emphasis in [7] has been given to a domain with discontinuous capillary pressure curves and requirement for a special treatment of the interface between heterogeneous parts of the domain. Similar problem was considered in numerous other papers. Here we mention only [30], where incompressible fluid flow was considered, since similar ideas are adapted in this chapter for compressible fluid flow. In this work for the spatial discretization we use the cell-centered finite volume approximation and for the time discretization we use an implicit Euler approximation. We also present test cases that were used for validation of the numerical method, with homogeneous and heterogeneous domains. All of the test cases are inspired by known test cases from the literature or are taken in its original form from available benchmarks.

The outline of this chapter is as follows. In Section 4.1 we give a brief description of the fractional flow/global pressure formulation from [5]. In Section 4.2 we present the finite volume discretization. The numerical results with the method described in Section 4.2 are presented in Section 4.3. More precisely, we will present five test cases modeling different scenarios of immiscible compressible two-phase flow in porous media. The first test case is the injection of gas (hydrogen) in a 2D homogeneous porous domain fully saturated with water. The second test is quasi-1D water-hydrogen flow in a homogeneous porous domain starting from non equilibrium state. The third test case describes secondary gas recovery by injecting water in a 2D homogeneous domain, while in the fourth test case we consider again water-hydrogen lock-exchange flow but this time in a 2D domain. The last test case is the injection of the hydrogen in a 3D homogeneous domain initially saturated with water.

Special attention is paid to the treatment of the heterogeneities and association to the numerical scheme and the transmission conditions. Therefore, in Section 4.4 we adapt the method to the case of domains composed of multiple rock types. More precisely, we introduce new variables at the interface between different rock types in order to enforce the flux continuity of both phases. Numerical simulations with the method described in Section 4.4 are presented in Section 4.5. The first test case in this part is the injection of the hydrogen in a 1D domain composed of two media with different capillary pressure curves, porosity, and permeability that is initially saturated with water. In the second test case we consider again water-hydrogen flow starting from non equilibrium state in a heterogeneous domain composed of two different media. Finally, a brief description of the implementation of the method is given in the Appendix A.

4.1 Mathematical formulation

The mathematical formulation describing the two-phase flow in terms of the global pressure p based on the total flux and the saturation of the wetting phase S_w as primary unknowns is given by the system composed of the mass balance equations for both phases:

$$\Phi\frac{\partial}{\partial t}\big(\rho_w S_w\big) + \operatorname{div}\left(f_w\mathbf{Q}_t + b_g\mathbb{K}\mathbf{g}\right) = -\operatorname{div}\left(\alpha\mathbb{K}\nabla p_c(S_w)\right) + F_w, \tag{4.1}$$

$$\Phi\frac{\partial}{\partial t}\big(\rho_n S_n\big) + \operatorname{div}\left(f_n\mathbf{Q}_t - b_g\mathbb{K}\mathbf{g}\right) = \operatorname{div}\left(\alpha\mathbb{K}\nabla p_c(S_w)\right) + F_n, \tag{4.2}$$

where we have denoted the total flux by $\mathbf{Q}_t = -\lambda\mathbb{K}\left(\omega\nabla p - \rho\mathbf{g}\right)$. A detailed description of the considered model is given in Chapter 1. We consider the proposed model in domain $Q_T = \Omega\times(0,T)$, where $T>0$ is fixed time and Ω is a polygonal domain. We assume that the boundary $\partial\Omega$ is divided in two disjoint parts $\partial\Omega = \Gamma_D\cup\Gamma_N$ where we impose the Neumann boundary conditions

$$\begin{cases} (f_w \mathbf{Q}_t + b_g \mathbb{K}\mathbf{g} + \alpha \mathbb{K} \nabla p_c) \cdot \mathbf{n} = q^w \\ (f_n \mathbf{Q}_t - b_g \mathbb{K}\mathbf{g} - \alpha \mathbb{K} \nabla p_c) \cdot \mathbf{n} = q^n \end{cases} \quad \text{on } \Gamma_N,$$

where **n** presents the outward unit normal to Γ_N, and the Dirichlet boundary conditions

$$\begin{cases} S_w = S_w^D \\ p = p^D \end{cases} \quad \text{on } \Gamma_D.$$

Instead of the system (4.1)–(4.2) we can consider the system composed of the total mass balance equation and the nonwetting phase mass balance equation:

$$\Phi \frac{\partial}{\partial t} \big(\rho_w S_w + \rho_n S_n\big) - \operatorname{div}\left(\lambda \mathbb{K}\left(\omega \nabla p - \rho \mathbf{g}\right)\right) = F_w + F_n, \tag{4.3}$$

$$\Phi \frac{\partial}{\partial t} \big(\rho_n S_n\big) + \operatorname{div}\left(f_n \mathbf{Q}_t - b_g \mathbb{K}\mathbf{g}\right) = \operatorname{div}\left(\alpha \mathbb{K} \nabla p_c\right) + F_n, \tag{4.4}$$

or the system composed of the wetting phase mass balance equation and the total mass balance equation:

$$\Phi \frac{\partial}{\partial t} \big(\rho_w S_w\big) + \operatorname{div}\left(f_w \mathbf{Q}_t + b_g \mathbb{K}\mathbf{g}\right) = -\operatorname{div}\left(\alpha \mathbb{K} \nabla p_c\right) + F_w, \tag{4.5}$$

$$\Phi \frac{\partial}{\partial t} \big(\rho_w S_w + \rho_n S_n\big) - \operatorname{div}\left(\lambda \mathbb{K}\left(\omega \nabla p - \rho \mathbf{g}\right)\right) = F_w + F_n. \tag{4.6}$$

For the primary variables, we can also choose the nonwetting phase saturation S_n and the global pressure p.

The phase pressures are obtained from the global pressure and the wetting phase saturation, using the capillary pressure law and the relation between nonwetting phase pressure, the global pressure and the saturation of the wetting phase:

$$\begin{aligned} p_n &= \pi(S_w, p), \\ p_w &= \pi(S_w, p) - p_c(S_w). \end{aligned} \tag{4.7}$$

The function π is given as a solution of the Cauchy problem (1.47). Once the phase pressures are computed one can easily compute all the remaining coefficients in the system (4.1)–(4.2), which are given by (1.43).

Finally, the problem is completed by the initial conditions that can be expressed in primary or phase variables.

4.2 Finite volume scheme

In this chapter we use the definition of the finite volume mesh on $\Omega \times (0,T)$ from [45], which is already given in Definition 3.2.1. All notation regarding finite volume mesh is the same as in Chapter 3.

We denote the weighted harmonic mean of the values u_K and u_L on two adjacent volumes K and L by $u_{K|L}$

$$u_{K|L} = \frac{d_{K|L}}{\frac{d_{K,\sigma}}{u_K} + \frac{d_{L,\sigma}}{u_L}}. \tag{4.8}$$

We introduce the following notation for the weighted arithmetic mean of the values u_K and u_L

$$\overline{u}_{K|L} = \frac{d_{K,\sigma}u_K + d_{L,\sigma}u_L}{d_{K|L}}. \tag{4.9}$$

Let us fix an integer N and set $\delta t = T/N$ and $t^k = k\delta t$, $k \in \{0, 1, ..., N\}$. For simplicity we will consider the case $\mathbb{K} = k(x)\mathbb{I}$, $x \in \Omega$. For the discretization of the total velocity on the edge $\sigma_{K|L}$ we use the approximation for the absolute permeability $k(x)$ given by (3.35) and for the function $\omega(S_w, p)$, arithmetic average for the mean density ρ, upwinding for the total mobility $\lambda(S_w, p)$, and two point approximation for the gradient of the global pressure. We obtain the following expression

$$Q_{K|L}^{k+1} = \lambda_{K|L}^{up,k+1} k_{K|L} \left(\omega_{K|L} \frac{p_K^{k+1} - p_L^{k+1}}{d_{K|L}} + \overline{\rho}_{K|L}^{k+1} \mathbf{g} \cdot \mathbf{n}_{K|L} \right), \tag{4.10}$$

where $\mathbf{n}_{K|L}$ denotes the outward unit normal to edge $\sigma_{K|L}$ pointing from K to L and

$$\lambda_{K|L}^{up,k+1} = \begin{cases} \lambda(S_{w,K}^{k+1}, p_K^{k+1}) & \text{if } \left(\omega_{K|L} \frac{p_K^{k+1} - p_L^{k+1}}{d_{K|L}} + \overline{\rho}_{K|L}^{k+1} \mathbf{g} \cdot \mathbf{n}_{K|L} \right) \geq 0 \\ \lambda(S_{w,L}^{k+1}, p_L^{k+1}) & \text{if } \left(\omega_{K|L} \frac{p_K^{k+1} - p_L^{k+1}}{d_{K|L}} + \overline{\rho}_{K|L}^{k+1} \mathbf{g} \cdot \mathbf{n}_{K|L} \right) < 0. \end{cases}$$

For the discretization of the term with the fractional flow functions $f_w(S_w, p)$ and $f_n(S_w, p)$ we use the upwind scheme:

$$F_{K|L}^{n,k+1} = \begin{cases} f_n(S_{w,K}^{k+1}, p_K^{k+1}) Q_{K|L}^{k+1} & \text{if } Q_{K|L}^{k+1} \geq 0 \\ f_n(S_{w,L}^{k+1}, p_L^{k+1}) Q_{K|L}^{k+1} & \text{if } Q_{K|L}^{k+1} < 0, \end{cases}$$

$$F_{K|L}^{w,k+1} = \begin{cases} f_w(S_{w,K}^{k+1}, p_K^{k+1}) Q_{K|L}^{k+1} & \text{if } Q_{K|L}^{k+1} \geq 0 \\ f_w(S_{w,L}^{k+1}, p_L^{k+1}) Q_{K|L}^{k+1} & \text{if } Q_{K|L}^{k+1} < 0. \end{cases}$$

The capillary diffusion term is discretized as follows

$$C_{K|L}^{k+1} = -\left(\alpha \mathbb{K} \nabla p_c(S_w) \cdot \mathbf{n}\right)|_{\sigma_{K|L}} = -\alpha_{K|L}^{k+1} k_{K|L} \frac{p_c(S_{w,L}^{k+1}) - p_c(S_{w,K}^{k+1})}{d_{K|L}}, \tag{4.11}$$

where $\alpha_{K|L}^{k+1}$ is given by the harmonic mean (4.8).

For the gravity term we use the discretization from [58] which is based on the fact that the heavier fluid goes down and that the lighter fluid goes up. The authors have considered a system composed of incompressible fluids. Since we have compressible fluid flow, we will use arithmetic mean for the approximation of the phase densities on the edge $\sigma_{K|L}$. We propose the following approximation

$$b_{g,K|L}^{k+1} = (b_g \mathbb{K} \mathbf{g} \cdot \mathbf{n})|_{\sigma_{K|L}} = \left(\overline{\rho}_{w,K|L}^{k+1} - \overline{\rho}_{n,K|L}^{k+1}\right) \frac{\overline{\rho}_{w,K|L}^{k+1} \overline{\rho}_{n,K|L}^{k+1} \lambda_{w,K|L}^{G,k+1} \lambda_{n,K|L}^{G,k+1}}{\overline{\rho}_{w,K|L}^{k+1} \lambda_{w,K|L}^{G,k+1} + \overline{\rho}_{n,K|L} \lambda_{n,K|L}^{G,k+1}} k_{K|L} \mathbf{g} \cdot \mathbf{n}_{K|L}. \tag{4.12}$$

Upwind values for the phase mobilities in the gravity term are given as follows

$$\lambda_{w,K|L}^{G,k+1} = \begin{cases} \lambda_w(S_{w,K}^{k+1}) & \text{if } \left(\overline{\rho}_{w,K|L}^{k+1} - \overline{\rho}_{n,K|L}^{k+1}\right) \mathbf{g} \cdot \mathbf{n}_{K|L} > 0 \\ \lambda_w(S_{w,L}^{k+1}) & \text{if } \left(\overline{\rho}_{w,K|L}^{k+1} - \overline{\rho}_{n,K|L}^{k+1}\right) \mathbf{g} \cdot \mathbf{n}_{K|L} \leq 0, \end{cases}$$

$$\lambda_{n,K|L}^{G,k+1} = \begin{cases} \lambda_n(S_{w,L}^{k+1}) & \text{if } \left(\overline{\rho}_{w,K|L}^{k+1} - \overline{\rho}_{n,K|L}^{k+1}\right) \mathbf{g} \cdot \mathbf{n}_{K|L} > 0 \\ \lambda_n(S_{w,K}^{k+1}) & \text{if } \left(\overline{\rho}_{w,K|L}^{k+1} - \overline{\rho}_{n,K|L}^{k+1}\right) \mathbf{g} \cdot \mathbf{n}_{K|L} \leq 0. \end{cases}$$

The finite volume scheme for the discretization of the problem (4.3)–(4.4) is given by the following set of equations with the unknowns $(p_K^{k+1})_{K\in\mathcal{T}}$ and $(S_{w,K}^{k+1})_{K\in\mathcal{T}}$, $k \in \{0, 1, ..., N-1\}$

$$\begin{aligned} |K|\Phi_K & \frac{\rho_{w,K}^{k+1} S_{w,K}^{k+1} + \rho_{n,K}^{k+1} S_{n,K}^{k+1} - (\rho_{w,K}^{k} S_{w,K}^{k} + \rho_{n,K}^{k} S_{n,K}^{k})}{\delta t} \\ & + \sum_{L\in N_D(K)} |\sigma_{K|L}| Q_{K|L}^{k+1} + \sum_{\sigma\in\partial K\cap\Gamma_N} |\sigma| q_\sigma^{t,k+1} = |K| F_{w,K}^{k+1} + |K| F_{n,K}^{k+1}, \end{aligned} \tag{4.13}$$

$$\begin{aligned} |K|\Phi_K \frac{\rho_{n,K}^{k+1} S_{n,K}^{k+1} - \rho_{n,K}^{k} S_{n,K}^{k}}{\delta t} & + \sum_{L\in N_D(K)} |\sigma_{K|L}| F_{K|L}^{n,k+1} + \sum_{L\in N_D(K)} |\sigma_{K|L}| C_{K|L}^{k+1} \\ - \sum_{L\in N_D(K)} |\sigma_{K|L}| b_{g,K|L}^{k+1} & + \sum_{\sigma\in\partial K\cap\Gamma_N} |\sigma| q_\sigma^{n,k+1} = |K| F_{n,K}^{k+1}. \end{aligned} \tag{4.14}$$

In the case of $\sigma_{K|L} \in N_D(K) \setminus N(K)$ we set $p_L^{k+1} = p_L^D$, $S_{w,L}^{k+1} = S_{w,L}^D$, $d_{K|L} = d_{K,\sigma}$, and $d_{L,\sigma} = 0$.

The wetting phase mass balance equation can be discretized in the following way

$$|K|\Phi_K \frac{\rho_{w,K}^{k+1} S_{w,K}^{k+1} - \rho_{w,K}^{k} S_{w,K}^{k}}{\delta t} + \sum_{L \in N_D(K)} |\sigma_{K|L}| F_{K|L}^{w,k+1} - \sum_{L \in N_D(K)} |\sigma_{K|L}| C_{K|L}^{k+1} \\ + \sum_{L \in N_D(K)} |\sigma_{K|L}| b_{g,K|L}^{k+1} + \sum_{\sigma \in \partial K \cap \Gamma_N} |\sigma| q_\sigma^{w,k+1} = |K| F_{w,K}^{k+1}. \tag{4.15}$$

This numerical method was implemented in the DuMu$^\text{x}$ framework, precisely in DuMu$^\text{x}$ 3, see [43, 66]. For solving the nonlinear system we have used DuMu$^\text{x}$ implementation of the Newton method with biconjugate gradient stabilized method (BiCGSTAB) as linear solver and Algebraic Multigrid (AMG) as preconditioner. In order to compute the nonwetting phase pressure p_n from the global pressure p and the wetting phase saturation S_w we have used the explicit Runge-Kutta-Fehlberg method in order to solve the Cauchy problem (1.47). For the computation of the function ω from (1.50) we have used composite trapezoidal rule. For a detailed description of the implementation check the Appendix A.

4.3 Numerical simulations in homogeneous case

In this section we present test cases which are used for the validation of the proposed finite volume scheme. In the following test cases we have assumed that the domain is homogeneous, in a sense that we have the same capillary pressure law on the whole domain. Presented results are validated by comparison with the results obtained with the DuMu$^\text{x}$ 2p module for two-phase, immiscible flow. In the next section we will consider the case with different capillary pressure curves on the different subdomains.

4.3.1 Injection of gas in homogeneous domain

The first test case is inspired by the test case from the MoMas benchmark [28], with simplification that the two-phase flow model is considered, instead of the two-phase two-component flow model. We consider quasi-1D flow with neglected gravity effect on a domain $\Omega = (0,200) \times (0,20)$. The porous domain is assumed to be homogeneous with porosity $\Phi = 0.15$ and absolute permeability $k = 5 \cdot 10^{-20}\text{m}^2$. The fluid system is composed of water, which is assumed incompressible, and hydrogen, with density given by the ideal gas law. The capillary pressure curve and the relative permeabilities are given by the Van-Genuchten law with parameters $\alpha = 0.5 \cdot 10^{-6}\text{Pa}^{-1}$, $n = 1.49$, and $S_{wr} = 0.4$.

The domain is initially fully saturated with water, namely the following initial conditions are taken

$$S_w(x,0) = 1, \quad p_w(x,0) = 10^6 \text{ Pa}, \quad x \in \Omega.$$

The corresponding global pressure p at initial time step is equal to 10^6 Pa. The duration of the simulation is 10^6 years. The bottom and the top part of the boundary are assumed impermeable. The left part of the boundary is the injection part of the boundary with the following boundary conditions:

$$q^w = 0 \text{ kg}/(\text{ms}), \quad q^n = 1.766 \cdot 10^{-13} \text{ kg}/(\text{ms}),$$

for the first 500 000 years. The Dirichlet boundary condition, identical to the initial condition, is imposed on the right part of the boundary. The temperature of the system is set to 303 K.

In the space domain an equidistant grid with $h = 2$ m is used. The initial time step is taken as $\delta t = 100$ s and the maximum time step size is set to $\delta t = 10000$ years. The obtained results are presented in Figures 4.1 - 4.6. In Figure 4.4 we can see that initially, the liquid phase pressure starts to increase, but after around 10000 years it starts to decrease, and by the end of the simulation it is tending to its initial value of 1 MPa. The gas phase pressure is increasing during the whole period of injection, and after the injection has finished it also tends to its initial value of 1 MPa. The gas saturation is slightly increasing due to the small amount of injected hydrogen near the injection boundary, but after the injection period has finished it starts to decrease. Due to the gas saturation growth, we also observe an increase in the capillary pressure in Figure 4.2 during the injection period, and afterwards it starts to decay. It is interesting to compare obtained results to the one of the original test case that are known from the literature. We observe that the increase of the gas saturation in the first 100000 years of the simulation is visible throughout the domain, and not just in the left part of the domain like in the results of the original test case, since we neglected dissolution of gas in water. Due to the same reason gas saturation is significantly larger in the end of the simulation than in the results of the original test case.

The correctness of the presented results is confirmed by comparison with the results obtained by the DuMu$^\text{x}$ 2p module for the two-phase, immiscible flow.

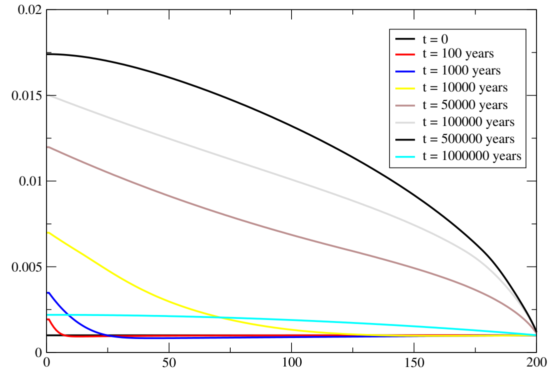

Figure 4.1: Gas saturation

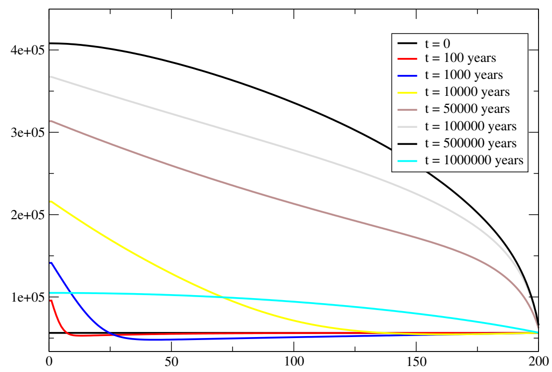

Figure 4.2: Capillary pressure

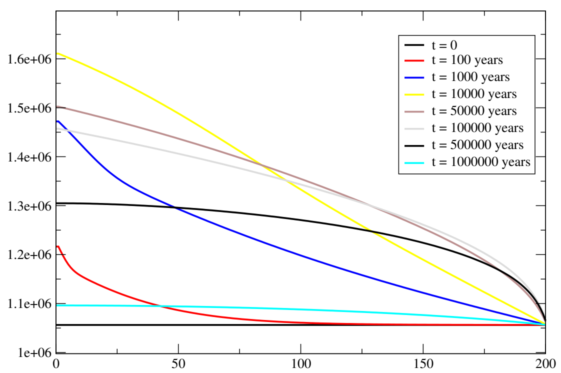

Figure 4.3: Gas phase pressure

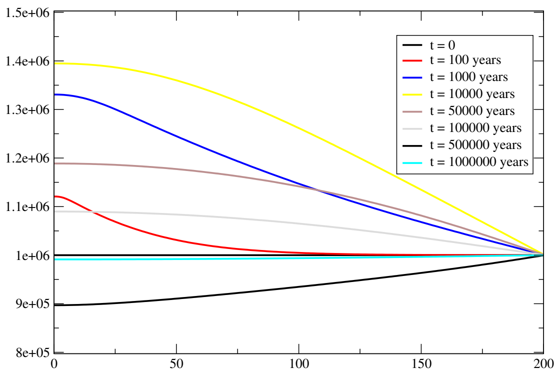

Figure 4.4: Liquid phase pressure

4.3.2 Compressible immiscible two-phase flow starting from non equilibrium state

This test case is also a simplified version of the test case from the MoMas benchmark [28]. In this test case an impermeable domain $\Omega = (0,1) \times (0,0.1)$ is considered. The domain is again assumed to be homogeneous with porosity $\Phi = 0.3$ and absolute permeability $k = 10^{-16}\text{m}^2$. The gravity term is once again neglected. The considered fluid system is the same as in the previous test case. The parameters for the capillary pressure and the relative permeability laws are given by $\alpha = 0.5 \cdot 10^{-6}\text{Pa}^{-1}$, $n = 1.54$ and $S_{wr} = 0.01$.

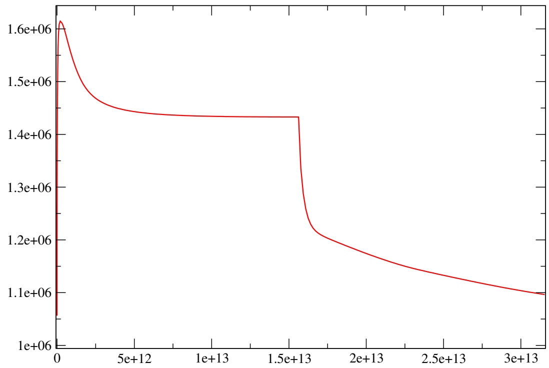

Figure 4.5: Evolution of the gas pressure on inlet over time

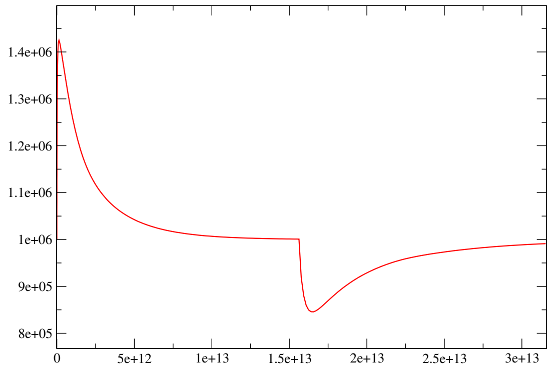

Figure 4.6: Evolution of the liquid pressure on inlet over time

The initial condition differs on the left and the right part of the domain, which represents additional difficulty while performing simulation. On the left part the initial condition is imposed as

$$S_w(x,0) = 0.962, \quad p_w(x,0) = 10^6 \text{ Pa}, \quad x \leq 0.5.$$

On the rest of the domain, the initial condition is set to be

$$S_w(x,0) = 0.842, \quad p_w(x,0) = 10^6 \text{ Pa}, \quad x > 0.5.$$

On the left part of the domain the initial global pressure is equal to 1.001 MPa and on the right part of the domain the initial global pressure is equal to 1.156 MPa. The duration of the simulation is 10^6 s. For the space domain, we have used an equidistant grid with $h = 2$ mm, and the initial time step is $\delta t = 0.01$ s. The obtained results are given in Figures 4.7 - 4.10. In Figure 4.7 we see that the gas phase starts to flow from the right part of the domain to the left part of the domain, and by the end of the simulation it is tending to a constant value $S_n = 0.1$ throughout the domain. As we see in Figure 4.8, due to the increase of the gas saturation in the left part of the domain, the capillary pressure is also increasing, while in the right part of the domain appears the decrease of the capillary pressure since there is also decrease in the gas phase saturation. By the end of the simulation, the capillary pressure is tending to the constant value of 1MPa. We observe the similar behavior for the gas phase pressure in Figure 4.9. At the beginning of the simulation, as one can see in Figure 4.10, the liquid phase pressure starts to increase at the center of the domain and by the end of the simulation it is tending to the constant value around 1.3 MPa.

Validation of the results was done through comparison with the DuMu^x 2p module. By comparison with results of the benchmark MoMas we note that we obtain physically correct behavior.

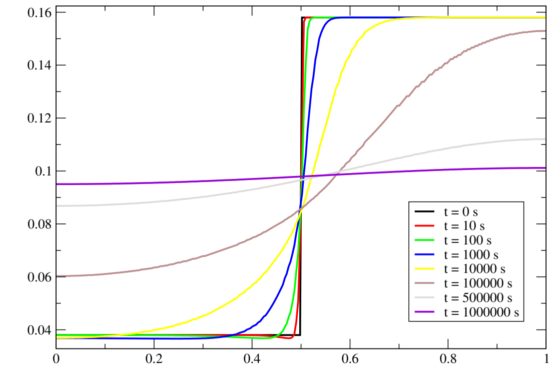

Figure 4.7: Gas saturation

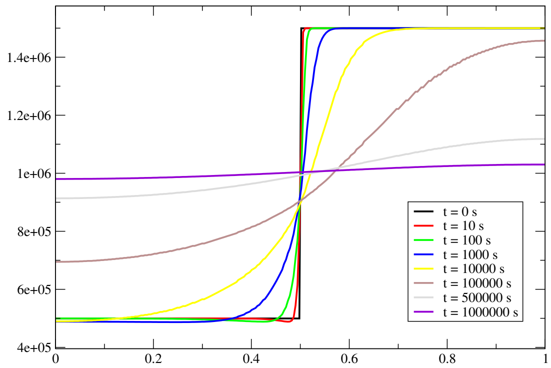

Figure 4.8: Capillary pressure

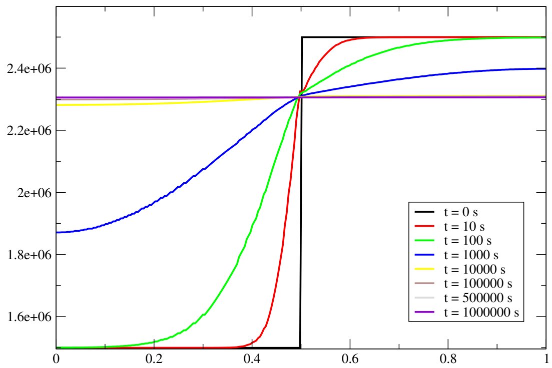

Figure 4.9: Gas phase pressure

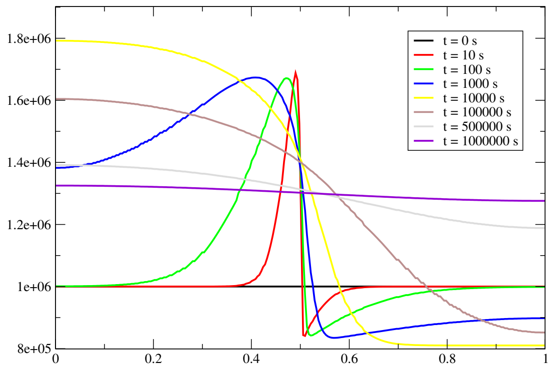

Figure 4.10: Liquid phase pressure

4.3.3 The secondary recovery of gas by injecting water

This test case is taken from [56], and results for this test obtained using numerical scheme (3.37)–(3.38) were already presented in this thesis in Section 3.9. Now we present the results obtained by the scheme (4.13)–(4.14).

The obtained results are given in Figures 4.11 - 4.14. In these figures one can see typical displacement of the nonwetting phase by the wetting phase. We observe that the front is not symmetric since the injection part of the boundary is set at the left part of the boundary. The presented results correspond to the one presented in [56] and to the one obtained by the DuMu^x 2p module and also to the one presented in Section 3.9.

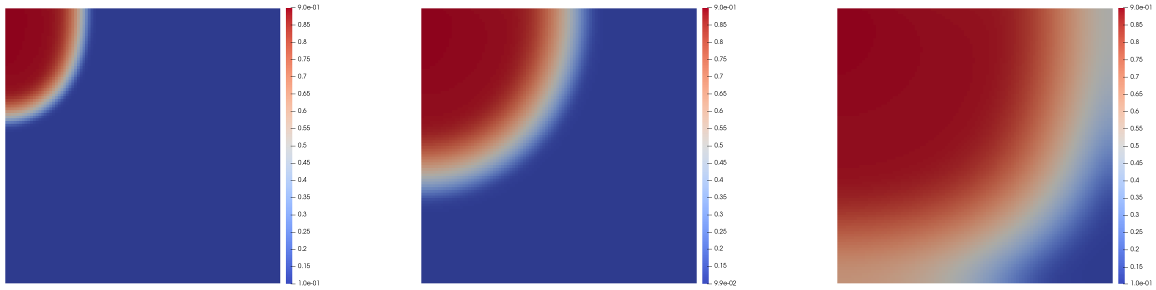

Figure 4.11: Water saturation at $t = 2$ s, 10 s, 40 s

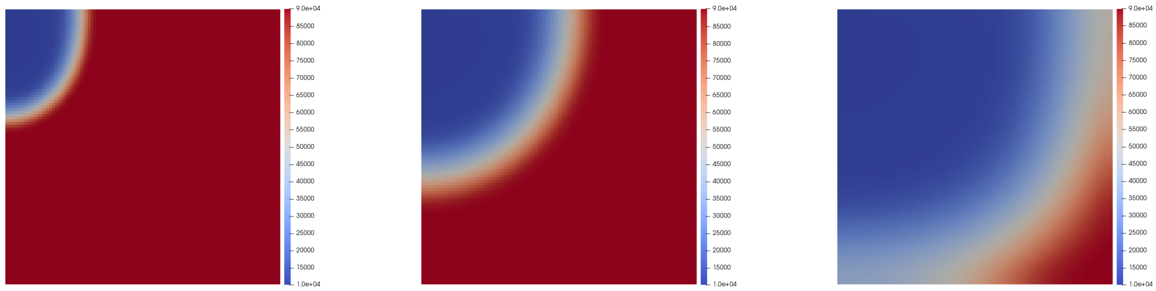

Figure 4.12: Capillary pressure at $t = 2$ s, 10 s, 40 s

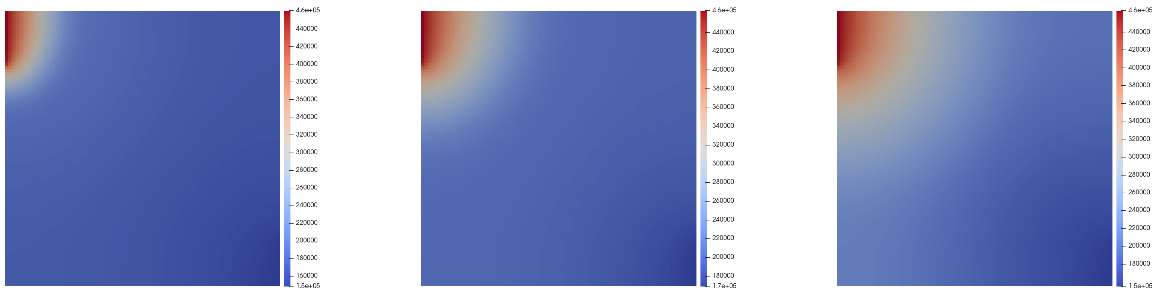

Figure 4.13: Gas phase pressure at $t = 2$ s, 10 s, 40 s

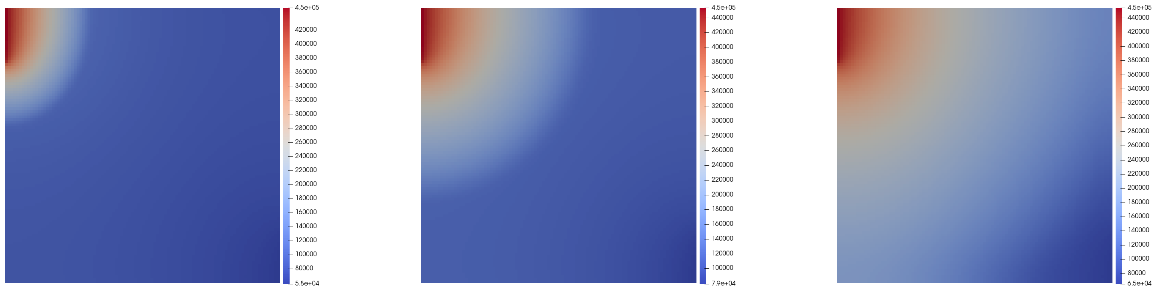

Figure 4.14: Liquid phase pressure at $t = 2$ s, 10 s, 40 s

4.3.4 Homogeneous two-phase compressible lock-exchange flow with viscous forces, buoyancy and capillary pressure

The next test case is inspired by the test case from [58]. The domain $\Omega = (0, 100)^2$ is homogeneous with absolute permeability $k = 5 \cdot 10^{-14}$ m^2 and porosity $\Phi = 0.4$. For the capillary pressure law, the Brooks Corey capillary pressure curve $p_c(S_{we}) = P_e S_{we}^{-\frac{1}{\lambda}}$ is used with parameters $P_e = 0.75$ MPa and $\lambda = 4$. The relative permeability functions are

$$kr_w(S_{we}) = S_{we}^{m_1}, \quad kr_n(S_{we}) = (1 - S_{we})^{m_2},$$

where we have set $S_{wr} = 0$, $m_1 = 2.5$ and $m_2 = 2$. Instead of an incompressible fluid system which was used in [58], we have used a fluid system composed of hydrogen and water. The boundary is assumed to be impermeable. The temperature is equal to 293.15 K. The initial pressure of the wetting phase is set to $p_w = 10^6$ Pa. An additional difficulty is introduced in this test case by imposing a discontinuity in the initial saturation of the nonwetting phase:

$$S_n(0, x) = \begin{cases} 0.1 & \text{if } x \leq 50, \\ 0.9 & \text{if } x > 50. \end{cases}$$

The initial global pressure on the left part of the domain is equal to $2.5 \cdot 10^5$ Pa and on the right part of the domain it is equal to $4.34 \cdot 10^5$ Pa. The time of simulation is 6000 days. In Figures 4.15 - 4.18, given below, one can see the obtained results. In Figure 4.15 we see that the water starts to flow from the left to the right side of the domain, and gas starts to flow from the right part to the left part of the domain. Since the water is heavier fluid it remains in the bottom part of the domain and the gas flows to the upper part of the domain. In Figure 4.16 we see that during the simulation the capillary pressure is decreasing in the bottom layers of the domain as the water is entering this region. Since the gas saturation is increasing in the upper layers of the domain, we observe an increase in the capillary pressure in this region. We observe a similar behavior of the phase pressures in the Figures 4.17 and 4.18.

Once again correctness of the presented results is confirmed by comparison with the results obtained with the DuMu^{x} module for two-phase, immiscible flow. Similar physical behavior was also observed in the results presented in [58] for incompressible fluid flow.

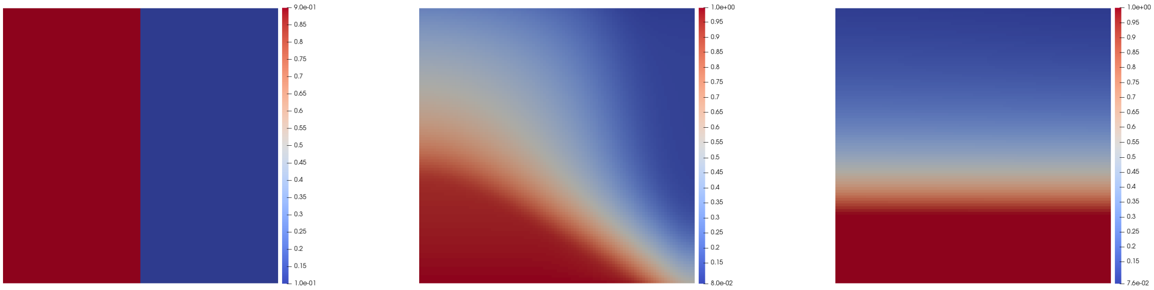

Figure 4.15: Water saturation at $t = 0, 500$ days, 6000 days

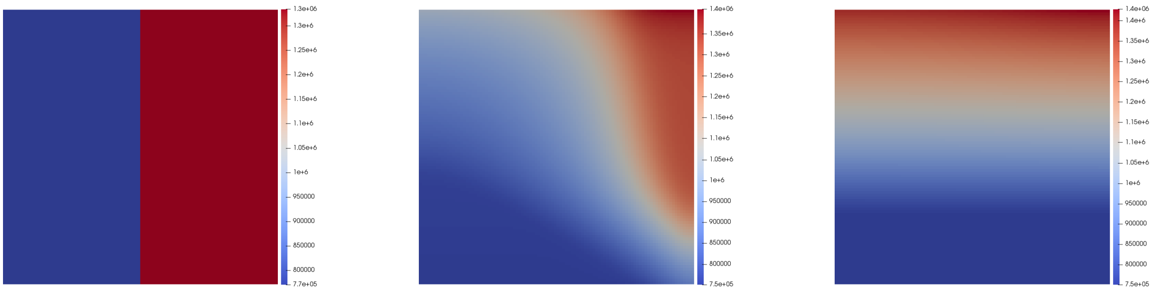

Figure 4.16: Capillary pressure at $t = 0, 500$ days, 6000 days

4.3.5 Injection of the hydrogen in a domain initially saturated with water

This test case is a simplified version of the test case 3.2.6 from [13], where we have once again used a two-phase flow model instead of a two-phase two-component flow model. A cubic domain with the volume of 10 m^3 is considered. A smaller cube with the volume of 1 m^3 at the bottom left corner is removed from a domain. The domain is initially fully saturated with water and the liquid phase pressure is assumed hydrostatic. Hydrogen is being injected in the domain

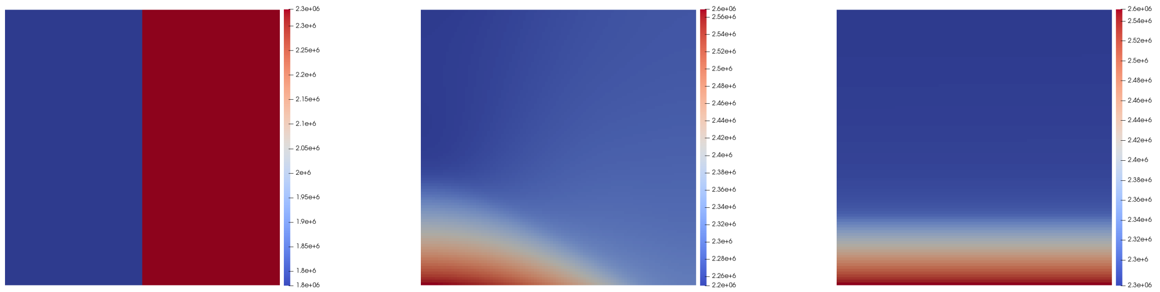

Figure 4.17: Gas phase pressure at $t = 0, 500$ days, 6000 days

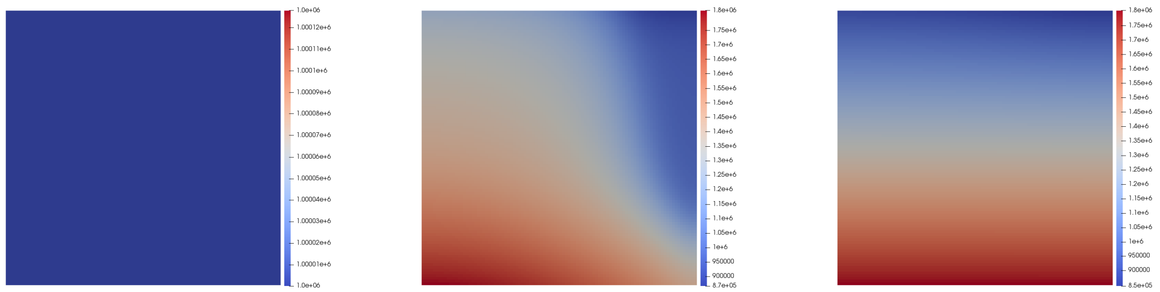

Figure 4.18: Water phase pressure at $t = 0, 500$ days, 6000 days

through the bottom left corner, with the following Neumann boundary condition:

$$q^w = 0 \text{ kg}/(\text{m}^2\text{s}), \quad q^n = 5.35 \cdot 10^{-11} \text{ kg}/(\text{m}^2\text{s}).$$

The Dirichlet boundary conditions corresponding to the initial boundary conditions are imposed on the top and the right part of the domain. The rest of the boundary is assumed impermeable. The duration of the simulation is 1000 years. The permeability is set to $k = 10^{-20}$ m^2 and porosity to 0.15. Van Genuchten's capillary pressure curve with parameters $n = 1.49$ and $\alpha = 0.067 \cdot 10^{-6}$ Pa^{-1} is used. The wetting phase is composed of water which is assumed incompressible and the gas phase is composed of hydrogen with density given by the ideal gas law.

The obtained results are shown in the Figures 4.19 - 4.21. In Figure 4.19 we can see a decrease in the water saturation around the injection hole. This decrease is visible during the first 100 years of simulation. Afterwards we can see the gas phase flow in the bottom of the domain, as a consequence of the imposed Dirichlet boundary conditions. In Figures 4.20 and 4.21 we can see that the phase pressures are increasing in the left bottom corner as a consequence of the gas injection. After around 100 years the phase pressures also start to decrease.

Validation of the results is done through comparison with the DuMu$^\text{x}$ 2p module. In the presented results one can observe behavior that is similar to the one presented in the results of the original test case in [13].

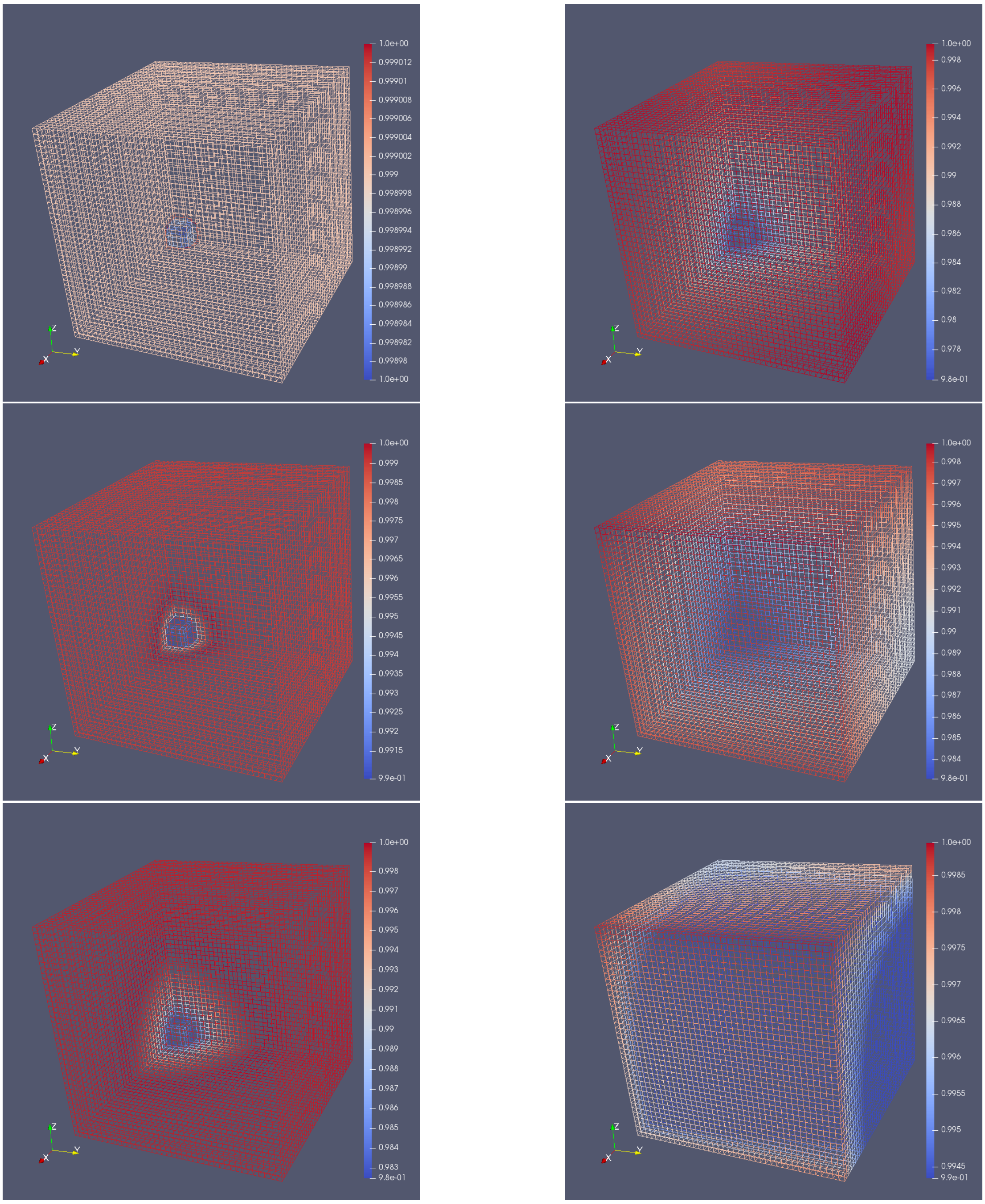

Figure 4.19: Water saturation at $t = 1$ day, 1 yr, 10 yrs in the first column, 100 yrs, 500 yrs, 1000 yrs in the second column

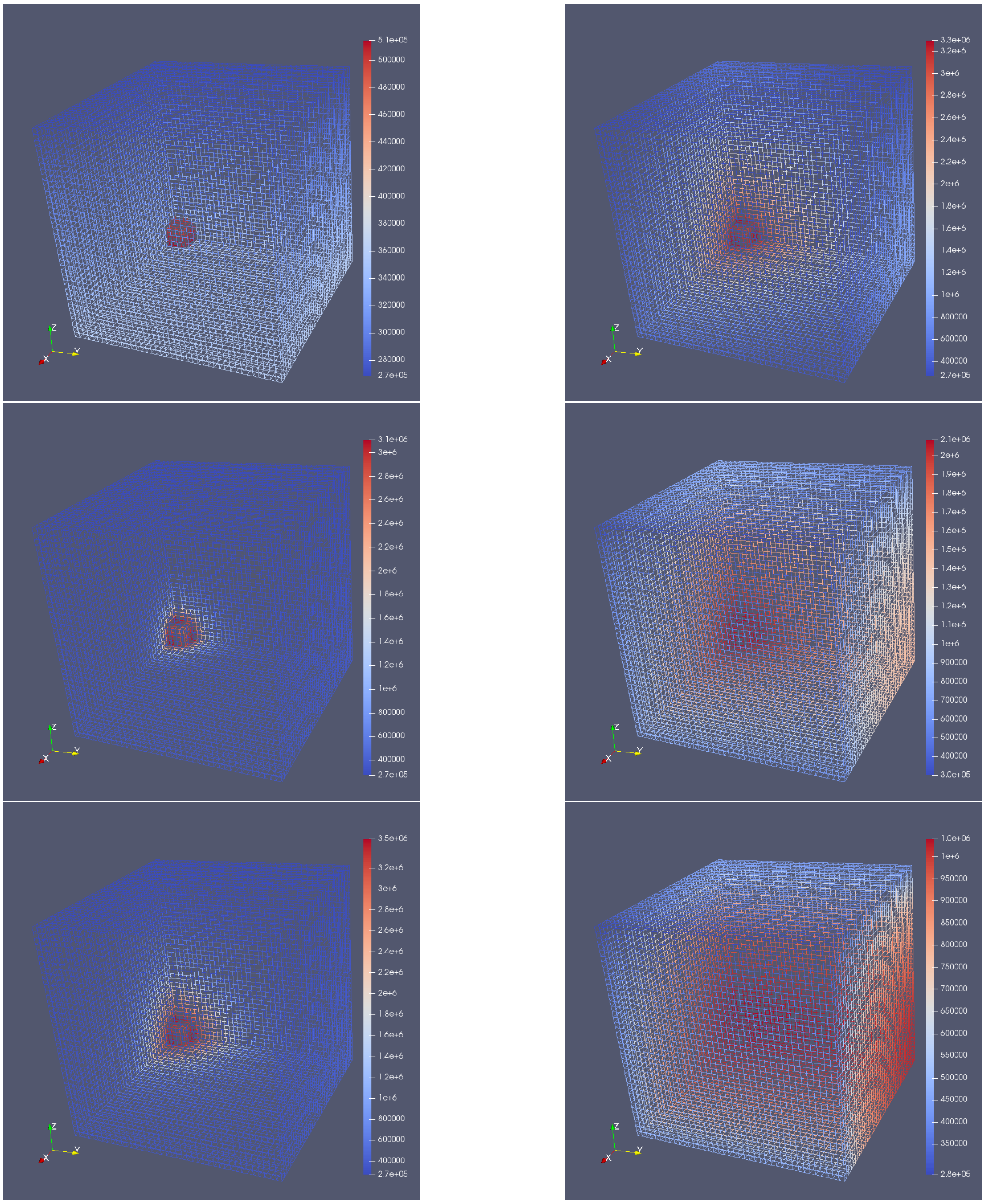

Figure 4.20: Gas phase pressure at $t = 1$ day, 1 yr, 10 yrs in the first column, 100 yrs, 500 yrs, 1000 yrs in the second column

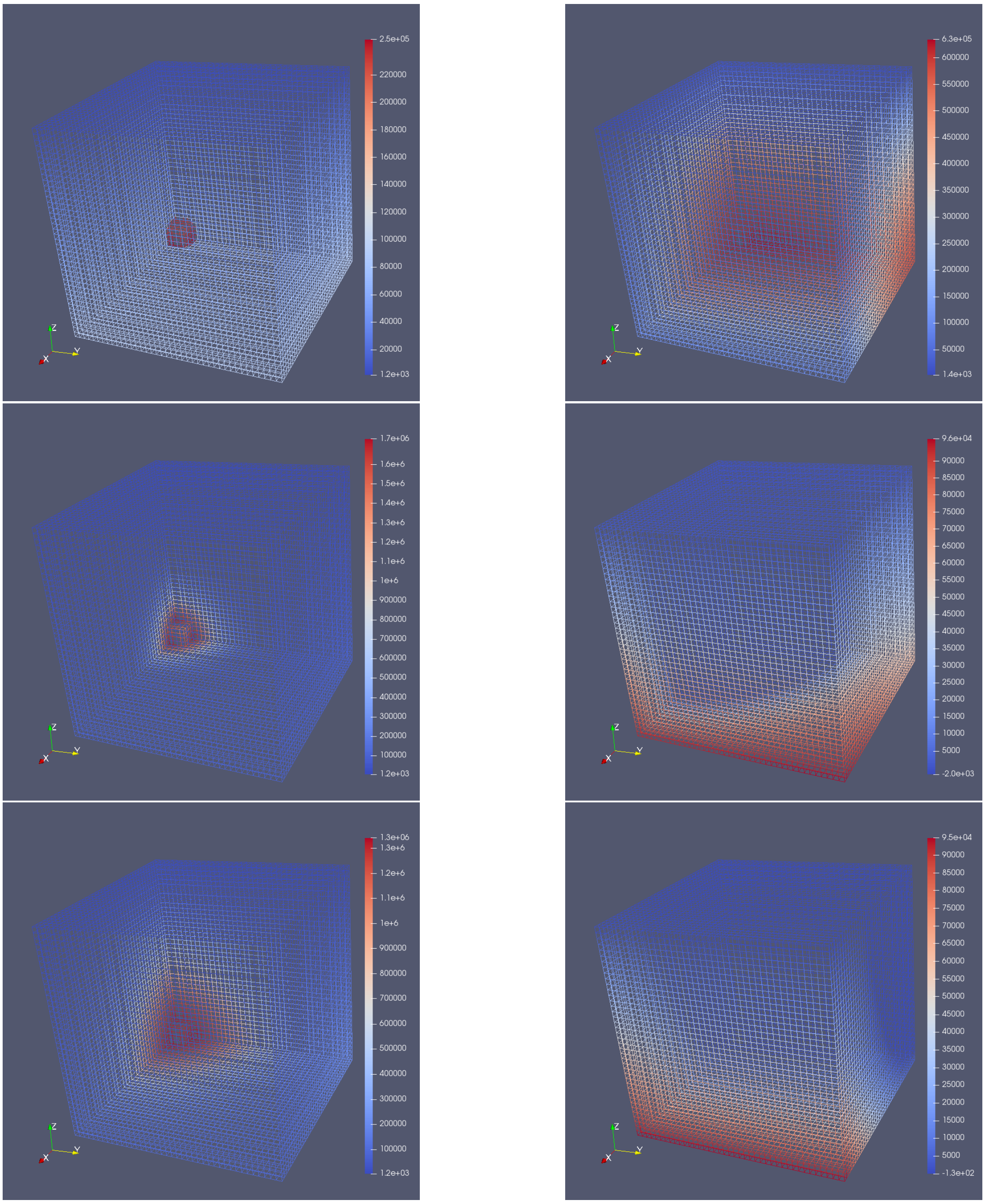

Figure 4.21: Liquid phase pressure at $t = 1$ day, 1 yr, 10 yrs in the first column, 100 yrs, 500 yrs, 1000 yrs in the second column

4.4 Discontinuous capillary pressure problem

Let us now consider a porous domain composed of multiple rock types. Each rock type has different properties, as well as different relative permeabilities and different capillary pressure curves. For simplicity let us consider a domain composed of two different rock types, $\Omega = \Omega_1 \cup \Omega_2$. We denote the interface between these two parts of the domain by Γ, and we emphasize dependency of the given function on domain Ω_i by the subscript $i, i \in \{1,2\}$. For example we will have

$$p_c(S_w(x,t)) = \begin{cases} p_{c,1}(S_w(x,t)) & \text{if } x \in \Omega_1 \\ p_{c,2}(S_w(x,t)) & \text{if } x \in \Omega_2. \end{cases}$$

To simplify the notation we will denote the wetting phase saturation S_w by S in the rest of this section. We will also omit writing the time step dependence. For simplicity, here we only consider capillary pressure curves that satisfies $p_{c,1}(S_w = 1) = 0$ and $p_{c,2}(S_w = 1) = 0$.

Approximation of the fluxes on the interface Γ has to be done carefully due to the strong effect of the discontinuity of the capillary pressure function on discretization of the diffusion term. Therefore, as already seen in [30] and [7], at the interface we need to introduce new variables in order to enforce the flux continuity of both phases. For simplicity we consider the two neighboring elements K and L with face $\sigma = \sigma_{K|L}$ belonging to the interface Γ. In the element K we have independent variables p_K and S_K and in the element L we have p_L and S_L. At the interface σ we attach new variables

$$p_{K,\sigma}, S_{K,\sigma}, p_{L,\sigma}, S_{L,\sigma}$$

which represent the one-sided limits of the global pressure ($p_{K,\sigma}$ and $p_{L,\sigma}$) and the wetting phase saturation ($S_{K,\sigma}$ and $S_{L,\sigma}$) at the interface σ. The continuity of the capillary pressure will lead to a jump in the saturation ($S_{K,\sigma} \neq S_{L,\sigma}$) and consequently to a jump in the global pressure ($p_{K,\sigma} \neq p_{L,\sigma}$).

At the interface σ the capillary pressure and the nonwetting phase pressure must be continuous. Therefore we have:

$$\begin{aligned} p_{c,K}(S_{K,\sigma}) &= p_{c,L}(S_{L,\sigma}) = u_\sigma \\ p_{n,K}(S_{K,\sigma}, p_{K,\sigma}) &= p_{n,L}(S_{L,\sigma}, p_{L,\sigma}) = p_{n,\sigma}, \end{aligned} \tag{4.16}$$

where we have denoted the corresponding material functions by indices K and L instead of 1 and 2. Notation u_σ and $p_{n,\sigma}$ denote the capillary pressure and the nonwetting phase pressure at the interface.

The fluxes at the interface will be calculated by the use of these new unknowns which will be eliminated by imposing the continuity of the fluxes.

The total flux is calculated in the following way

$$Q_{K,\sigma} = k_K \lambda(S_K, p_K)\omega(S_K, p_K)\frac{p_K - p_{K,\sigma}}{d_{K,\sigma}} + k_K \mathbf{g}\cdot\mathbf{n}_{K,\sigma}(\lambda\rho)(S_K, p_K). \tag{4.17}$$

The total flux continuity can be expressed as

$$Q_{K,\sigma} + Q_{L,\sigma} = 0 \tag{4.18}$$

Similarly, the nonwetting phase flux at the interface will be calculated as follows

$$\mathscr{F}_{K,\sigma} = f_n(\overline{S}_{K,\sigma}, \overline{p}_{K,\sigma})Q_{K,\sigma} + \alpha(S_K, p_K)k_K\frac{p_c(S_K) - p_c(S_{K,\sigma})}{d_{K,\sigma}} - b_{g,K,\sigma}. \tag{4.19}$$

For the nonwetting phase fractional flow we perform upwind in the following way

$$\overline{S}_{K,\sigma} = \begin{cases} S_K & \text{if } Q_{K,\sigma} \geq 0 \\ S_{K,\sigma} & \text{if } Q_{K,\sigma} < 0, \end{cases} \qquad \overline{p}_{K,\sigma} = \begin{cases} p_K & \text{if } Q_{K,\sigma} \geq 0 \\ p_{K,\sigma} & \text{if } Q_{K,\sigma} < 0. \end{cases}$$

For the gravity convection term, the approximation is taken as follows

$$b_{g,K,\sigma} = (\rho_{w,K} - \rho_{n,K})\frac{\rho_{w,K}\rho_{n,K}\lambda^G_{w,K,\sigma}\lambda^G_{n,K,\sigma}}{\rho_{w,K}\lambda^G_{w,K,\sigma} + \rho_{n,K}\lambda^G_{n,K,\sigma}}k_K \mathbf{g}\cdot\mathbf{n}_{K,\sigma}.$$

Upwind values for phase mobilities in the gravity term are given as follows

$$\lambda^G_{w,K,\sigma} = \begin{cases} \lambda_w(S_K) & \text{if } (\rho_{w,K} - \rho_{n,K})\,\mathbf{g}\cdot\mathbf{n}_{K,\sigma} > 0 \\ \lambda_w(S_{K,\sigma}) & \text{if } (\rho_{w,K} - \rho_{n,K})\,\mathbf{g}\cdot\mathbf{n}_{K,\sigma} \leq 0, \end{cases} \tag{4.20}$$

$$\lambda^G_{n,K\sigma} = \begin{cases} \lambda_n(S_{K,\sigma}) & \text{if } (\rho_{w,K} - \rho_{n,K})\,\mathbf{g}\cdot\mathbf{n}_{K,\sigma} > 0 \\ \lambda_n(S_K) & \text{if } (\rho_{w,K} - \rho_{n,K})\,\mathbf{g}\cdot\mathbf{n}_{K,\sigma} \leq 0. \end{cases} \tag{4.21}$$

The nonwetting phase flux continuity can be expressed as

$$\mathscr{F}_{K,\sigma} + \mathscr{F}_{L,\sigma} = 0. \tag{4.22}$$

Calculation procedure. First we need an efficient procedure to calculate the global pressure as a function of the capillary pressure and the nonwetting phase pressure, therefore we introduce the following notation

$$p = \hat{v}(u, p_n).$$

Then, we consider (4.18) which gives,

$$Q_{K,\sigma}+Q_{L,\sigma}=k_K(\lambda\omega)(S_K,p_K)\frac{p_K-p_{K,\sigma}}{d_{K,\sigma}}+k_K\mathbf{g}\cdot\mathbf{n}_{K,\sigma}(\lambda\rho)(S_K,p_K)$$
$$+k_L(\lambda\omega)(S_L,p_L)\frac{p_L-p_{L,\sigma}}{d_{L,\sigma}}+k_L\mathbf{g}\cdot\mathbf{n}_{L,\sigma}(\lambda\rho)(S_L,p_L)=0.$$

We simplify the notation by introducing

$$A_K=k_K(\lambda\omega)(S_K,p_K),\quad G_K=k_K\mathbf{g}\cdot\mathbf{n}_{K,\sigma}(\lambda\rho)(S_K,p_K),$$

and rewriting (4.18) as

$$A_K\frac{p_K-p_{K,\sigma}}{d_{K,\sigma}}+G_K+A_L\frac{p_L-p_{L,\sigma}}{d_{L,\sigma}}+G_L=0$$

or

$$\frac{A_K}{d_{K,\sigma}}p_{K,\sigma}+\frac{A_L}{d_{L,\sigma}}p_{L,\sigma}=\frac{A_K}{d_{K,\sigma}}p_K+\frac{A_L}{d_{L,\sigma}}p_L+G_K+G_L.$$

To the side σ on the interface we associate two values: the capillary pressure of the interface u_σ and the gas pressure of the interface $p_{n,\sigma}$. These are continuous functions across the interface and therefore have a unique value at the interface. The total flux continuity (4.18) can now be expressed as

$$\frac{A_K}{d_{K,\sigma}}\hat{v}_K(u_\sigma,p_{n,\sigma})+\frac{A_L}{d_{L,\sigma}}\hat{v}_L(u_\sigma,p_{n,\sigma})=\frac{A_K}{d_{K,\sigma}}p_K+\frac{A_L}{d_{L,\sigma}}p_L+G_K+G_L,\tag{4.23}$$

since $p_{K,\sigma}=\hat{v}_K(u_\sigma,p_{n,\sigma}),\ p_{L,\sigma}=\hat{v}_L(u_\sigma,p_{n,\sigma})$. For fixed u_σ the function

$$p_{n,\sigma}\mapsto\frac{A_K}{d_{K,\sigma}}\hat{v}_K(u_\sigma,p_{n,\sigma})+\frac{A_L}{d_{L,\sigma}}\hat{v}_L(u_\sigma,p_{n,\sigma})$$

is monotone increasing, and the equation (4.23) has a unique solution $p_{n,\sigma}$ for fixed u_σ. By solving the equation (4.23) we obtain $p_{n,\sigma}$ as a function of u_σ:

$$p_{n,\sigma}=\hat{p}_n(u_\sigma).$$

If we chose u_σ we can directly calculate $S_{K,\sigma}=p_{c,K}^{-1}(u_\sigma)$ and $S_{L,\sigma}=p_{c,L}^{-1}(u_\sigma)$. By solving the equation (4.23) we get $p_{n,\sigma}$ and then we have $p_{K,\sigma}=\hat{v}_K(u_\sigma,p_{n,\sigma})$ and $p_{L,\sigma}=\hat{v}_L(u_\sigma,p_{n,\sigma})$. Then we can define the total fluxes in both cells:

$$Q_{K,\sigma}=A_K\frac{p_K-p_{K,\sigma}}{d_{K,\sigma}}+G_K,\quad Q_{L,\sigma}=-Q_{K,\sigma}.$$

Now we have a single value to determine, the capillary pressure u_σ, and it will be determined from the continuity of the nonwetting phase flux across the interface (4.22), which can be written as

$$\begin{aligned} f_n(\overline{S}_{K,\sigma},\overline{p}_{K,\sigma})Q_{K,\sigma} + \alpha(S_K,p_K)k_K \frac{p_c(S_K)-p_c(S_{K,\sigma})}{d_{K,\sigma}} - b_{g,K,\sigma} \\ + f_n(\overline{S}_{L,\sigma},\overline{p}_{L,\sigma})Q_{L,\sigma} + \alpha(S_L,p_L)k_L \frac{p_c(S_L)-p_c(S_{L,\sigma})}{d_{L,\sigma}} - b_{g,L,\sigma} = 0. \end{aligned} \tag{4.24}$$

To simplify notation let us denote $D_K = \alpha(S_K,p_K)k_K$, $D_L = \alpha(S_L,p_L)k_L$, $u_K = p_c(S_K)$, $u_L = p_c(S_L)$, and

$$\overline{u}_{K,\sigma} = \begin{cases} u_K & \text{if } Q_{K,\sigma} \geq 0 \\ u_\sigma & \text{if } Q_{K,\sigma} < 0. \end{cases}$$

Now we can rewrite equation (4.24) as $\Psi(u_\sigma) = 0$, where

$$\begin{aligned} \Psi(u_\sigma) = \big(f_n(\overline{S}_{K,\sigma},\hat{v}_K(\overline{u}_{K,\sigma},\hat{p}_n(\overline{u}_{K,\sigma}))) - f_n(\overline{S}_{L,\sigma},\hat{v}_L(\overline{u}_{L,\sigma},\hat{p}_n(\overline{u}_{L,\sigma})))\big)\, Q_{K,\sigma}(u_\sigma) \\ + D_K \frac{u_K - u_\sigma}{d_{K,\sigma}} - b_{g,K,\sigma} + D_L \frac{u_L - u_\sigma}{d_{L,\sigma}} - b_{g,L,\sigma}. \end{aligned} \tag{4.25}$$

Lemma 4.4.1. *Let $s_K, s_L \in [0,1]$. Then there exists $u_\sigma \in [0, \max_i p_{c,i}(0)]$ such that $\Psi(u_\sigma) = 0$.*

Proof. For the proof of the lemma we use a technique similar to the one from the proof of Lemma 2.1. in [30]. We will show that the limits of the function $\Psi(u_\sigma)$ when $u_\sigma \to 0$ and $u_\sigma \to \max_i p_{c,i}$ have different signs and then the result follows from the continuity of the function $\Psi(u_\sigma)$.

Since the function $u \mapsto \hat{v}(u,\hat{p}_n(u))$ is continuous on $[0,\max_i p_{c,i}(0))$ we can pass to the limit when $u \to 0$ to obtain

$$\begin{aligned} p_{K,\sigma} &= \lim_{u\to 0} \hat{v}_K(u,\hat{p}_n(u)) = \hat{p}_n(0), \\ p_{L,\sigma} &= \lim_{u\to 0} \hat{v}_L(u,\hat{p}_n(u)) = \hat{p}_n(0). \end{aligned}$$

If we pass to the limit $u \to 0$ in equation (4.23) we obtain

$$\frac{A_K}{d_{K,\sigma}}\hat{p}_n(0) + \frac{A_L}{d_{L,\sigma}}\hat{p}_n(0) = \frac{A_K}{d_{K,\sigma}}p_K + \frac{A_L}{d_{L,\sigma}}p_L + G_K + G_L. \tag{4.26}$$

From the previous equation we conclude

$$\hat{p}_n(0) = \frac{\dfrac{A_K}{d_{K,\sigma}}p_K + \dfrac{A_L}{d_{L,\sigma}}p_L + G_K + G_L}{\dfrac{A_K}{d_{K,\sigma}} + \dfrac{A_L}{d_{L,\sigma}}},$$

i.e. the function $Q_{K,\sigma}(u_\sigma)$ has a finite limit when $u_\sigma \to 0$. For passing to the limit $u_\sigma \to \max_i p_{c,i}(0)$ we will apply Remark 1.3.3 to obtain the following inequalities

$$\begin{aligned} \hat{v}_K(u_\sigma, \hat{p}_n(u_\sigma)) \le \hat{p}_n(u_\sigma) \le \hat{v}_K(u_\sigma, \hat{p}_n(u_\sigma)) + M_K, \\ \hat{v}_L(u_\sigma, \hat{p}_n(u_\sigma)) \le \hat{p}_n(u_\sigma) \le \hat{v}_L(u_\sigma, \hat{p}_n(u_\sigma)) + M_L, \end{aligned} \tag{4.27}$$

for some $M_K, M_L > 0$. If we apply these estimates to (4.23) we have

$$\frac{A_K}{d_{K,\sigma}}(\hat{p}_n(u_\sigma) - M_K) + \frac{A_L}{d_{L,\sigma}}(\hat{p}_n(u_\sigma) - M_L) \le \frac{A_K}{d_{K,\sigma}} p_K + \frac{A_L}{d_{L,\sigma}} p_L + G_K + G_L, \tag{4.28}$$

which leads to

$$\hat{p}_n(u_\sigma) \le \frac{\frac{A_K}{d_{K,\sigma}} p_K + \frac{A_L}{d_{L,\sigma}} p_L + G_K + G_L}{\frac{A_K}{d_{K,\sigma}} + \frac{A_L}{d_{L,\sigma}}} + \max\{M_K, M_L\}.$$

Therefore, we conclude that $\hat{v}_K(u_\sigma, \hat{p}_n(u_\sigma))$ is bounded and consequently we have the boundedness of the function $Q_{K,\sigma}(u_\sigma)$ when $u_\sigma \to \max_i p_{c,i}(0)$.

Now we consider the first term in the function $\Psi(u_\sigma)$. Let us assume $Q_{K,\sigma}(0) > 0$. Then we have $Q_{K,\sigma}(u_\sigma) > 0$ for $u_\sigma \in [0, \varepsilon)$, for some $\varepsilon > 0$, and consequently

$$\begin{aligned} &\left(f_n(\overline{S}_{K,\sigma}, \hat{v}_K(\overline{u}_{K,\sigma}, \hat{p}_n(\overline{u}_{K,\sigma}))) - f_n(\overline{S}_{L,\sigma}, \hat{v}_L(\overline{u}_{L,\sigma}, \hat{p}_n(\overline{u}_{L,\sigma})))\right) Q_{K,\sigma}(u_\sigma) \\ &\qquad = f_n(S_K, p_K) Q_{K,\sigma}(u_\sigma) - f_n(S_{L,\sigma}, \hat{v}_L(u_\sigma, \hat{p}_n(u_\sigma))) Q_{K,\sigma}(u_\sigma). \end{aligned}$$

Since $f_n(1, p_{n,\sigma}) = 0$ and the function $Q_{K,\sigma}(u_\sigma)$ has a finite limit when $u_\sigma \to 0$ we conclude

$$\lim_{u_\sigma \to 0} f_n(S_{L,\sigma}, \hat{v}_L(u_\sigma, \hat{p}_n(u_\sigma))) Q_{K,\sigma}(u_\sigma) = 0,$$

which leads to

$$\lim_{u_\sigma \to 0} \left(f_n(\overline{S}_{K,\sigma}, \hat{v}(\overline{u}_{K,\sigma}, \hat{p}_n(\overline{u}_{K,\sigma}))) - f_n(\overline{S}_{L,\sigma}, \hat{v}_L(\overline{u}_{L,\sigma}, \hat{p}_n(\overline{u}_{L,\sigma})))\right) Q_{K,\sigma}(u_\sigma) \ge 0. \tag{4.29}$$

In the case $Q_{K,\sigma}(0) = 0$ we have

$$\lim_{u_\sigma \to 0} \left(f_n(\overline{S}_{K,\sigma}, \hat{v}_K(\overline{u}_{K,\sigma}, \hat{p}_n(\overline{u}_{K,\sigma}))) - f_n(\overline{S}_{L,\sigma}, \hat{v}_L(\overline{u}_{L,\sigma}, \hat{p}_n(\overline{u}_{L,\sigma})))\right) Q_{K,\sigma}(u_\sigma) = 0,$$

and in the case $Q_{K,\sigma}(0) < 0$ we can apply the same reasoning as in the first case since

$$\left(f_n(\overline{S}_{K,\sigma}, \hat{v}_K(\overline{u}_{K,\sigma}, \hat{p}_n(\overline{u}_{K,\sigma}))) - f_n(\overline{S}_{L,\sigma}, \hat{v}_L(\overline{u}_{L,\sigma}, \hat{p}_n(\overline{u}_{L,\sigma})))\right) Q_{K,\sigma}(u_\sigma)$$

$$= f_n(S_{K,\sigma}, \hat{v}_K(u_\sigma, \hat{p}_n(u_\sigma)))Q_{K,\sigma}(u_\sigma) - f_n(S_L, p_L)Q_{K,\sigma}(u_\sigma),$$

which leads to a nonnegative limit at $u_\sigma \to 0$.

For the term $-b_{g,K,\sigma}$ we have

$$-\lim_{u_\sigma \to 0} b_{g,K,\sigma} \geq 0, \tag{4.30}$$

since in the case $(\rho_{w,K} - \rho_{n,K})\mathbf{g} \cdot \mathbf{n}_{K,\sigma} > 0$ we get (see 4.21)

$$\lambda^G_{n,K,\sigma} = \lambda_n(S_{K,\sigma}) \to 0, \text{ when } u_\sigma \to 0.$$

We can perform the same calculations for the term $b_{g,L,\sigma}$, leading to

$$-\lim_{u_\sigma \to 0} b_{g,L,\sigma} \geq 0. \tag{4.31}$$

From the estimates (4.29), (4.30) and (4.31) we conclude

$$\lim_{u_\sigma \to 0} \Psi(u_\sigma) \geq D_K \frac{u_K}{d_{K,\sigma}} + D_L \frac{u_L}{d_{L,\sigma}} \geq 0. \tag{4.32}$$

Now we pass to the limit $u_\sigma \to \max_i p_{c,i}(0)$ i.e. $S_{K,\sigma} \to 0$ and $S_{L,\sigma} \to 0$. In the case $Q_{K,\sigma}(\max_i p_{c,i}(0)) > 0$ we have

$$\lim_{u_\sigma \to \max_i p_{c,i}(0)} (f_n(S_K, p_K) - f_n(S_{L,\sigma}, \hat{v}_L(u_\sigma, \hat{p}_n(u_\sigma))))Q_{K,\sigma}(u_\sigma) \leq 0 \tag{4.33}$$

due to $f_n(0, p_{n,\sigma}) = 1, |f_n(S_K, p_K)| \leq 1$ and the boundedness of the function $Q_{K,\sigma}(u_\sigma)$. The case $Q_{K,\sigma}(u_\sigma) = 0$ is again trivial, and for the case $Q_{K,\sigma}(u_\sigma) < 0$ we get the same conclusion

$$\lim_{u_\sigma \to \max_i p_{c,i}(0)} (f_n(S_{K,\sigma}, \hat{v}_K(u_\sigma, \hat{p}_n(u_\sigma))) - f_n(S_L, p_L))))Q_{K,\sigma}(u_\sigma) \leq 0.$$

For the term $-b_{g,K,\sigma}$ we conclude

$$-\lim_{u_\sigma \to \max_i p_{c,i}(0)} b_{g,K,\sigma} \leq 0, \tag{4.34}$$

since in the case $(\rho_{w,K} - \rho_{n,K})\mathbf{g} \cdot \mathbf{n}_{K,\sigma} \leq 0$ by (4.20) we have

$$\lambda^G_{w,K,\sigma} = \lambda_w(S_{K,\sigma}) \to 0 \text{ when } u_\sigma \to \max_i p_{c,i}(0).$$

The same conclusion is valid for $-b_{g,L,\sigma}$, therefore we conclude

$$\lim_{u_\sigma \to \max_i p_{c,i}(0)} \Psi(u_\sigma) \leq D_K \frac{u_K - \max_i p_{c,i}(0)}{d_{K,\sigma}} + D_L \frac{u_L - \max_i p_{c,i}(0)}{d_{L,\sigma}} \leq 0.$$

Since the function Ψ is continuous, we conclude that there exists u_σ such that $\Psi(u_\sigma) = 0$. □

Algorithms In order to find a solution to the nonlinear equation $\Psi(u_\sigma) = 0$ by some iterative procedure, in each iteration we have to find $p_{n,\sigma}$ from the nonlinear equation

$$\frac{A_K}{d_{K,\sigma}}\hat{v}_K(u_\sigma, p_{n,\sigma}) + \frac{A_L}{d_{L,\sigma}}\hat{v}_L(u_\sigma, p_{n,\sigma}) = \frac{A_K}{d_{K,\sigma}}p_K + \frac{A_L}{d_{L,\sigma}}p_L + G_K + G_L,$$

for fixed u_σ. Therefore, we define the function

$$g_{u_\sigma}(p_{n,\sigma}) = \frac{A_K}{d_{K,\sigma}}\hat{v}_K(u_\sigma, p_{n,\sigma}) + \frac{A_L}{d_{L,\sigma}}\hat{v}_L(u_\sigma, p_{n,\sigma}) - \frac{A_K}{d_{K,\sigma}}p_K - \frac{A_L}{d_{L,\sigma}}p_L - G_K - G_L.$$

Algorithm 1 for given u_σ finds $p_{n,\sigma}$ which is the solution to the nonlinear equation $g_{u_\sigma}(p_{n,\sigma}) = 0$, using the Newton iterations. Algorithm 2 solves the equation $\Psi(u_\sigma) = 0$ by the Newton method. So instead of solving the nonlinear system of two equations with unknowns $p_{n,\sigma}$ and u_σ we are searching for solutions of the two decoupled nonlinear equations.

Data: capillary pressure u_σ, precision EPS, maximum number of iterations $maxIter$

Result: $p_{n,\sigma}$

Set initial approximation:

$p^0_{n,\sigma} = \frac{t_K p_{n,K} + t_L p_{n,L}}{t_K + t_L}$, where $t_K = \frac{k_K}{d_{K,\sigma}}, t_L = \frac{k_L}{d_{L,\sigma}}$;

Compute $g_{u_\sigma}(p^0_{n,\sigma})$ and $g'_{u_\sigma}(p^0_{n,\sigma})$;

while $N < maxIter$ **do**

  $p^1_{n,\sigma} = p^0_{n,\sigma} - \frac{g_{u_\sigma}(p^0_{n,\sigma})}{g'_{u_\sigma}(p^0_{n,\sigma})}$;

  Compute $g_{u_\sigma}(p^1_{n,\sigma})$ **if** ($|g_{u_\sigma}(p^1_{n,\sigma})| < EPS$ *or* $|p^1_{n,\sigma} - p^0_{n,\sigma}|/|p^0_{n,\sigma}| < EPS$) **then**

    return $p^1_{n,\sigma}$;

  end

  $N = N + 1$;

  Set $p^0_{n,\sigma} = p^1_{n,\sigma}$, $g_{u_\sigma}(p^0_{n,\sigma}) = g_{u_\sigma}(p^1_{n,\sigma})$;

  Compute $g'_{u_\sigma}(p^0_{n,\sigma})$;

end

Algorithm 1: $p_{n,\sigma}$ computation

Data: unknowns on the elements K, L, precision EPS, $maxIter$
Result: $p_{n,\sigma}$ and u_σ
Set initial approximation:
$u_\sigma^0 = \frac{t_K u_K + t_L u_L}{t_K + t_L}$, where $t_K = \frac{k_K}{d_{K,\sigma}}, t_L = \frac{k_L}{d_{L,\sigma}}$;
For given u_σ^0 compute $p_{n,\sigma}^0$ by Algorithm 1;
Compute $\Psi(u_\sigma^0)$ and $\Psi'(u_\sigma^0)$;
while $N < maxIter$ **do**
  $u_\sigma^1 = u_\sigma^0 - \frac{\Psi(u_\sigma^0)}{\Psi'(u_\sigma^0)}$;
  For given u_σ^1 compute $p_{n,\sigma}^1$ by Algorithm 1 ;
  Compute $\Psi(u_\sigma^1)$;
  if ($|\Psi(u_\sigma^1)| < EPS$ *or* $|u_\sigma^1 - u_\sigma^0|/|u_\sigma^0| < EPS$) **then**
    return u_σ^1 and $p_{n,\sigma}^1$;
  end
  $N = N + 1$;
  Set $u_\sigma^0 = u_\sigma^1$, $\Psi(u_\sigma^0) = \Psi(u_\sigma^1)$;
  Compute $\Psi'(u_\sigma^0)$;
end

Algorithm 2: u_σ computation

4.5 Numerical simulations in a heterogeneous case

In this section we present numerical results for test cases with heterogeneous domain. First we present the test case based on test case from the MoMas benchmark with simplification that the immiscible two-phase flow model is considered. In this test case heterogeneous porous domain $I = (0, 200)$ is composed of two media $I_1 = (0, 20]$ and $I_2 = (20, 200)$ with different capillary pressure curves, porosity, and permeability. For both media we have used Van Genuchten's capillary pressure curves, but with different parameters. The parameters used in the simulation are given in Table 4.1. The duration of the simulation is 10^6 years. The Dirichlet boundary

Table 4.1: Van Genuchten's parameters and rock properties

	$n(-)$	$\alpha(1/\text{Pa})$	$S_{wr}(-)$	$S_{gr}(-)$	Φ	$k(\text{m}^2)$
I_1	1.54	$0.5 \cdot 10^{-6}$	0.01	0.0	0.3	10^{-18}
I_2	1.49	$0.067 \cdot 10^{-6}$	0.4	0.0	0.15	$5 \cdot 10^{-20}$

conditions are imposed on the right part of the boundary:

$$p_w = 10^6 \text{ Pa}, \quad p_n = 1.5 \cdot 10^6 \text{ Pa}, \quad x = 200,$$

and the Neumann boundary conditions are imposed on the left part:

$$q^w = 0 \text{ kg/s}, \quad q^n = 1.766 \cdot 10^{-13} \text{ kg/s}, \quad x = 0.$$

The initial conditions are equal to the Dirichlet boundary conditions on the right part of the domain. Consequently the initial global pressure in I_1 is equal to 1.002 MPa and in I_2 it is equal to 1.0 MPa. Gravity effects are neglected. For the fluid system we use the following properties: $\mu_w = 10^{-3}$ Pa·s, $\mu_n = 9 \cdot 10^{-6}$ Pa·s, $\rho_w = 1000$ kg/m^3, $\rho_n(p_n) = c_g p_n$, where $c_g = 0.794 \cdot 10^{-6}$ kg/$\left(\text{m}^3\text{Pa}\right)$. The temperature is set to 303 K.

An equidistant mesh is used for the space grid with $h = 1$ m. Initial step is taken as $\delta t = 1$ s. The obtained results are shown in Figures 4.22 - 4.25. In Figure 4.22 we observe that the water saturation remains practically unchanged since the injection rate of hydrogen is very small. After 1000 years the water saturation starts to decay in the left part of the domain, and in the end of the simulation it is equal approximately 0.87. Decrease of the water saturation in the right part of the domain is much smaller due to the smaller absolute permeability in this part of the domain. In Figure 4.24 we see that the gas phase pressure is increasing during the whole simulation. The water phase pressure is increasing for the around 10^5 years and afterwards it starts to decay, as one can see in Figure 4.25.

The obtained results correspond to the results obtained by the DuMu$^\text{x}$ 2p module. They also show physical behavior close to the one seen in the results of the original test case.

The second test case is the BOBG (French acronym of Engineered Barrier Geological Barrier) test case from [28]. In this test case a heterogeneous porous domain $I = (0,1) = I_1 \cup I_2$ is used. The subdomains I_1 and I_2 are equal to $I_1 = (0, 0.5]$ and $I_2 = (0.5, 1)$. The fluid system is composed of water, which is assumed incompressible, and hydrogen, with density given by the ideal gas law. In this test case the domain boundary is assumed impermeable. Beside heterogeneity of the domain, an additional difficulty in this test case is heterogeneous initial condition for the water saturation

$$S_w(x,0) = \begin{cases} 0.77, & x \le 0.5 \\ 1, & x > 0.5, \end{cases}$$

which is out of equilibrium and leads to high flow rate in the first few steps of the simulation. The initial gas phase pressure is set to $p_n(x,0) = 0.1$ MPa, $x \in I$. The initial global pressure is

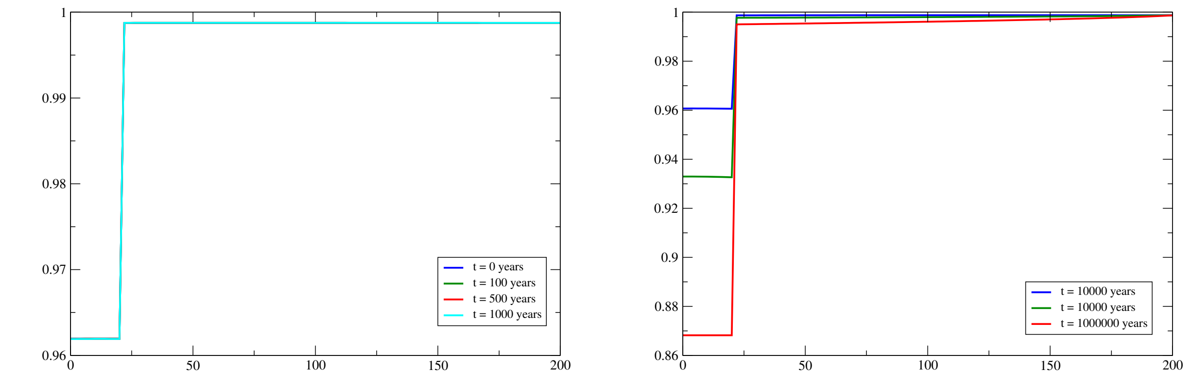

Figure 4.22: Water saturation

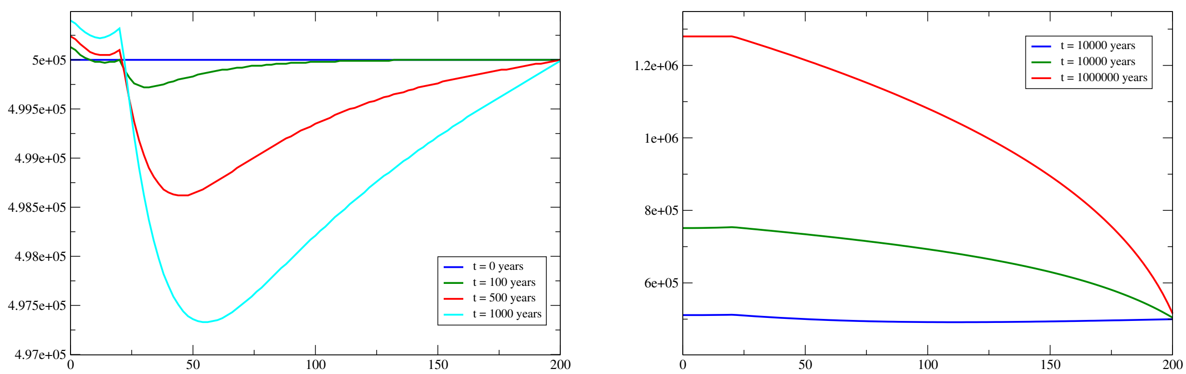

Figure 4.23: Capillary pressure

equal to -88.8449 MPa in I_1 and it is equal to 0.1 MPa in I_2. Like in the previous test cases Van Genuchten's capillary pressure curves are used, but with different parameters. For the relative permeability the following functions are used

$$kr_n(S_w) = (1-S_w)^2\left(1-S_w^{\frac{5}{3}}\right), \quad kr_w(S_w) = (1+A(S_w^{-B}-1)^C)^{-D}.$$

The parameters for Van Genuchten's capillary pressure curve and relative permeability functions are given in Table 4.2.

The temperature is set to $T = 300$ K. The time of simulation is 1000 years. For the space grid we have used a mesh with 256 elements with a finer grid around the interface point. The

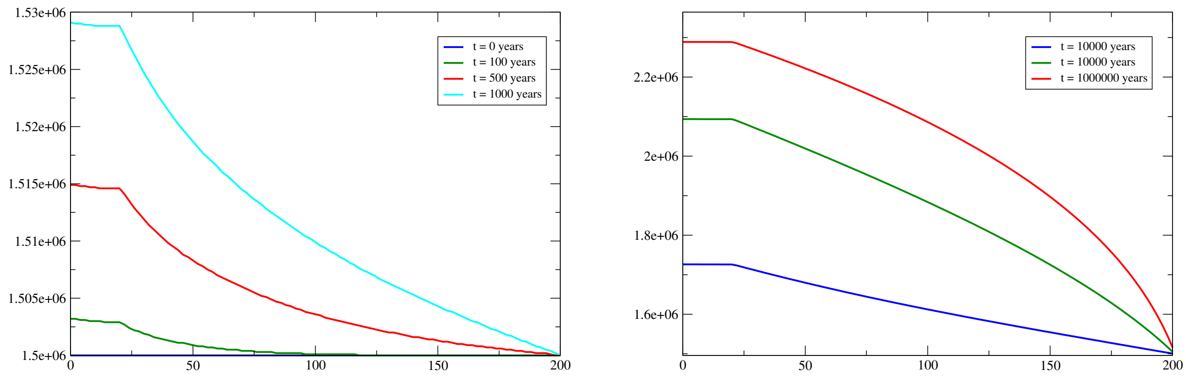

Figure 4.24: Gas phase pressure

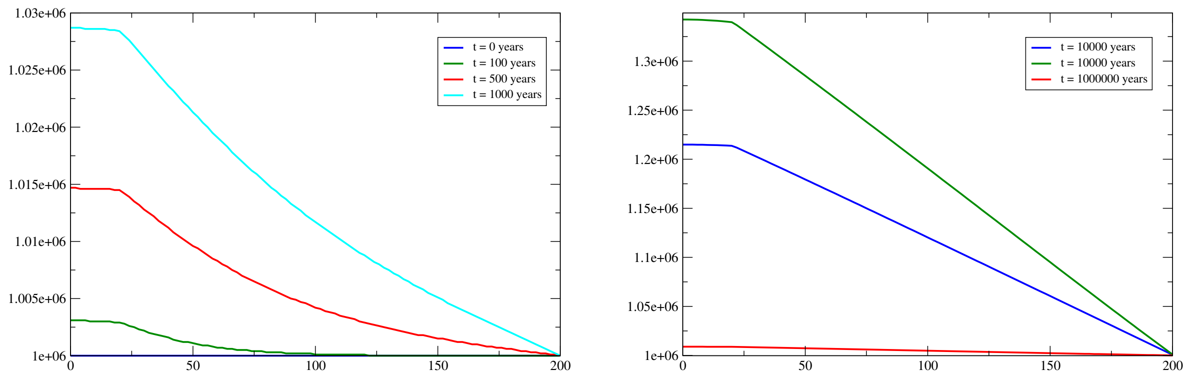

Figure 4.25: Liquid phase pressure

initial time step is taken as $\delta t = 10^{-5}$ s and by the end of simulation it is increased to $\delta t = 10^8$ s. The obtained results are given in Figures 4.26 - 4.29.

In the proposed test the right part of the domain is initially fully saturated with water as one can see in Figure 4.26. From the very beginning of the simulation the water starts to flow to the left part of the domain, while the gas is entering the right part of the domain. Due to this behavior there is a significant increase of the gas pressure at the interface as one can see in Figure 4.28. After around 10^5 s the gas pressure on the interface starts to decay since a significant amount of gas has entered the right part of the domain. By the end of the simulation the gas pressure

Table 4.2: Van Genuchten's parameters and rock properties

	$m(-)$	$\alpha(1/\text{Pa})$	A	B	C	D	Φ	k
I_1	0.06	$0.67\cdot10^{-6}$	0.25	16.67	1.88	0.5	0.3	10^{-20}
I_2	0.412	$0.1\cdot10^{-6}$	1.0	2.429	1.176	1.0	0.05	10^{-19}

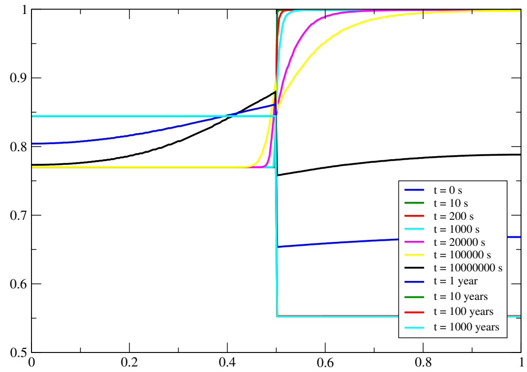

Figure 4.26: Water saturation

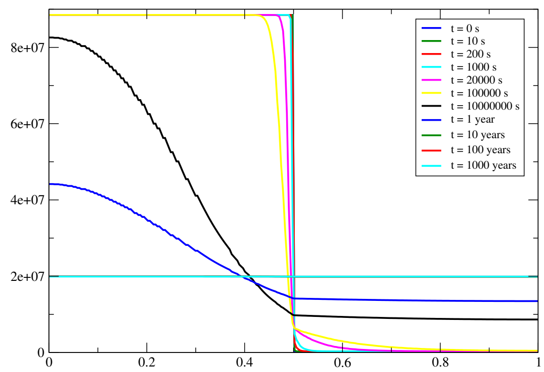

Figure 4.27: Capillary pressure

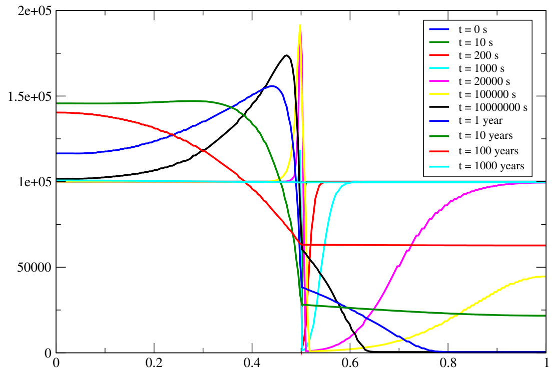

Figure 4.28: Gas phase pressure

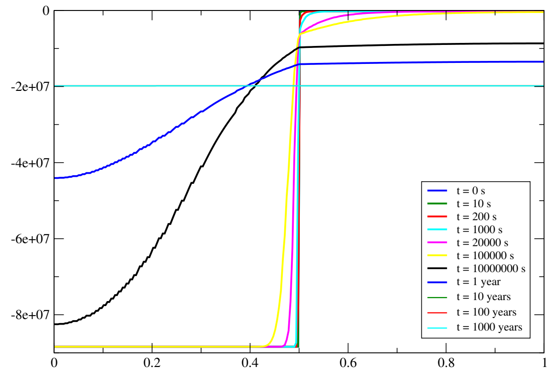

Figure 4.29: Liquid phase pressure

is increasing in the right part of the domain and it is decreasing on the left part of the domain to eventually reach the initial value of 10^5 Pa. During the whole simulation the water pressure is decreasing in the right part of the domain and it is increasing in the left part of the domain as shown in Figure 4.29. At the end of the simulation the water pressure is tending to the value of -20 MPa. In Figure 4.27 one can see the opposite behavior of the capillary pressure since the amount of gas in the left part of the domain becomes smaller during the simulation, and the amount of gas in the right part of the domain is increasing. At the end of the simulation the capillary pressure is attaining the value of around 20 MPa. If we look closely to Figure 4.26 we can see that the water saturation is attaining the value of $S_w = 0.844$ on the left part of the domain and on the right part of the domain it is equal $S_w = 0.548$ at the end of the simulation.

The presented results show physically correct behavior and they are validated through comparison with the DuMu^x 2p module.

4.6 Conclusion

In this chapter numerical simulations obtained by the cell-centered finite volume discretization of the fractional flow/global pressure formulation are presented. With regard to benchmark test cases, obtained results correspond to the known results from the literature. Regarding test cases that were inspired by some benchmark problems, obtained results show physically correct behavior. Results are additionally validated through comparison with results obtained by the DuMu^x 2p module. Even though the proposed method has shown some shortcomings regarding running time, due to the computation of the global pressure, it is expected that these shortcomings will be less important when the method is applied to the two-phase two-component model. That motivation is drawn from the fact that the global pressure can be used as a persistent variable in the model describing fluid flow with mass exchange between the phases.

Appendix A

Implementation of the finite volume method in DuMu^x

In this section we describe the implementation in the DuMu^x framework of the cell-centered finite volume method for two-phase, immiscible, compressible flow based on the fractional flow formulation presented in Chapter 4. The DuMu^x, [43], is a platform for implementation and application of models describing the flow and transport processes in porous media. It comes with a number of modules for simulation of various processes in porous media and it allows addition of new modules into the framework. In this section we describe a construction of a new module and in particular the calculation of coefficients depending on the global pressure.

A.1 DuMu^x `2p-gp` module

In order to implement the cell-centered finite volume method for two-phase, immiscible flow based on the fractional flow formulation and the concept of global pressure based on the total flux, we have created a new DuMu^x module called `2p-gp` module. The new module is based on the DuMu^x `2p` module which implements classical engineering finite volume scheme for two-phase, immiscible flow. Here we give list of classes that were modified for purpose of the implementation of our method:

- `PorousMediumFlowProblem` (file `dumux/porousmediumflow/problem.hh`) - Base class for all fully implicit porous media problems was altered in order to initialize computation of tables storing the nonwetting phase pressure which will be described in detail in Section

A.2.

- `TwoPFormulation` (file `dumux/porousmediumflow/2p/formulation.hh`) - class that specifies primary variable choice was altered in order to support formulations `ps1` which uses the global pressure and the nonwetting phase saturation as primary unknowns and `ps0` which uses the global pressure and the wetting phase saturation as primary unknowns. Default formulation is set to `ps0`.

- `ImmiscibleFluidState` (file`dumux/material/fluidstates/immiscible.hh`) - class that stores current state of fluid was adapted so that it provides computation of the nonwetting phase pressure from the global pressure and the saturation and also computation of the global pressure for given nonweting phase pressure and saturation. These processes will be described in more detail in Section A.2.

- `TwoPVolumeVariables` (file `dumux/porousmediumflow/2p/volumevariables.hh`) - class that computes the quantities which are constant within a finite volume was modified to use the global pressure and the saturation as primary variables. These quantities are the phase pressures p_w and p_n, and all coefficients from the system given by (1.43).

- `ImmiscibleLocalResidual` (file `dumux/porousmediumflow/immiscible/localresidual.hh`) - class that calculates element-wise the residual for problems was modified to compute the fluxes in a way given by the finite volume scheme (4.13)–(4.14). The computation of the fluxes is described in more detail in Section A.4.

- `TwoPModel` (file `dumux/porousmediumflow/2p/model.hh`) - Property system of the `TwoPModel` was modified in order to take into account previously mentioned alterations and to add new property `numMaterials` which is used to indicate number of different materials in porous media. Default value for `numMaterials` is set to one. Here is also defined property `ReplaceCompEqIdx`, which suggest which of the equations from (4.1)–(4.2) should be replaced by the total mass balance equation. Default system is set to the system (4.3)–(4.4) by imposing `ReplaceCompEqIdx = 0`. We change it by imposing `ReplaceCompEqIdx = 2` for the system (4.1)–(4.2) and `ReplaceCompEqIdx = 1` for the system (4.5)–(4.6).

The most challenging part of the implementation is a computation of the nonwetting phase pressure from the given saturation and global pressure. Therefore, we give a detailed description of the corresponding implementation in the next section.

A.2 Calculation of the gas pressure and the function ω

The function π is given as a solution of the Cauchy problem (1.47) which can be written in a simpler form with the capillary pressure as unknown. If we denote $u = p_c(S_w)$, due to the invertibility of the capillary pressure, we can write $S_w = S_w(u)$. Consequently, we can replace any function $f(S_w)$ of the wetting phase saturation by the corresponding function of the capillary pressure $\overline{f}(u) = f(S_w(u))$. Instead of solving the problem (1.47), we find a solution $\overline{p}_n(u,p)$ of the following problem

$$\begin{cases} \dfrac{d\overline{p}_n(u,p)}{du} = \dfrac{\overline{\hat{\rho}}_w(\overline{p}_n(u,p)-u)\overline{\lambda}_w(u)}{\overline{\hat{\rho}}_w(\overline{p}_n(u,p)-u)\overline{\lambda}_w(u)+\overline{\hat{\rho}}_n(\overline{p}_n(u,p))\overline{\lambda}_n(u)}, \quad u>0 \\ \overline{p}_n(0,p) = p + p_c(1). \end{cases} \tag{A.1}$$

The solution to the problem (1.47) is given by a change of variables as $p_n(S_w,p) = \overline{p}_n(p_c(S_w),p)$. For the numerical solution of (A.1), we introduce the class

```
class GlobalExactTables: public GlobalTables
```

These two classes implement a table of values $\overline{p}_n(u,p)$ for a given number of the global pressure values ranging from `pMin` to `pMax` and a given number of capillary pressure values ranging from 0 to `pcMax`. $\overline{p}_n(u,p)$ is computed as a solution of the initial problem (A.1) by using the GSL ODE solver [57]. These classes also contain the implementation of a table of values $\omega(u,p)$. The function $\omega(S_w,p)$ is given by (1.50), which can be written in a simpler way if we introduce the change of variables $u = p_c(S_w)$ as in the system (1.47)

$$\omega(S_w,p) = \exp\left(-\int_0^{p_c(S_w)} (\overline{v}_n(u,p)-\overline{v}_w(u,p))\frac{\overline{\rho}_w(u,p)\overline{p}_n(u,p)\overline{\lambda}_w(u)\overline{\lambda}_n(u)}{\overline{\lambda}(u,p)^2}\,du\right). \tag{A.2}$$

Therefore, in order to compute the function $\omega(u,p)$ we have to perform a numerical integration. Thereby we have used the trapezoidal rule. Let us look closely at how these computations are done. The class `GlobalTables` is base class for the class `GlobalExactTables`. This class does not calculate the tables, but it offers all the functions necessary for the interpolation and the allocation of the tables:

- Allocation of the tables is done in function `GlobalTables::init()`.

- Functions `GlobalTables::gas_pressure(Scalar u, Scalar p)` and `GlobalTables::omega(Scalar u, Scalar p)` provide the values $p_n(u,p)$ and $\omega(u,p)$ from corresponding tables using cubic spline interpolation in two variables. For the interpolation we used ALGLIB library [25].

An important member of the class `GlobalTables` is the variable `materialParams` which stores the parameters for the capillary pressure law and the relative permeabilities. The calculation of the tables is implemented in the class `GlobalExactTables`. Let us note that in the case of the domain with heterogeneous material law parameters, we are going to have more than one table for $p_n(u,p)$ and more than one table for $\omega(u,p)$. These tables will be stored in an object of type `ImmiscibleFluidStateGP`, obtained by modification of the class `ImmiscibleFluidState`. Therefore, the class `ImmiscibleFluidStateGP` has a member

```
static std::vector<GlobalExactTables> table_
```

which stores all necessary tables. This vector will have as many elements as there are different rock types in domain. Variable `table_` is of type `static` because these tables are computed only once, at the beginning of the numerical simulation. Some of the member functions of the class `ImmiscibleFluidStateGP` which are important at this point are:

- `pn(Scalar sn, Scalar p, MaterialLawParams materialParams)` which computes the gas pressure for a given saturation of the nonwetting phase and the global pressure. This function calls the function `GlobalTables::gas_pressure(Scalar u, Scalar p)`. The parameter `materialParams` is necessary in order to know which table to look up.

- `omega(Scalar sn, Scalar p, MaterialLawParams materialParams)` which computes the value of ω for a given saturation of the nonwetting phase and the global pressure. This function calls the function `GlobalTables::omega(Scalar u, Scalar p)`.

- `global_pressure(Scalar sn, Scalar pn, MaterialLawParams materialParams)` which computes the global pressure for a given nonwetting phase saturation and a nonwetting phase pressure using the Newton method for finding a solution of the nonlinear equation `pn(sn, p, materialParams) - pn = 0`. It is used only for imposing the initial and Dirichlet boundary condition in terms of the global pressure and the saturation, which will be further commented in Section A.3.

Computations of the tables are initialized by calling the function

```
initializeTables(std::shared_ptr<const FVGridGeometry> fvGridGeometry)
```

from the class `PorousMediumFlowProblemGP` (modified `PorousMediumFlowProblem`). This function reads from the input file values of the variables `pMax`, `pMin`, and `noOfGlobalPressurePoints` and checks the domain for different rock types. Afterwards it starts the computation of the tables.

A.3 Implementation of initial and boundary conditions

Neumann boundary conditions in DuMu^{x} are implemented in the class `FVProblem<TypeTag>` by imposing the exact value of the flux for every equation in the system. This is done in the function `neumannAtPos(const GlobalPosition &globalPos)`. Therefore we do not have to make any alteration in the DuMu^{x} code for implementing the Neumann boundary condition in the module based on the global pressure, but we must be careful when imposing the value since it depends on the system of equations that we are using. As previously mentioned for implementing the Dirichlet boundary condition, we have to compute the global pressure from the gas pressure and the saturation since the boundary conditions are normally given in terms of the phase pressures. We impose the obtained value in the function `dirichletAtPos(const GlobalPosition &globalPos)`. The initial conditions for the system are given by $p(x,0) = p^0(x)$, $S_w(x,0) = S_w^0(x)$. The initial conditions are imposed in the function `initialAtPos(const GlobalPosition &globalPos)`.

A.4 Computation of the storage term and the fluxes

In order to calculate the storage term and the flux we have modified the class `ImmiscibleLocalResidual`(file `dumux/porousmediumflow/immiscible/localresidual.hh`) to obtain

```
class TwoPGPLocalResidual
```

In order to implement the discretization of the advective term we have modified the class `CCTpfaDarcysLaw` (file `dumux/discretization/cellcentered/tpfa/darcyslaw.hh`) to obtain

```
class CCTpfaDarcysLawGP
```

which is used for the computation of the term $Q_{K,\sigma}$, given by (4.10)
(file `dumux/discretization/cellcentered/tpfa/darcyslaw-gp.hh`). Upwinding is implemented as part of the class `TwoPGPLocalResidual`. The capillary and gravity terms, which are given by (4.11) and (4.12), are implemented as part of the

```
class CCTpfaCapillaryFlux
```

(file `dumux/discretization/cellcentered/tpfa/capillaryflux-gp.hh`) and they are summed into overall flux in

```
class TwoPGPLocalResidual
```

For the implementation of the interface condition for discontinuous capillary pressure problem, which is currently supported only for the system (4.3)–(4.4), we have added the function `computeFluxOnInterface()` (file `dumux/porousmediumflow/2p-gp/computefluxinterace.hh`). The interface between the heterogeneous parts of the domain is detected inside class `TwoPGPLocalResidual`. In the function `computeFluxOnInterface()` is given the implementation of the algorithms 1 and 2, which are used for the calculation of the flux over the interface using (4.17) and (4.19).

Conclusion

This thesis offers both mathematical and numerical analysis of models describing two-phase compressible flow in porous media. Contributions of the thesis to mathematical modeling and analysis of multiphase, multicomponent flow in porous media are done by proving the existence of a weak solution for a model describing two-phase two-component flow.The model is completed with the assumption of the low solubility of the gas. The low solubility assumption is essential for the derivation of the energy estimate without any unphysical assumptions on the diffusive parts of the model, that was imposed in some previous works on this subject.

Contribution to the numerical analysis of the finite volume methods is done through the convergence analysis of a classical engineering cell-centered finite volume method for immiscible compressible two-phase flow in porous media. The convergence proof is based on the equivalent global pressure/fractional flow formulation, and its cell-centered finite volume discretization. This equivalence between two different discretization was essential for the derivation of the energy estimate.

Contribution to the numerical simulation of the two-phase fluid flow is done through construction and implementation of the cell-centered finite volume method for a model describing immiscible, compressible two-phase flow based on the concept of the global pressure and fractional flow form of the equations. Implementation of the method is done with use of the DuMu^{x} library, considering also the case of heterogeneous porous media, and it is verified on important benchmark problems. Even though the proposed method did not meet the expectation in the case of the immiscible two-phase flow as far as running time was concerned, it is strongly believed that the method will bring great advantages when employed for multicomponent flow. That motivation is drawn from the fact that the global pressure can be used as a persistent variable, well defined in both one-phase and two-phase regions. Obtained implementation will therefore be used as the groundwork for the future research regarding multiphase, multicomponent flow in porous media.

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Curriculum Vitae

Ivana Radišić was born on November 17, 1990, in Zagreb, Croatia. After obtaining secondary education in Čitluk, she started undergraduate studies in Mathematics in 2009, and in 2012 she started graduate studies in Applied Mathematics, both at the University of Zagreb, Faculty of Science, Department of Mathematics. In 2014, she graduated with diploma thesis *Double Porosity Model* under supervision of Prof. Mladen Jurak.

From 2014 to 2015 she worked as an IT developer for Ruby Monday d.o.o, Zagreb. She has been working as a a teaching and research assistant at the Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, since September 2015. In the same year, she enrolled in the PhD program in Mathematics at Faculty of Science, Department of Mathematics, under supervision of prof. Mladen Jurak and she became a member of the Seminar for differential equations and numerical analysis at the same faculty. From September to October, 2017, and also from September to December, 2018, she was a PhD intern at Laboratorie de Mathematiques et de leur Appliquees, University of Pau and Pays de l'Adour, under supervision of Prof. Brahim Amaziane.

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