DEPARTMENT OF MATHEMATICS
FACULTY OF SCIENCE
UNIVERSITY OF ZAGREB

Ana Žgaljić Keko

Modelling, Analysis and Numerical Simulations of Immiscible Compressible Two-phase Fluid Flow in Heterogeneous Porous Media

PhD Thesis

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This thesis has been submitted for evaluation to the Department of Mathematics, Faculty of Science, University of Zagreb for the fulfillment of the Degree of Doctor of Philosophy.

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PRIRODOSLOVNO-MATEMATIČKI FAKULTET
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Chapter 1

Introduction

This work is closely related to the area of modelling of multiphase flow in porous media which is significant for many petroleum and environmental engineering problems. In present-day industry, chlorinated hydrocarbons, petroleum products and similar materials are essential and very frequent. Uncontrolled spreading of such materials may have strong environmental influence. Furthermore, the storage of nuclear waste and recent advances towards underground storage of CO_2 additionally raise safety and environment concerns. A certain risk of accidental spillage of harmful materials always exists. Such spills may result in release of these materials into the environment, which may cause pollution of the groundwaters. With regards to geological repositories of nuclear waste, problems are related to the flow of water and gas. In such cases the gas is most commonly hydrogen and the most important source of the gas is the corrosion of metallic components (waste containers) and water radiolysis by radiation issued from nuclear waste. It is important to model and predict underground gas migration, in order to avoid overpressure and prevent mechanical damages. Mathematical models and numerical simulations of multiphase flows help in the development of cost-efficient, safe and suitable methods for the storage of hazardous materials. Numerical simulations of such models can give an answer about the pressure, saturation and velocity of the fluids involved in the flow, as functions of the space and time.

This thesis is devoted to the study of immiscible, compressible two-phase flow in porous media, taking into account gravity, capillary effects, and heterogeneity. A general case of two compressible fluids will be considered. The usual set of equations describing this type of flow is given by the mass balance law and Darcy-Muscat law for each phase, which leads to the system of strongly coupled nonlinear partial differential equations. In such systems there are several choices of primary variables. By algebraic manipulation over these equations a fractional flow formulation can be obtained. In the fractional flow approach, the two phase problem is seen as a total fluid flow of a one mixed fluid. In such a formulation, the saturation of one of the phases and the global pressure are independent variables.

Motivation for introducing the global pressure is due to the strong coupling of the equations. Setting the global pressure as a primary unknown lessens the strength of coupling between the coupled equations: the global pressure equation and the saturation equation.

The global pressure was first introduced in [15, 25] and afterwards considered by other authors, see [28]. The study of immiscible incompressible two-phase flow using the feature of global pressure is well known, see [15, 25, 30]. This is not the case for two compressible phases, except in the case of low capillary pressure so that the densities are assumed to depend upon the global pressure which gives an approximative model, see [25, 43] and the references therein. In these situations, it is assumed that the nonlinear functions appearing in the system depend upon the global pressure by ignoring the error caused by calculating fluid phase densities at the global pressure instead of calculating them at the phase pressure. These assumptions have limited the use of the global pressure formulation in numerical simulations algorithmic implementations. A fully equivalent global pressure formulation to the original system for the flow of water and gas was derived in [7]. A fractional flow formulation for the general case of immiscible compressible two-phase flow was recently derived in [8] without any simplifying assumptions, and this formulation is fully equivalent to the original phase equations formulation, i.e. where the phase pressures and the phase saturations are primary unknowns. A fully equivalent formulation for a case of three phase flow was established in [24], and it has been further investigated in [31–33].

Comparison with other formulations [30] shows the computational effectiveness of the global pressure when it can be employed. This may explain the current revival of interest for the concept of global pressure for numerical modelling of multiphase flow in porous media, especially in the case of compressible flow. Recently, the most common numerical methods used to approximate derived systems are finite volume method combined with mixed finite element method and discontinuous Galerkin finite element method. Methods where mixed finite elements are used for the pressure equation have proven efficient in the case of incompressible flow. In this thesis the vertex centred finite volume method is applied on the derived system of equations. Vertex centred finite volume method allows the application of an approximation of the finite element type so it can be naturally implemented with libraries implementing finite elements [50].

Discontinuous porous media is a special problem for numerical methods, since at the discontinuities the fluxes and (in general) phase pressures are continuous through the discontinuity of the medium, which would generally produce discontinuities in the main unknowns of the derived system. All these values need to be calculated locally, from the globally assigned values. The discontinuous media has been a problem of study of many authors, see [17, 46, 54–56, 59].

Mathematical analysis of the two-phase flow in porous media has been a problem of interest for many years and many methods have been developed. One may refer to [6, 15, 16, 20, 25, 27, 36, 38, 40, 49, 66, 67] for more information on the analysis, especially on the existence of solutions of immiscible incompressible two-phase flow in porous media. The case of miscible compressible flow in porous media is treated in [10–12, 34, 39]. However, the situation is quite different for immiscible compressible two-phase flow in porous media, where only recently a few results were obtained. In the case of immiscible two-phase flows with one (or more) compressible fluids without any exchange between the phases, some approximate models were studied in [41–43]. In [41] certain terms related to the compressibility are neglected, and in [42, 43] the mass densities are assumed not to depend on the physical pressure, but on the Chavent's global pressure. In [44, 48], a more general immiscible compressible two-phase flow model in homogeneous porous media is considered with the assumption of the bounded capillary pressure function, which is too restrictive for some realistic problems. In the case of immiscible two-phase flows with one (or more) compressible fluids with the exchange between the phases, i.e. a multicomponent model, the existence of weak solutions for these equations under some assumptions on the compressibility of the fluids has been recently established in [51, 62, 63].

This thesis is organized as follows: in chapter 2 basic terms and equations on the description of the two-phase flow model in porous media are presented [17–19, 25, 30, 46]. At the end of the chapter several formulations of the model are presented with different primary variables chosen. Also, since most of the simulations in chapter 4 involve heterogeneous porous medium, general treatment of the heterogeneity in the porous media is discussed.

A new model using global pressure as a primary variable, fully equivalent to original equations, derived in chapter 2, is described in chapter 3. The new model was introduced in [7] for water-gas flow. In this chapter, the model is presented for the flow of two compressible fluids, and is mainly represented in the article [8]. By setting the global pressure as primary variable in the new fractional flow formulation, a computation of phase pressures corresponding to a given global pressure requires a solution of a differential equation (see (3.14)). The evaluation of the coefficients depending on phase pressures requires more calculation in the fully equivalent fractional flow model (3.23)–(3.25) as compared to the original model (2.20), (2.21). Numerically, this calculation can be performed by using standard numerical libraries present in the literature. For this reason, a simplified fractional flow formulation, which is not fully equivalent to the corresponding phase equations, is presented. The simplified fractional flow formulation is compared to fully equivalent fractional flow formulation by comparing the coefficients. The goal of the comparison is to recognize situations in which approximate fractional flow formulation can be safely used and to show differences in approximate and fully equivalent formulations in the cases where these are significant.

In chapter 4 the finite volume method in one dimensional case for the new model is presented. Special attention is paid to the treatment of the heterogeneities. In numerical simulations, the fluids observed are water, considered as incompressible, and compressible gas, such as hydrogen, concerning the gas migration through engineered and geological barriers for the deep repository of radioactive waste. In the development and usage of numerical models for immiscible compressible flow in porous media it is important to verify the numerical model by means of adequate benchmark problems.

Recently, the French research group MoMaS (http://www.gdrmomas.org/) proposed benchmark tests (http://www.gdrmomas.org/ex_qualifications.html) designed to improve the simulation of the water–hydrogen flow related to corrosion of nuclear waste containers in an underground storage.

The verification of the new global pressure model is shown on several test cases [52] in the heterogeneous porous media. In the first test case, the initial conditions for phase pressures are taken to be continuous and constant in the whole domain, so that the capillary pressure is continuous and nonzero at the initial moment. The new and the simplified model are applied to this test case, and the results are compared afterwards. In the second test case, the initial capillary pressure is taken to be discontinuous, and the intensity of the capillary pressure is taken to be very high compared to the initial gas pressure, which can lead to numerical difficulties. The third test case is chosen to represent the effect of the entry pressure, when the porous medium is initially fully saturated by the water.

In chapter 5 existence results of weak solutions for this new formulation for the two-phase compressible flows are obtained. This section contains results from [9]. The equations are rewritten by expressing the phase fluxes in terms of nonwetting saturation and global pressure. Under certain realistic assumptions on the data also presented in this chapter, an existence result, with the help of appropriate regularizations and the time discretization is obtained. The system is firstly regularized with a parameter $\eta > 0$ in order to make capillary pressure bounded, and a small constant is added to diffusivity term to obtain the ellipticity of the discretized system. The existence of the weak solution for a regularized system is shown, by introducing time discretization, so a small parameter $h > 0$ relating to the time discretization is introduced. Afterwards, the existence of the solution for a discretized problem is shown by applying Schauder's fixed point theorem. A set of suitable test functions is employed to get a priori estimates independent on h and the regularization parameter η, in order to pass to the limit in nonlinear terms when h tends to zero. This gives the existence result for a regularized system. To pass to the limit as η tends to zero a generalization of compactness lemma from [25, 43, 48] and a compactness lemma from [60] is used. This approach permits considering heterogeneous media.

Appendix A contains further explanation on the implementation of the coefficients of the fully equivalent global pressure formulation of compressible, immiscible two-phase flow. The numerical code for their calculation is developed and implemented in C++ programming language.

Chapter 2

Two-phase Flow in Porous Media

In this chapter the basic terms and equations for immiscible compressible two-phase fluid flow in porous media are explained. The chapter is organized as follows: in the first section the basic terms and laws regarding the porous media are presented. The second section is devoted to two-phase immiscible compressible flow, and explanation of the terms needed to describe this flow. The third section starts with the presentation of the governing equations describing two-phase immiscible flow in porous media, written on macroscopic level, and afterwards some basic formulations are presented. At the end of the chapter, the treatment of the heterogeneous porous media is considered. Most of this chapter follows the references [19], [17], [25], [46].

2.1 Porous Media

2.1.1 Basic Definitions

Every material composed of a solid part called **solid matrix** and a connected **pore space** (void space) can be identified as a **porous medium**. The pore space can be filled with one or more fluids. In order to derive valid mathematical model of fluid flow through a porous medium, the medium must satisfy some additional properties [35], [17]:

- *Pore space is interconnected.*
- *The smallest dimension of the pore space must be large enough to contain fluid particles.* This property allows the application of the continuum approach at the pore space scale.

- *Dimensions of the pore space must be small enough so that the fluid flow is controlled by adhesive forces of fluid-solid interfaces and cohesive forces of fluid-fluid interfaces.* This property eliminates the case of network pipes.

Some of the examples of the porous media are: sand, soil, clay, sponge, etc.

If the pore space is filled by a single, or by several, completely miscible fluids, one speaks about single-phase fluid flow in porous media. The term **phase**, as employed in [46] is used to differentiate one or more fluids separated by a sharp interface. Two fluids are said to be **immiscible** if a strictly defined interface between them exists. In such a system, each fluid represents a different phase. The solid matrix is considered to be the solid phase. Different phase properties are assigned to each phase, one fluid phase may differ from the others by its density, dynamic viscosity and compressibility. Phases can also be composed of different components. However, multicomponent flows are not considered in the scope of this work. Further details may be found in [17, 25, 46].

2.1.2 Fluid Properties

Mass density of the fluid will be denoted by ρ. Generally, it is assumed to be a function of the fluid pressure P, and temperature T. In this work, only the isothermal flow is considered, which means that it is assumed that the density depends only upon the pressure, and temperature T is involved only as a parameter. The density is constant if the fluid is **incompressible**. In the case of the ideal gas the density is given by the equation of the state:

$$\rho(P) = \frac{PM}{RT},$$

where R is the universal gas constant ($R = 8.31 J/Kmol$), T is the temperature, and M is the fluid molar mass.

Compressibility of the fluid is defined as

$$\nu = \frac{1}{\rho(P)} \frac{d\rho(P)}{dP}.$$

It is usually assumed to be a constant so, generally, the density can be given as

$$\rho(P) = \rho_0 e^{\nu(P-P_0)},$$

where P_0 is the reference pressure and $\rho_0 = \rho(P_0)$.

In the case of liquids, ν is usually assumed to be very low. For example, the compressibility of water is $5.1 \times 10^{-10} Pa^{-1}$. Fluids with low compressibility can be modeled as incompressible, or the density is modeled as

$$\rho(P) = \rho_0 + \nu(P - P_0) \tag{2.1}$$

Such fluids are called *slightly compressible* fluids.

Another property of the fluid is **dynamic viscosity** $[Pas, cP]$ which, in this work, will be called simply viscosity. In this work it is assumed constant, though it can also depend on pressure and temperature.

2.1.3 Macroscopic Scale

In the mathematical modelling of flow through porous media, different scales can be used. Besides *molecular* scale ($\approx 10^{-9} m$) one can use *microscopic* and *macroscopic* scale.

At the *microscopic* scale the system of Navier-Stokes equations is used, with some assigned boundary conditions. The task of solving the Navier-Stokes equations in the pore space is not practical due to the unknown pore space geometry. Moreover, the fluid flow variations at the pore space scale, are not of interest. Therefore, one needs to set up mathematical model at a larger scale.

Because of these reasons, the *macroscopic* scale is usually used, and in the flow description a *continuum approach* is applied. At the macroscopic scale, the porous medium is assumed to be a continuum in which one does not distinguish the solid phase from the fluid phases present in the pore space. On macroscopic level, macroscopic quantities represent average values of the quantities given on the microscopic level. Therefore, quantities appearing in the macroscopic model, i.e. pressure and velocity, actually represent average values over sufficiently large volumes.

Porous medium is called **homogeneous** if its properties do not vary in space or time. Otherwise, the medium is called **heterogeneous**.

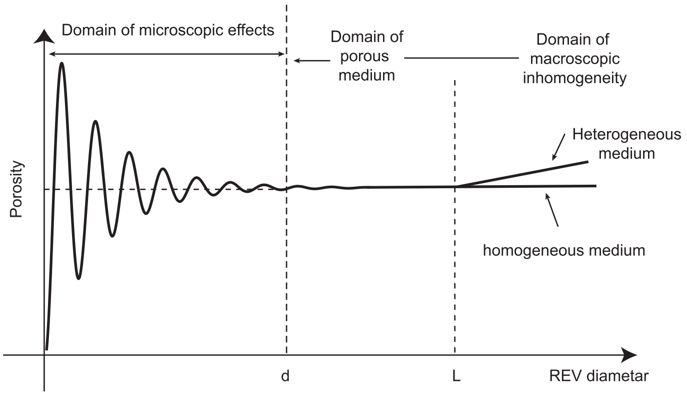


Figure 2.1: Determination of the REV

Rock Properties

The **porosity** is obtained by an averaging procedure over elementary volume of the following pore space indicator function defined at the microscopic level

$$\varphi(\mathbf{x}) = \begin{cases} 1 & \mathbf{x} \in \text{pore space} \\ 0 & \mathbf{x} \in \text{solid} \end{cases} \qquad \forall \mathbf{x} \in \Omega. \tag{2.2}$$

The porosity at the position $\mathbf{x}_0$ is the following value:

$$\phi(\mathbf{x}_0) = \frac{1}{\text{meas}(K(\mathbf{x}_0, r))} \int_{K(\mathbf{x}_0,r)} \varphi(\mathbf{x})\, dx.$$

Here, $K(\mathbf{x}_0, r) = \{\mathbf{x} : d(\mathbf{x}, \mathbf{x}_0) < r\}$ is called *representative elementary volume* (REV).

In the definition of macroscopic properties it is important to determine which radius can be used to obtain a valid model. For example, when defining the porosity at the point $\mathbf{x}_0$, the porosity is calculated for different radii. For very small radius the oscillatory behavior is obtained, and after a certain value of the radius, the values of the porosity stop behaving oscillatory. This is presented in the figure (2.1). A similar observation can be found in [17], [19]. As explained in [19], the radius of the REV should satisfy

$$d \leq 2r \leq L$$

where d is the length that characterizes the microscopic structure of the void space, and L is the characteristic length of the porous medium domain.

The porosity is therefore a function of space, but, in more complex models, where the rock is deformable, it is assumed to be a function of the pressure.

Another macroscopic property of the porous medium is the **absolute permeability** $\mathbb{K}$ [m^2,Darcy], usually a symmetric tensor describing the ability of the porous media to transmit fluids. In the heterogeneous media it is space dependent and the media is **isotropic** if $\mathbb{K} = k\mathbb{I}$.

The absolute permeability appears in Darcy's law, which will be described in the next subsection. In the two-phase flow system, besides the absolute permeability, the relative permeabilities must be introduced, since the flow of each phase depends upon the presence of other phases.

2.1.4 Derived Macroscopic Equations

At the macroscopic level, the **macroscopic balance law** for the one-phase system in a porous medium $\Omega \subseteq \mathbb{R}^n$ can be rewritten as [17], [25]:

$$\frac{\partial(\Phi\rho(P))}{\partial t} + \operatorname{div}(\rho(P)\mathbf{q}) = \mathcal{F} \tag{2.3}$$

where $\mathbf{q}$ $[m/day]$ is a macroscopic apparent velocity, and $\mathcal{F}$ is a source (sink) term.

The macroscopic apparent velocity or Darcy velocity $\mathbf{q}$ [m/year] relates to the pressure of the fluid with the equation called **Darcy's law**.

$$\mathbf{q} = -\frac{1}{\mu}\mathbb{K}(\nabla P - \rho\mathbf{g}) \tag{2.4}$$

where $\mathbf{g}$ is the gravitational, downward-pointing, constant vector and, as already mentioned, ρ is the fluid density, and P is the fluid pressure. Darcy's law is actually the momentum conservation of the Navier-Stokes equation on the macroscopic level [17].

Therefore, the equation which describes monophasic flow in the porous domain $\Omega \subseteq \mathbb{R}^n$, with P as unknown (and $\mathbf{q}$ as unknown which is calculated by Darcy's law) is:

$$\frac{\partial(\Phi\rho(P))}{\partial t} - \operatorname{div}(\frac{\rho(P)}{\mu}\mathbb{K}\,(\nabla P - \rho(P)\mathbf{g})) = \mathcal{F}, \quad \text{in } \Omega. \tag{2.5}$$

To this equation the following initial and boundary conditions are usually assigned:

$$P(\mathbf{x},0) = P_0(\mathbf{x}), \quad P(\mathbf{x},t) = P_d(\mathbf{x},t) \text{ on } \Gamma_d \quad \rho\mathbf{q}\cdot\mathbf{n} = q_n \text{ on } \Gamma_n,$$

where $\partial\Omega = \Gamma_d \cup \Gamma_n$.

In the case of incompressible fluid flow, the initial condition for the pressure is not necessary, since in that case one deals with an elliptic equation. Equations (2.4)-(2.3) can also be rewritten for the case of a two-phase flow. In that case, however, several additional definitions are needed. These will be presented in the next section.

2.2 Two-phase Flow in Porous Media

In the two-phase flow system, a wetting and a nonwetting phase are introduced. One example of this kind of system is water-gas system, where the water is the wetting phase. In the flow of oil and water, water is considered as a wetting phase, and in the flow of oil and gas, oil is considered to be the wetting fluid. The wetting phase can be easily determined by the following action: if one looks at a capillary tube, the convexity of meniscus is always oriented towards wetting fluid, as presented in the figure (2.2). In this work the indices $\alpha = w, g$, will denote the wetting and nonwetting phases respectively. To rewrite the equations (2.3) and (2.4) in a two-phase flow case one needs to introduce aditional terms: saturations, capillary pressure and relative permeabilities.

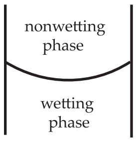


Figure 2.2: Determining the wetting fluid

2.2.1 Saturation

Phase saturations S_α, $\alpha = w, g$ are macroscopic variables introduced in order to describe the quantity of the volume of the phase at the point $\mathbf{x}_0$ of the porous medium. Its definition is similar to the definition of the porosity. For a phase $\alpha = w, g$ the phase indicator function is [17]:

$$\varphi_\alpha(\mathbf{x},t) = \begin{cases} 1 & \mathbf{x} \in \text{phase } \alpha \text{ at time } t \\ 0 & \mathbf{x} \notin \text{phase } \alpha \text{ at time } t \end{cases}$$

The saturation of the phase α is defined as

$$S_\alpha(\mathbf{x_0},t) = \frac{\int_{REV} \varphi_\alpha(\mathbf{x,t})\,dx}{\int_{REV} \varphi(\mathbf{x})\,dx}. \quad \forall \mathbf{x_0} \in \Omega$$

where $\varphi(\mathbf{x})$ is the function defined by (2.2), and REV is assigned to the point $\mathbf{x_0}$

It clearly follows $\sum_\alpha S_\alpha(\mathbf{x},t) = 1$, and $0 \leq S_\alpha \leq 1, \alpha = w, g$.

2.2.2 Capillary Pressure

On the microscopic level two immiscible fluids are separated by clearly defined interface which leads to a jump of pressure. This jump of pressure is called capillary pressure and is equal to

$$P_c = P_g - P_w. \tag{2.6}$$

It is described by

$$P_c = \sigma\left(\frac{1}{r_1} + \frac{1}{r_2}\right) \tag{2.7}$$

where σ is the interfacial tension, and r_1 and r_2 are the main curvature radii of the surface between the fluids. For smaller meniscus radii the capillary pressure is higher and vice versa, for larger radii the capillary pressure is lower. One can conclude from this, that, in the case of drainage - injection of the nonwetting phase in the area fully saturated by the wetting phase - the wetting phase flows to smaller pores. On the contrary, when the imbibition -injection of the wetting phase in the area fully saturated by the nonwetting phase - is performed the wetting phase starts to fill the largest pores first.

Capillary pressure is always positive since the pressure of the nonwetting phase is higher than the pressure of the wetting phase.

Macroscopic capillary pressure is an average value of the microscopic capillary pressure. On the macroscopic level, there is no interface between phases, and in every point of the porous medium domain one observes wetting and nonwetting pressure P_w and P_g, and these are the average values of the values of the fluid pressures defined on the microscopic level. Thus the equation (2.6) is also valid at the macroscopic level.

The macroscopic capillary pressure is assumed to depend on the saturation since, for example, when drainage is performed one can conclude from the previous discussion that the decrease of wetting phase saturation would produce the increase of the capillary pressure. The values of capillary pressure function can be obtained experimentally by performing drainage, or by performing imbibition. Since the measurements require certain amount of time, theoretical formulae are commonly used in practice.

When the saturation of the wetting phase in the porous medium is equal to a certain small value S_{wr}, the increase of the gas pressure will not displace the wetting phase. Value S_{wr} is called the *residual saturation* of the wetting phase. The capillary pressure is expected to have vertical asymptote at that point. Similarly, in the case of imbibition, certain amount of nonwetting phase that cannot be displaced by a wetting phase exists, so the saturation of the nonwetting phase cannot be lower than S_{nr}, (the *residual nonwetting saturation*). Therefore, the capillary pressure is naturally defined on the interval $]S_{wr}, 1 - S_{nr}]$.

It is natural to introduce the effective saturation

$$S_{ew} = \frac{S_w - S_{wr}}{1 - S_{wr} - S_{gr}} \quad S_{eg} = \frac{S_g - S_{gr}}{1 - S_{wr} - S_{gr}} \tag{2.8}$$

which means that

$$S_w = S_{wr} \Rightarrow S_{ew} = 0 \text{ and } S_w = 1 - S_{gr} \Rightarrow S_{ew} = 1$$

and clearly:

$$S_{ew} + S_{eg} = 1.$$

The capillary pressure is usually considered to be a function of the effective saturation.

Several analytical expressions of the capillary pressure exist. The two most important, usually used in the description of water-gas flows are:

- Van Genuchten capillary pressure [64]

$$P_c(S_{ew}) = Pr(S_{ew}^{-\frac{1}{m}} - 1)^{\frac{1}{n}} \quad S_{ew} \in]0, 1], \tag{2.9}$$

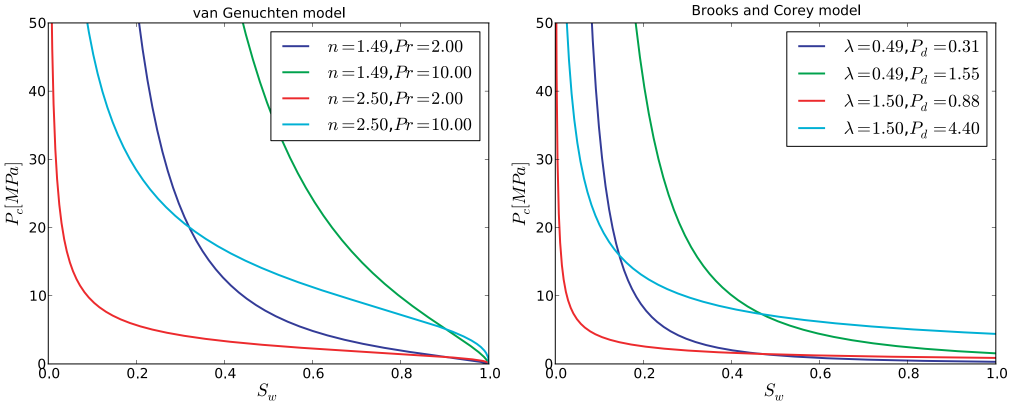


Figure 2.3: Capillary pressure for the van Genuchten and the Brooks and Corey models

where $m = 1 - \frac{1}{n}$, and usually $n \in [1.49, 5.0]$.

- Brooks and Corey capillary pressure [23]

$$P_c(S_{ew}) = P_d S_{ew}^{-\frac{1}{\lambda}} \quad S_{ew} \in]0,1], \tag{2.10}$$

P_d is the *entry pressure* and the parameter λ is related to the structure of the porous medium. A value that is commonly used is $\lambda \in [0.2, 3.0]$.

Macroscopic capillary pressure can also depend on temperature and surface tension, but, in this work, it is assumed that it is a function of the saturation only.

Remark 2.1. *An equivalence can be established between the Brooks and Corey and van Genuchten parameters. The main results are given in [53], and the equivalence is given by the formulae*

$$\lambda = n - 1, \quad P_d = Pr\frac{(p+3)}{2p(p-1)}\left(\frac{147.8 + 8.1p + 0.092p^2}{55.6 + 7.4p + p^2}\right), \quad \text{where} \quad p = 3 + \frac{2}{\lambda}. \tag{2.11}$$

Figure 2.3 presents a graphical illustration of the capillary pressures of the van Genuchten and the Brooks and Corey models, for the equivalent respective parameters.

2.2.3 Relative Permeabilities

Each phase's relative permeability is considered to be an increasing function of its own saturation, which means that the phase is more mobile if it is more present in the domain. It is always valid $kr_w(S_{ew} = 0) = 0$ and $kr_g(S_{ew} = 1) = 0$. Two models of deriving the relative permeability functions form the given capillary pressure function are described here, (*Mualem's* and *Burdine's*). More detailed presentations of these models can be found in [26], [46].

- In the *Mualem* model, relative permeability functions are defined by the following formulae

$$k_{rw}(S_{ew}) = S_{ew}^{\frac{1}{2}} \left(\frac{\int_0^{S_{ew}} \frac{ds}{P_c(s)}}{\int_0^1 \frac{ds}{P_c(s)}} \right)^2 \tag{2.12}$$

$$k_{rg}(S_{ew}) = (1 - S_{ew})^{\frac{1}{2}} \left(\frac{\int_{S_{ew}}^1 \frac{ds}{P_c(s)}}{\int_0^1 \frac{ds}{P_c(s)}} \right)^2 . \tag{2.13}$$

- In the *Burdine* model, relative permeability functions are defined by the following formulae

$$kr_w(S_{ew}) = S_{ew}^2 \left(\frac{\int_0^{S_{ew}} \frac{ds}{P_c^2(s)}}{\int_0^1 \frac{ds}{P_c^2(s)}} \right) \tag{2.14}$$

$$kr_g(S_{ew}) = (1 - S_{ew})^2 \left(\frac{\int_{S_{ew}}^1 \frac{ds}{P_c^2(s)}}{\int_0^1 \frac{ds}{P_c^2(s)}} \right) . \tag{2.15}$$

Calculation gives the following van Genuchten Mualem relative permeability functions:

$$kr_w(S_{ew}) = S_{ew}^{\frac{1}{2}} \left(1 - (1 - S_{ew}^{\frac{1}{m}})^m \right)^2 \tag{2.16}$$

$$kr_g(S_{ew}) = (1 - S_{ew})^{\frac{1}{2}} (1 - S_{ew}^{\frac{1}{m}})^{2m} . \tag{2.17}$$

Also, the following Brooks and Corey Burdine functions are obtained:

$$kr_w(S_{ew}) = S_{ew}^{3+\frac{2}{\lambda}} \tag{2.18}$$

$$kr_g(S_{ew}) = (1 - S_{ew})^2 \left(1 - S_{ew}^{\frac{2+\lambda}{\lambda}} \right) . \tag{2.19}$$

These functions are presented in the figure 2.4 for the $S_{wr} = S_{gr} = 0.05$.

Remark 2.2. *For the formulae (2.16)-(2.19) one obtains:*

1. $\lim_{S_{ew} \to 0} kr_w(S_w) P_c'(S_w) = 0$ *for Brooks and Corey functions and for van Genuchten functions.*

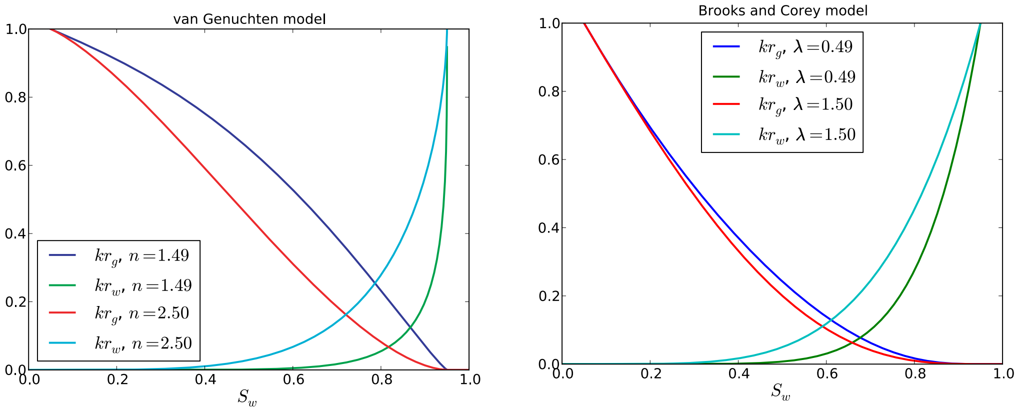


Figure 2.4: Relative permeability functions in the van Genuchten and Brooks and Corey models for $S_{wr} = S_{gr} = 0.05$.

2. $\lim\limits_{S_{ew}\to 1} kr_g(S_w)P_c'(S_w) = 0$ *for Brooks and Corey functions and for van Genuchten functions.*

3. $kr_w(S_w)P_c'(S_w) < \infty$ *as* $S_{ew} \to 1$ *for Brooks and Corey functions, but not for van Genuchten functions.*

In this work it is mostly considered that $S_{wr} = S_{gr} = 0$, unless it is other specified.

2.3 Governing Equations

The equations describing the immiscible, compressible two-phase fluid flow in the porous medium are given by the mass balance equation for each phase and the Darcy-Muscat law which relates the phase pressure gradient and volumetric phase velocity (see, e.g., [18, 25, 30, 46]):

$$\Phi\frac{\partial}{\partial t}(\rho_\alpha S_\alpha) + \operatorname{div}(\rho_\alpha \mathbf{q}_\alpha) = \mathcal{F}_\alpha \quad \text{and} \quad \mathbf{q}_\alpha = -\mathbb{K}\frac{kr_\alpha(S_\alpha)}{\mu_\alpha}(\nabla P_\alpha - \rho_\alpha \mathbf{g}), \tag{2.20}$$

where, as mentioned previously, Φ and $\mathbb{K}$ are the porosity and the absolute permeability, of the porous medium, which depend only on the space variable; and for $\alpha = w, g$ ρ_α, S_α, P_α, $\mathbf{q}_\alpha$ and μ_α are, the mass density, saturation, pressure, volumetric velocity, and viscosity of the α-phase; $\mathcal{F}_\alpha$ is the source/sink term, kr_α is the relative permeability of the α-phase, and $\mathbf{g}$ is the gravitational, downward-pointing, constant vector. In addition to (2.20), the following equations apply

$$S_w + S_g = 1, \quad \text{and} \quad P_c(S_w) = P_g - P_w. \tag{2.21}$$

The primary variables are S_α, P_α, and $\mathbf{q}_\alpha$. Here the porosity Φ and the absolute permeability $\mathbb{K}$ are functions of space and the viscosities μ_w, μ_g are constant. Finally, the capillary pressure and relative permeabilities are considered to be functions of the saturation only. To simplify the notation their spatial dependence is omitted. The governing equations (2.20)–(2.21) are strongly coupled, nonlinear partial differential equations. These equations can be transformed in other forms (see [29], [30]) by algebraic manipulation over these equations and choice of primary unknowns.

2.3.1 Pressure-Pressure Formulation

In the system (2.20)-(2.21) one may select phase pressures as the main unknowns. Given that the capillary pressure is an invertible function, the phase saturations are

$$S_\alpha = S_\alpha(P_c) = S_\alpha(P_g - P_w).$$

Thus the governing equations can be reformulated in the following way

$$\Phi \frac{\partial}{\partial t}(\rho_g(P_g) S_g(P_g - P_w)) + \operatorname{div}(\rho_g(P_g)\mathbf{q}_g) = \mathcal{F}_g \tag{2.22}$$

$$\Phi \frac{\partial}{\partial t}(\rho_w(P_w) S_w(P_g - P_w)) + \operatorname{div}(\rho_w(P_w)\mathbf{q}_w) = \mathcal{F}_w \tag{2.23}$$

$$\mathbf{q}_g = -\mathbb{K}\frac{kr_g(S_g(P_g - P_w))}{\mu_g}(\nabla P_g - \rho_g(P_g)\mathbf{g}) \tag{2.24}$$

$$\mathbf{q}_w = -\mathbb{K}\frac{kr_w(S_w(P_g - P_w))}{\mu_w}(\nabla P_w - \rho_w(P_w)\mathbf{g}). \tag{2.25}$$

The derived system is strongly coupled through the expression for the saturation. This formulation is not commonly used [46], since it is inefficient for very small capillary pressure gradients, which often occur in heterogeneous porous media.

2.3.2 Pressure-Saturation Formulation

This approach will be explained on a system where the wetting phase saturation and the nonwetting pressure are chosen as main unknowns. From (2.21) one easily obtains

$$S_g = 1 - S_w \quad P_w = P_g - P_c(S_w).$$

Putting this into (2.20) the following system of equations in the porous domain $\Omega \subseteq \mathbb{R}^n$is obtained:

$$\Phi \frac{\partial}{\partial t}(\rho_g(P_g)(1 - S_w)) + \operatorname{div}(\rho_g(P_g)\mathbf{q}_g) = \mathcal{F}_g \tag{2.26}$$

$$\Phi \frac{\partial}{\partial t}(\rho_w(P_w)S_w) + \operatorname{div}(\rho_w(P_w)\mathbf{q}_w) = \mathcal{F}_w \tag{2.27}$$

$$\mathbf{q}_g = -\mathbb{K}\frac{kr_g(S_w)}{\mu_g}(\nabla P_g - \rho_g(P_g)\mathbf{g}) \tag{2.28}$$

$$\mathbf{q}_w = -\mathbb{K}\frac{kr_w(S_w)}{\mu_w}(\nabla P_g - \nabla P_c(S_w) - \rho_w(P_w)\mathbf{g}) \tag{2.29}$$

The derived system is strongly coupled and it can be assumed as a parabolic system. By reformulation, one can see that this is not true [17]. The boundary and initial conditions can be chosen as [17]:

$$S_w(\mathbf{x}, 0) = S_w^0(\mathbf{x}) \quad P_g(\mathbf{x}, 0) = P_g^0(\mathbf{x}) \ \mathbf{x} \in \Omega \tag{2.30}$$

$$S_w(\mathbf{x}, t) = S_w^d(\mathbf{x}, t) \text{ on } \Gamma_d^{S_w} \quad P_g(\mathbf{x}, t) = P_g^d(\mathbf{x}, t) \text{ on } \Gamma_d^{P_g} \tag{2.31}$$

$$\rho_w(P_w)\mathbf{q}_w \cdot \mathbf{n} = Q_w \text{ on } \Gamma_n^{S_w} \quad \rho_g(P_g)\mathbf{q}_g \cdot \mathbf{n} = Q_g \text{ on } \Gamma_n^{P_g} \tag{2.32}$$

Note that in the above: $\partial\Omega = \Gamma_d^{P_g} \cup \Gamma_n^{P_g} = \Gamma_d^{S_w} \cup \Gamma_n^{S_w}$.

In order to reveal the type of the system (2.26)-(2.29), it is worthwhile to examine an another formulation which also includes one pressure, and one saturation as the main unknowns. Therefore, the phase mobility functions are introduced:

$$\lambda_\alpha(S_w) = \frac{kr_\alpha(S_w)}{\mu_\alpha}, \quad \alpha = w, g \tag{2.33}$$

and the total mobility is

$$\lambda(S_w, P_g) = \rho_w(P_w)\lambda_w(S_w) + \rho_g(P_g)\lambda_g(S_w). \tag{2.34}$$

Then the fractional flow functions

$$f_\alpha(S_w, P_g) = \frac{\rho_\alpha(P_\alpha)\lambda_\alpha(S_w)}{\lambda(S_w, P_g)}, \quad \alpha = w, g, \tag{2.35}$$

and also the following nonlinear functions:

$$\rho(S_w, P_g) = \frac{(\lambda_w(S_w)\rho_w(P_w)^2 + \lambda_g(S_w)\rho_g(P_g)^2)}{\lambda(S_w, P_g)}, \tag{2.36}$$

$$\alpha(S_w, P_g) = \frac{\rho_w(P_w)\rho_g(P_g)\lambda_w(S_w)\lambda_g(S_w)}{\lambda(S_w, P_g)}, \tag{2.37}$$

$$b_g(S_w, P_g) = (\rho_w(P_w) - \rho_g(P_g))\alpha(S_w, P_g), \quad a(S_w, P_g) = -\alpha(S_w, P_g)P_c'(S_w). \tag{2.38}$$

are introduced. In the above formulae the nonwetting pressure P_g and the wetting phase saturation S_w are chosen as independent variables.

Rewriting the equations (2.20)–(2.21) by summation of the two equations and introduction of total flux, $\mathbf{Q}_t = \rho_w(P_w)\mathbf{q}_w + \rho_g(P_g)\mathbf{q}_g$, one obtain the following:

$$\begin{aligned}&\Phi\frac{\partial}{\partial t}(S_w\rho_w(P_w) + (1 - S_w)\rho_g(P_g)) \\ &\qquad - \operatorname{div}\left(\lambda(S_w, P_g)\mathbb{K}\left[\nabla P_g - f_w(S_w, P_g)\nabla P_c(S_w) - \rho(S_w, P_g)\mathbf{g}\right]\right) = \mathcal{F}_w + \mathcal{F}_g,\end{aligned} \tag{2.39}$$

$$\mathbf{Q}_t = -\lambda(S_w, P_g)\mathbb{K}\left(\nabla P_g - f_w(S_w, P_g)\nabla P_c(S_w) - \rho(S_w, P_g)\mathbf{g}\right), \tag{2.40}$$

$$\Phi\frac{\partial}{\partial t}(\rho_w(P_w)S_w) + \operatorname{div}(f_w(S_w, P_g)\mathbf{Q}_t + b_g(S_w, P_g)\mathbb{K}\mathbf{g}) - \operatorname{div}(a(S_w, P_g)\mathbb{K}\nabla S_w) = \mathcal{F}_w. \tag{2.41}$$

The governing equation for the saturation (2.41) is a nonlinear convection-diffusion PDE and the equation for pressure (2.39) is a nonlinear PDE strongly coupled to the saturation equation through the gradient of capillary pressure and the time derivative term. The boundary and initial conditions for this system can be again defined with (2.30)-(2.32).

Remark 2.3. *Phase fluxes can be expressed through the total flux as:*

$$\rho_w(p_w)\mathbf{q}_w = f_w(S_w, P_g)\mathbf{Q}_t - a(S_w, P_g)\mathbb{K}\nabla S_w + b_g(S_w, P_g)\mathbb{K}\mathbf{g}, \tag{2.42}$$

$$\rho_g(P_g)\mathbf{q}_g = f_g(S_w, P_g)\mathbf{Q}_t + a(S_w, P_g)\mathbb{K}\nabla S_w - b_g(S_w, P_g)\mathbb{K}\mathbf{g}. \tag{2.43}$$

Remark 2.4. *Starting with the (S_g, P_w) formulation the coefficients (2.33)-(2.38) may be rewritten as a functions of the variables (S_g, P_w) by changing the variable as follows: $S_g = 1 - S_w$ and $P_w = P_g - P_c(S_g)$. This way one obtain the following system of equations:*

$$\begin{aligned}&\Phi\frac{\partial}{\partial t}((1-S_g)\rho_w(P_w)+S_g\rho_g(P_g))\\&\qquad - div\left(\lambda(S_g,P_w)\mathbb{K}\left[\nabla P_w+f_g(S_w,P_w)\nabla P_c(S_g)-\rho(S_g,P_w)\mathbf{g}\right]\right)=\mathcal{F}_w+\mathcal{F}_g,\end{aligned} \tag{2.44}$$

$$\mathbf{Q}_t=-\lambda(S_g,P_w)\mathbb{K}\left(\nabla P_w+f_g(S_g,P_w)\nabla P_c(S_g)-\rho(S_g,P_w)\mathbf{g}\right), \tag{2.45}$$

$$\Phi\frac{\partial}{\partial t}(\rho_g(P_g)S_g)+div(f_g(S_w,P_w)\mathbf{Q}_t-b_g(S_g,P_w)\mathbb{K}\mathbf{g})-div(a(S_g,P_w)\mathbb{K}\nabla S_g)=\mathcal{F}_g. \tag{2.46}$$

Incompressible Case

In the case where the two fluids in the porous medium are incompressible, the mass balance law for each phase can be divided by the phase density. By introducing the total velocity

$$\mathbf{q}_t=\mathbf{q}_w+\mathbf{q}_g$$

and the coefficients

$$\begin{aligned}\lambda^{inc}(S_w)&=\lambda_w(S_w)+\lambda_g(S_w)\\ f_w^{inc}(S_w)=\lambda_w(S_w)/\lambda^{inc}(S_w)\quad f_g(S_w)&=\lambda_g(S_w)/\lambda^{inc}(S_w)\\ \rho^{inc}(S_w)&=(\lambda_w(S_w)\rho_w+\lambda_g(S_w)\rho_g)/\lambda^{inc}(S_w)\\ \alpha^{inc}(S_w)&=\lambda_w(S_w)\lambda_g(S_w)/\lambda^{inc}(S_w)\\ b_g(S_w)&=(\rho_w-\rho_g)\alpha^{inc}(S_w)\\ a(S_w)&=-\alpha^{inc}(S_w)P_c'(S_w).\end{aligned}$$

one obtains the following equations:

$$\mathrm{div}(\mathbf{q}_t)=\mathcal{F}_w/\rho_w+\mathcal{F}_g/\rho_g \tag{2.47}$$

$$\Phi\frac{\partial S_w}{\partial t}+\mathrm{div}(f_w^{inc}(S_w)\mathbf{q}_t+\mathbb{K}\mathbf{g}b_g^{inc}(S_w))-\mathrm{div}(a^{inc}(S_w)\mathbb{K}\nabla S_w)=\mathcal{F}_w/\rho_w. \tag{2.48}$$

where

$$\mathbf{q}_t=-\lambda^{inc}(S_w)\mathbb{K}\left[\nabla P_g-f_w^{inc}(S_w)P_c'(S_w)\nabla S_w-\rho^{inc}(S_w)\mathbf{g}\right] \tag{2.49}$$

and the following expressions for the velocities:

$$\mathbf{q}_w = f_w^{inc}(S_w)\mathbf{q}_t - \mathbb{K}a^{inc}(S_w)\nabla S_w + \mathbb{K}\mathbf{g}b_g^{inc}(S_w)$$
$$\mathbf{q}_g = f_g^{inc}(S_w)\mathbf{q}_t + \mathbb{K}a^{inc}(S_w)\nabla S_w - \mathbb{K}\mathbf{g}b_g^{inc}(S_w).$$

One can see that in the incompressible case the coupling between the two equations is less strong since the time derivative term does not appear in equation (2.47). It is shown [15, 25](see also section 3.1) that by introducing a new variable called global pressure this coupling can be weaken even more, giving the system well defined mathematical structure.

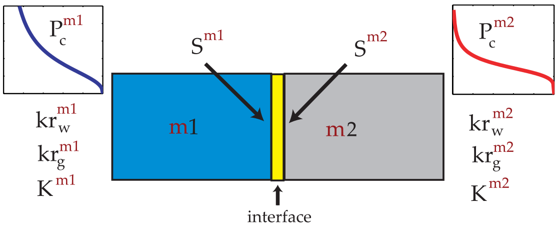
2.4 Discontinuous Porous Media. Interface Conditions

Porous media are usually heterogeneous, which introduces additional difficulties in mathematical modelling, since the heterogeneity must be treated properly, and some additional conditions at the interfaces must be introduced. Assume that the porous medium Ω is composed of different rock types. Without loss of generality and for the sake of simplicity, the case of two different rock types will be considered ($\Omega = \Omega^{m1} \cup \Omega^{m2}$), as presented in the figure (2.4). In heterogeneous media, each rock type can have different permeability, porosity, relative permeability and capillary pressure functions. The main difficulty that arises from heterogeneity is that, in general, primary unknowns can have discontinuities across the interface. The case when $P_c(1) = 0$ is firstly considered. At the interface the following conditions must be satisfied:

1. There is no loss or production of the mass, resulting in the condition that

   $$\rho_w(P_w)\mathbf{q}_n \cdot \mathbf{n}, \rho_g(P_g)\mathbf{q}_g \cdot \mathbf{n} \text{ are continuous across the interface.}$$

   $\mathbf{n}$ is taken here to be the vector normal to the interface pointing in the direction Ω^{m2}.



2. If the two-phase system is present at each side of the interface, and both phases are mobile (which means $\lambda_w(S_w), \lambda_g(S_g) > 0$), it is assumed that the intensive state variables are continuous at the interface, which means that the phase and capillary pressures satisfy:

$$\begin{aligned} P_c^{m1}(x_{interface}, t) &= P_c^{m2}(x_{interface}, t) \\ P_g^{m1}(x_{interface}, t) &= P_g^{m2}(x_{interface}, t) \\ P_w^{m1}(x_{interface}, t) &= P_w^{m2}(x_{interface}, t) \end{aligned}$$

The second condition is derived from the boundedness of the phase fluxes, in the case when both phases are mobile at the interface.

The consequence of the continuity of the capillary pressure is that the saturation variable is generally discontinuous at the interface, and has two limiting values S_w^{m1} and S_w^{m2} in the interface point.

However, a common situation is having the entry pressure involved in the model describing capillary pressure (like in Brooks and Corey capillary pressure) which means

$$P_c(1) = P_d.$$

In such a case capillary pressure does not need to be continuous. One can observe situations like the one presented in the figure 2.5, where the entry pressures for different rock types are not the same. In these situations one phase pressure is also discontinuous, since the phase and capillary pressures are connected by the equation (2.21).

Remark 2.5. *As described in [37] when the porous media is initially saturated by the wetting phase, and the nonwetting phase is injected, the meaning of the "entry pressure", can be described as follows: the nonwetting phase will cross the interface only when the capillary pressure P_c^{m1} is greater then the entry pressure P_d^{m2}. When this happens, the capillary pressure becomes continuous at the interface. If the capillary pressure P_c^{m1} is smaller than P_d^{m2}, the nonwetting phase will not cross the interface, and the capillary pressure will be discontinuous. Since, in this example, the wetting phase is mobile, the wetting phase pressure will be continuous at the interface, which is not the situation for the nonwetting phase pressure.*

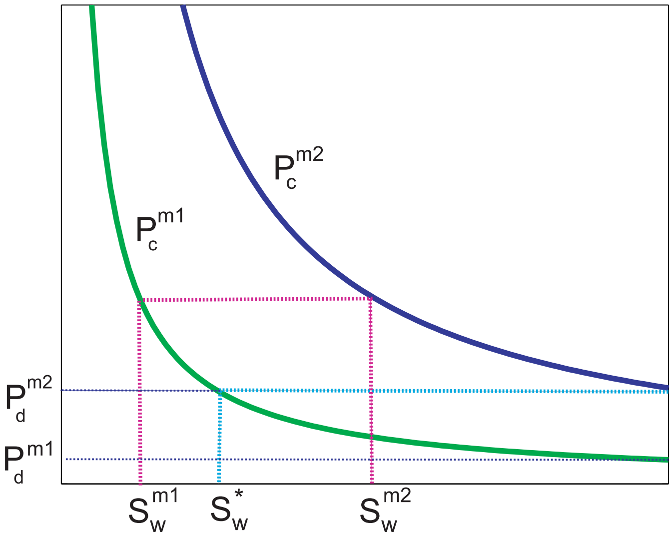


Figure 2.5: Capillary pressure with the entry pressure

One can describe the behavior of the saturation in such a case by this simple condition, as described in [17], [37], [59] called "*extended capillary pressure condition*":

$$S_w^{m2} = \begin{cases} 1 & \text{for } S_w^{m1} > S_w^* \\ (P_c^{m2})^{-1}(P_c^{m1}(S_w^{m1})) & \text{for } S_w^{m1} \leq S_w^* \end{cases} \tag{2.50}$$

Here the *threshold saturation* S_w^* is introduced by the formula

$$S_w^* = (P_c^{m1})^{-1}(P_d^{m2}).$$

For van Genuchten model, the capillary pressure is always continuous, so one may safely assume the threshold saturation S_w^* to be equal to 1.

Remark 2.6. *In the case of multiple rock types, in higher dimensions, the interface conditions are the same, assuming that these conditions for each pair of the materials are observed.*

2.5 Conclusion

In this chapter the basic properties of the porous media are described and the basic notation is laid out. The equations (2.39)-(2.41) have been presented with the wetting saturation and the nonwetting pressure as the main unknowns. The derived equations are strongly coupled and in order to make this coupling less strong, in the next chapter a new model of compressible two phase flow based on the concept of the global pressure is derived.

Chapter 3

A New Global Pressure Formulation for Immiscible Compressible Flow in Porous Media

The concept of global pressure was first introduced by [15,25] and investigated by the other authors afterwards (e.g. [28], [30]). Motivation for introducing the global pressure is due to the strong coupling of the equations describing two-phase immiscible flow. By setting the global pressure as a primary unknown, the coupling of the derived equations becomes less strong. Also, equations with well defined mathematical structure are obtained. The global pressure has been used in a wide range of numerical simulations, especially in hydrology and petroleum reservoir engineering, see for instance [30]. In the incompressible case, the fractional flow formulation has been proven far more computationally efficient, if compared to the two-pressure approach [30].

In the case of immiscible compressible two-phase flow, the concept of global pressure has not been applied until recently. An exception is its application in certain approximative models, see [25, 43] and references therein. Since comparisons with other formulations [30] have shown the computational effectiveness of the global pressure, it is worthwile to investigate its effectiveness in the compressible flow case.

A fully equivalent global pressure formulation to the original equations (2.20)-(2.21) for water-gas flow was derived in [7]. For the three-phase compressible flows case a global pressure formulation fully equivalent to the original equations was derived in [24], and afterwards considered in [31–33].

In this chapter a fully equivalent fractional flow formulation is introduced with the global pressure as a primary variable [8]. The general case of two immiscible compressible fluids is considered. This formulation leads to a system which consists of a nonlinear parabolic global pressure equation and a nonlinear diffusion-convection saturation equation.

In section 3.3 a simplified fractional flow formulation described in [25] is recalled and its deficiency for certain pressure ranges is shown. Subsequently, a modification that makes the model more applicable is proposed. A comparison of the fully equivalent fractional flow model with the simplified one is given in section 3.4. The two models differ solely in calculation of coefficients. Thus the coefficients are compared in order to recognize situations where the simplified formulation can be safely used. The comparison also elaborates the differences between the simplified and fully equivalent formulation where the differences are significant. This will be also commented in the chapter on numerical simulations. Finally, for the purpose of numerical simulations, treatment of heterogeneity in global pressure models is discussed.

3.1 Global Pressure in Incompressible Case

In order to make coupling of equations (2.47)-(2.48) less strong, a new variable called *global pressure* was introduced [15, 25]. This new pressure-like variable is intended to give the total velocity (2.49) the form of Darcy's law, and eliminate the saturation gradient in total velocity formulation [17, 25]. The idea is to have:

$$\nabla P_g - f_w^{inc}(S_w) P_c'(S_w) \nabla S_w = \nabla P \tag{3.1}$$

and this equation is going to be satisfied if

$$P = P_g - P_c(1) + \int_{S_w}^{1} f_w^{inc}(s) P_c'(s)\, ds, \tag{3.2}$$

$$\tag{3.3}$$

which gives

$$P_w \leq P \leq P_g. \tag{3.4}$$

After rewriting equations (2.47)-(2.48) the following equations including P as primary unknown are obtained:

$$\mathbf{q}_t = -\lambda^{inc}(S_w)\mathbb{K}(\nabla P - \rho^{inc}(S_w)\mathbf{g}), \tag{3.5}$$

$$\operatorname{div}(\mathbf{q}_t) = \mathcal{F}_w/\rho_w + \mathcal{F}_g/\rho_g \tag{3.6}$$

$$\Phi\frac{\partial S_w}{\partial t} + \operatorname{div}(f_w^{inc}(S_w)\mathbf{q}_t + \mathbb{K}\mathbf{g}b_g^{inc}(S_w)) - \operatorname{div}(a^{inc}(S_w)\mathbb{K}\nabla S_w) = \mathcal{F}_w/\rho_w. \tag{3.7}$$

The equation (3.7) is a nonlinear convection-diffusion equation. The diffusion term is degenerate, which means that $a^{inc} = 0$ when the wetting saturation is $S_w = 0, 1$. The equation for the pressure is a family of elliptic equations (one for each $t \in]0, T[$). These two equations are connected through the total velocity and the coefficients which depend on S_w. By introducing the global pressure in the equation, the system is less strongly coupled and derived equations are well mathematically structured. In the next section the case of two compressible fluids is considered.

3.2 A Fully Equivalent Fractional Flow Formulation

In the case of two compressible fluids the same idea as in the case of the incompressible fluids is followed. The capillary pressure gradient term can be eliminated from (2.39) by expressing the total flux $\mathbf{Q}_t$ as the Darcy flux of some *mean pressure* P, which leads to

$$\nabla P_g - f_w(S_w, P_g)P_c'(S_w)\nabla S_w = \omega(S_w, P)\nabla P, \tag{3.8}$$

where the function $\omega(S_w, P)$ is to be determined. To that aim assume that nonwetting pressure is an unknown function P_g such that

$$P_g = P_g(S_w, P), \tag{3.9}$$

and this function relates to new variable P (*the global pressure*) and a nonwetting pressure P_g. The global pressure is expected to be an intermediate pressure between P_w and P_g. From (3.8) and (3.9) one have

$$\nabla P_g = \omega(S_w, P)\nabla P + f_w(S_w, P_g(S_w, P))P_c'(S_w)\nabla S_w,$$

or

$$\frac{\partial P_g}{\partial S_w}(S_w, P)\nabla S_w + \frac{\partial P_g}{\partial P}(S_w, P)\nabla P = \omega(S_w, P)\nabla P + f_w(S_w, P_g(S_w, P))P_c'(S_w)\nabla S_w.$$

Since P and S_w are independent variables one must have

$$\frac{\partial P_g}{\partial S_w}(S_w, P) = f_w(S_w, P_g(S_w, P))P_c'(S_w) \tag{3.10}$$

$$\frac{\partial P_g}{\partial P}(S_w, P) = \omega(S_w, P). \tag{3.11}$$

The equation (3.10) will be integrated to obtain $P_g(S_w, P)$, and use (3.11) as a definition of ω. By setting $P_g(1, P) = P + P_c(1)$, it follows

$$P_g(S_w, P) = P + P_c(1) + \int_1^{S_w} f_w(s, P_g(s, P))P_c'(s)\,ds, \tag{3.12}$$

which gives

$$P \leq P_g(S_w, P) \leq P + P_c(S_w),$$

and therefore $P_w \leq P \leq P_g$. The formula for the wetting phase pressure can be obtained easily

$$P_w(S_w, P) = P - \int_1^{S_w} f_g(s, P_g(s, P))P_c'(s)\,ds. \tag{3.13}$$

The integral equation (3.12) can be rewritten in a form of the Cauchy problem for an ordinary differential equation as follows:

$$\begin{cases} \dfrac{dP_g(S, P)}{dS} = \dfrac{\rho_w(P_g(S, P) - P_c(S))\lambda_w(S)P_c'(S)}{\rho_w(P_g(S, P) - P_c(S))\lambda_w(S) + \rho_g(P_g(S, P))\lambda_g(S)}, & S < 1 \\ P_g(1, P) = P + P_c(1). \end{cases} \tag{3.14}$$

The problem (3.14) can be given in a form that is easier to solve by introducing the capillary pressure as an independent variable. Since the capillary pressure is invertible, $u = P_c(S_w)$ can be written as $S_w = S_w(u)$; any function of the wetting saturation $f(S_w)$ can be replaced by the corresponding function of capillary pressure $\hat{f}(u) = f(S_w(u))$.

Remark 3.1. *A common situation is also to have* $P_c(S_w = 1) = P_0$, *where* $P_0 > 0$ *is an* *entry pressure. In that case wetting and nonwetting relative permeabilities, for capillary pressures in the interval* $(0, P_0)$*, are naturally defined as one and zero respectively.*

The function $\hat{P}_g(u, P)$ as a solution of the Cauchy problem (P is a parameter) is introduced,

$$\begin{cases} \dfrac{d\hat{P}_g(u,P)}{du} = \dfrac{\rho_w(\hat{P}_g(u,P)-u)\hat{\lambda}_w(u)}{\rho_w(\hat{P}_g(u,P)-u)\hat{\lambda}_w(u)+\rho_g(\hat{\pi}(u,P))\hat{\lambda}_g(u)}, \quad u > 0. \\ \hat{\pi}(0,P) = P + P_c(1). \end{cases} \tag{3.15}$$

For problem (3.15) it is easy to see that it has a global solution $\hat{P}_g(u, P)$, and then a solution of (3.14) is given by

$$P_g(S_w, P) = \hat{P}_g(P_c(S_w), P).$$

Having found the function P_g one obtains a formula for ω based on the equation (3.11). In the first place, a new notation for the coefficients which now depend on the global pressure P instead of the phase pressures P_g and P_w is introduced. All these functions are denominated by a superscript $''n''$ as new:

$$\rho_w^n(S_w,P) = \rho_w(P_g(S_w,P) - P_c(S_w)), \quad \rho_g^n(S_w,P) = \rho_g(P_g(S_w,P)), \tag{3.16}$$

$$\lambda^n(S_w,P) = \rho_w^n(S_w,P)\lambda_w(S_w) + \rho_g^n(S_w,P)\lambda_g(S_w), \tag{3.17}$$

$$f_w^n(S_w,P) = \frac{\rho_w^n(S_w,P)\lambda_w(S_w)}{\lambda^n(S_w,P)}, \quad f_g^n(S_w,P) = \frac{\rho_g^n(S_w,P)\lambda_g(S_w)}{\lambda^n(S_w,P)} \tag{3.18}$$

$$\rho^n(S_w,P) = \rho(S_w,P_g(S_w,P)), \quad a^n(S_w,P) = a(S_w,P_g(S_w,P)), \tag{3.19}$$

$$b_g^n(S_w,P) = b_g(S_w,P_g(S_w,P)). \tag{3.20}$$

Note that the coefficients (3.16)–(3.20) are obtained from (2.33)–(2.38) by replacing P_g by $P_g(S_w, P)$ and P_w by $P_g(S_w, P) - P_c(S_w)$. Fluid compressibilities are defined as:

$$\nu_w^n(S,p) = \frac{\rho_w'(P_g(S,P) - P_c(S))}{\rho_w(P_g(S,P) - P_c(S))}, \quad \nu_g^n(S,P) = \frac{\rho_g'(P_g(S,P))}{\rho_g(P_g(S,P))}. \tag{3.21}$$

From (3.10) and (3.11) it follows that $\omega(S_w, P)$ satisfies a linear ordinary differential equation

$$\frac{\partial \omega}{\partial S_w}(S_w,P) = \partial_{P_g} f_w(S_w, P_g(S_w,P))P_c'(S_w)\omega(S_w,P),$$

(P being a parameter) which has a solution

$$\omega(S_w,P)=\exp\left(\int_{S_w}^{1}(\nu_g^n(s,P)-\nu_w^n(s,P))\frac{\rho_w^n(s,P)\rho_g^n(s,P)\lambda_w(s)\lambda_g(s)P_c'(s)}{(\rho_w^n(s,P)\lambda_w(s)+\rho_g^n(s,P)\lambda_g(s))^2}\,ds\right),\quad (3.22)$$

where $\omega(1,P)=1$, as a consequence of $P_g(1,P)=P+P_c(1)$. From (3.22) it is evident that ω is strictly positive function and it is less than one if the nonwetting phase compressibility is greater that the wetting phase compressibility.

Finally by replacing P_g with $P_g(S_w,P)$ in equations (2.39)–(2.41), and using (3.8), one obtains the following system of equations:

$$\Phi\frac{\partial}{\partial t}(S_w\rho_w^n(S_w,P)+\rho_g^n(S_w,P)(1-S_w)) \qquad (3.23)$$
$$-\operatorname{div}\Big(\lambda^n(S_w,P)\mathbb{K}(\omega(S_w,P)\nabla P-\rho^n(S_w,P)\mathbf{g})\Big)=\mathcal{F}_w+\mathcal{F}_g,$$

$$\mathbf{Q}_t=-\lambda^n(S_w,P)\mathbb{K}(\omega(S_w,P)\nabla P-\rho^n(S_w,P)\mathbf{g}), \qquad (3.24)$$

$$\Phi\frac{\partial}{\partial t}(S_w\rho_w^n(S_w,P))+\operatorname{div}(f_w^n(S_w,P)\mathbf{Q}_t+b_g^n(S_w,P)\mathbb{K}\mathbf{g})=\operatorname{div}(a^n(S_w,P)\mathbb{K}\nabla S_w)+\mathcal{F}_w. \qquad (3.25)$$

The system (3.23)–(3.25) is expressed in the variables S_w and P. The phase pressures P_g and P_w are given as smooth functions of S_w and P through $P_g=P_g(S_w,P)$ and $P_w=P_g(S_w,P)-P_c(S_w)$. Since the derivative $\partial P_g(S_w,P)/\partial P=\omega(S_w,P)$ is strictly positive, one can find the global pressure P in the form $P=\eta_g(S_w,P_g)$, with certain smooth function η_g, allowing the conclusion that the flow equations (3.23)–(3.25) are fully equivalent to equations (2.39)–(2.41), and therefore to (2.20), (2.21).

Using the global pressure the total flow $\mathbf{Q}_t$ can be rewritten in the form of the Darcy-Muskat law. The global pressure can be then interpreted as a mixture pressure where the two phases are considered as mixture constituents (see [65]). Note that the sum of "phase energies" can be decomposed as

$$\begin{aligned}&\rho_w(P_w)\lambda_w(S_w)\mathbb{K}\nabla P_w\cdot\nabla P_w+\rho_g(P_g)\lambda_g(S_w)\mathbb{K}\nabla P_g\cdot\nabla P_g\\&\quad=\lambda^n(S_w,P)\omega(S_w,P)^2\mathbb{K}\nabla P\cdot\nabla P+\alpha^n(S_w,P)\mathbb{K}\nabla P_c(S_w)\cdot\nabla P_c(S_w).\end{aligned}\qquad (3.26)$$

The equation (3.26) shows again physical relevance of the global pressure. The way how the formula (3.26) is obtained is going to be shown in the chapter 5.

Remark 3.2. *If the nonwetting saturation S_g is chosen as a main variable, one obtains* *the following formula for the nonwetting and the wetting pressure.*

$$P_g(S_g, P) = P + P_c(0) + \int_0^{S_g} f_w(s, P_g(s, P))P_c'(s)\, ds \tag{3.27}$$

where is taken that fractional flow function depends on nonwetting saturation and nonwetting phase pressure and it is obtain from (2.35) by setting $S_w = 1 - S_g$*. The wetting phase pressure is given by*

$$P_w(S_g, P) = P_g(S_g, P) - P_c(S_g). \tag{3.28}$$

$$\omega(S_g, P) = \frac{\partial P_w(S_g, P)}{\partial P} = \frac{\partial P_g(S_g, P)}{\partial P},$$

and a calculation shows that it can be expressed by the formula:

$$\omega(S_g, P) = \exp\left(-\int_0^{S_g} (\nu_g^n(s, P) - \nu_w^n(s, P))\frac{\rho_w^n(s, P)\rho_g^n(s, P)\lambda_w(s)\lambda_g(s)P_c'(s)}{(\rho_w^n(s, P)\lambda_w(s) + \rho_g^n(s, P)\lambda_g(s))^2}\, ds\right), \tag{3.29}$$

In such a case, as explained in remark 2.4, the coefficients (3.16)-(3.20) depend on the nonwetting saturation and the global pressure P *just by a simple change of variable* $S_g = 1 - S_w$*. The formulae are the same, only the dependence is changed. For the diffusivity coefficient one obtains*

$$a(S_g, P) = \frac{\rho_w^n(S_g, P)\rho_g^n(S_g, P)\lambda_w(S_w)\lambda_g(S_g)P_c'(S_g)}{\lambda^n(S_g, P)}.$$

This formulation with the nonwetting saturation is going to be used in the chapter 5, in proving an existence theorem. For the sake of problem formulation and notational simplicity, the main variable will be chosen to make the capillary pressure an increasing function.

In numerical simulations based on the system (3.23)–(3.25), one has to compute the coefficients (3.16)–(3.22) by integrating the equation (3.15) for different initial values of the global pressure P. From a practical point of view, one can solve (3.15) approximately for certain values of initial data and then use an interpolation procedure to extend these values to the whole range of interest. The necessary calculations can be done in a preprocessing phase, without penalizing the flow simulation. This approach is employed in the implementation of the practical part of this thesis.

3.3 A Simplified Fractional Flow Formulation

In the existing literature the concept of global pressure in two and three phase compressible flow models is always introduced by means of an approximation. More precisely, it is assumed that one can ignore the error caused by calculating the phase density ρ_α at the global pressure P instead of the phase pressure P_α. This assumption is introduced in [25] and used in petroleum engineering applications (see, e.g., [29,30]), but it cannot be satisfied for all the existing immiscible compressible two-phase flow. The simplified global pressure formulation will be described for the case of two phase flow. It will also be compared to the new formulation introduced in the previous section.

Assuming that one can replace the wetting pressure in the fractional flow phase function with the global pressure P, the equation (3.8) is transformed to

$$\nabla P_g - f_w(S_w, P)P_c'(S_w)\nabla S_w = \omega(S_w, P)\nabla P,$$

which can be satisfied by

$$P_g = P + P_c(1) - \gamma(S_w, P), \quad \gamma(S_w, P) = -\int_0^{P_c(S_w)} \hat{f}_w(u, P)\, du, \tag{3.30}$$

where, as before, $\hat{f}_w(u, P) = f_w(S_w, P)$ for $u = P_c(S_w)$, and relative permeabilities are for $P_c(1) \neq 0$ defined as in remark 3.1. From (3.30) it follows

$$\nabla P = \nabla P_g + \frac{\partial}{\partial P}\gamma(S_w, P)\nabla P - f_w(S_w, P)P_c'(S_w)\nabla S_w,$$

which means that

$$\omega(S_w, P) = 1 - \frac{\partial}{\partial P}\gamma(S_w, P). \tag{3.31}$$

The total flux now obtains a form of Darcy's law:

$$\mathbf{Q}_t = -\lambda(S_w, P)\mathbb{K}(\omega(S_w, P)\nabla P - \rho(S_w, P)\mathbf{g}). \tag{3.32}$$

The system (2.39)–(2.41), written in the unknowns P and S_w, now takes the form:

$$\Phi\frac{\partial}{\partial t}(S_w\rho_w(P)+(1-S_w)\rho_g(P)) \tag{3.33}$$

$$-\operatorname{div}(\lambda(S_w,P)\mathbb{K}[\omega(S_w,P)\nabla P-\rho(S_w,P)\mathbf{g}])=\mathcal{F}_w+\mathcal{F}_g,$$

$$\mathbf{Q}_t=-\lambda(S_w,P)\mathbb{K}(\omega(S_w,P)\nabla P-\rho(S_w,P)\mathbf{g}), \tag{3.34}$$

$$\Phi\frac{\partial}{\partial t}(S_w\rho_w(P))+\operatorname{div}(f_w(S_w,P)\mathbf{Q}_t+\mathbb{K}\mathbf{g}b_g(S_w,P))=\operatorname{div}(\mathbb{K}a(S_w,P)\nabla S_w)+\mathcal{F}_w, \tag{3.35}$$

where, according to the initial assumption, one systematically approximates $\rho_g(P_g)$ with $\rho_g(P)$ and $\rho_w(P_w)$ with $\rho_w(P)$. The coefficients in (3.33)–(3.35) are, therefore, given by

$$\lambda(S_w,P)=\rho_w(P)\lambda_w(S_w)+\rho_g(P)\lambda_g(S_w). \tag{3.36}$$

$$f_\alpha(S_w,P)=\rho_\alpha(P)\lambda_\alpha(S_w)/\lambda(S_w,P),\quad \alpha=w,g, \tag{3.37}$$

$$\rho(S_w,P)=(\lambda_w(S_w)\rho_w(P)^2+\lambda_g(S_w)\rho_g(P)^2)/\lambda(S_w,P), \tag{3.38}$$

$$\alpha(S_w,P)=\rho_w(P)\rho_g(P)\lambda_w(S_w)\lambda_g(S_w)/\lambda(S_w,P), \tag{3.39}$$

$$b_g(S_w,P)=(\rho_w(P)-\rho_g(P))\alpha(S_w,P), \tag{3.40}$$

$$a(S_w,P)=-\alpha(S_w,P)P_c'(S_w), \tag{3.41}$$

and (3.31). It is clear that the systems (3.33)–(3.35) and (3.23)–(3.25) differ only in the way their coefficients are calculated.

Remark 3.3. *Note that (3.30) defines* P_g *as a function of* S_w *and* P *in a form* $P_g = P_g(S_w,P)=P+P_c(1)-\gamma(S_w,P)$, *but for fixed* P_g *and* S_w, *(3.30) is a nonlinear equation in* P *and its solvability is to be demonstrated if one wants to have an invertible change of variables. From (3.30) it also follows that the new global pressure* P *is between the two phase pressures:*

$$P_w\le P\le P_g.$$

With regards to the question of well-posedness of the simplified global formulation, the system (3.33)–(3.35) is physically relevant only if the function ω, introduced by (3.31), is strictly positive since ω is a certain correction factor of the total mobility that takes into account that the nonwetting pressure is now a nonlinear function of the global pressure.

This function can be written as

$$\begin{aligned}\omega(S_w, P) &= 1 + \int_0^{P_c(S_w)} \frac{\partial}{\partial P}\hat{f}_w(u, P)\, du \\ &= 1 - \int_0^{P_c(S_w)} \frac{\hat{\lambda}_w(u)\hat{\lambda}_g(u)}{(\hat{\lambda}_w(u) + M(P)\hat{\lambda}_g(u))^2}\, du\, M'(P),\end{aligned} \tag{3.42}$$

where

$$M(P) = \frac{\rho_g(P)}{\rho_w(P)}, \quad M'(P) = M(P)\left(\frac{\rho_g'(P)}{\rho_g(P)} - \frac{\rho_w'(P)}{\rho_w(P)}\right). \tag{3.43}$$

The condition $\omega > 0$ is critical only in the case where the nonwetting phase compressibility is greater than the wetting phase compressibility, which is usually the case. In that case

$$\int_0^{\infty} \frac{\hat{\lambda}_w(u)\hat{\lambda}_g(u)}{(\hat{\lambda}_w(u) + M(P)\hat{\lambda}_g(u))^2}\, du\, M'(P) < 1, \tag{3.44}$$

for all pressures P in the range of interest. Under the condition (3.44) the change of variables $(S_w, P) \mapsto (S_w, P_g)$ is invertible.

Lemma 3.1. *For given $P_g > 0$ and $0 < S_w \leq 1$, assume that the condition (3.44) is satisfied for $P \in (P_w, P_g)$, with $P_w = P_g - P_c(S_w)$. Then, the global pressure P is well defined by the equation (3.30).*

Proof. For $S_w = 1$ is obviously $P = P_w \leq P_g$. For $S_w \in (0, 1)$ one defines a function

$$\Phi_{S_w}(P) = P + P_c(1) - P_g + \int_0^{P_c(S_w)} \frac{\rho_w(P)\hat{\lambda}_w(u)}{\rho_w(P)\hat{\lambda}_w(u) + \rho_g(P)\hat{\lambda}_g(u)}\, du.$$

The global pressure P is defined by $\Phi_{S_w}(P) = 0$. Note that $\Phi'_{S_w}(P) = \omega(S_w, P)$, and by (3.44) one has $\Phi'_{S_w}(P) > 0$ for all $P \in (P_w, P_g)$. It easily follows that $\Phi_{S_w}(P_g) > 0$, and $\Phi_{S_w}(P_w) < 0$, so that Φ_{S_w} must have a unique zero in interval (P_w, P_g). $\square$

Note that the condition (3.44) is not always satisfied in the whole range of the global pressure P. Taking, for example, incompressible wetting phase and the ideal gas law $\rho_g(P) = c_g P$ for a nonwetting phase, (3.44) reduces to

$$\int_0^{\infty} \frac{c_g \rho_w \hat{\lambda}_w(u)\hat{\lambda}_g(u)}{(\rho_w \hat{\lambda}_w(u) + c_g P \hat{\lambda}_g(u))^2}\, du < 1.$$

In the terms of wetting saturation variable this integral can be rewritten as

$$\int_0^1 \frac{c_g \rho_w(-\lambda_w(s)\lambda_g(s)P_c'(s))}{(\rho_w \lambda_w(s) + c_g P \hat{\lambda}_g(s))^2}\, ds < 1,$$

and since in the case of the van Gencuhten and Brooks and Corey functions the function $|\lambda_w(S_w)\lambda_g(S_w)P_c'(S_w)|$ is always bounded for $S_w \in]0,1[$ with finite limits for $S_w \to 0$ and $S_w \to 1$, and for $P > 0$ the denominator in the above formula is always strictly positive, the above integral exists, and it's value can be controled by P. So, the above integral will be generally lower than 1 only for P sufficiently large. Therefore, the simplified fractional flow model is not well defined if the field pressure in the porous domain is not sufficiently large.

In order to correct this deficiency of the simplified fractional flow model the function ω will be redefined. The formula (3.42) was obtained as a consequence of calculation of mass densities ρ_w and ρ_g in the global pressure instead of the appropriate phase pressure. One can make this kind of approximation directly in the formula (3.22) for ω in a fully equivalent fractional flow model, leading to

$$\begin{aligned} \omega(S_w, P) &= \exp\left(\int_{S_w}^1 (\nu_g(P) - \nu_w(P)) \frac{\rho_w(P)\rho_g(P)\lambda_w(s)\lambda_g(s)P_c'(s)}{(\rho_w(P)\lambda_w(s) + \rho_g(P)\lambda_g(s))^2}\, ds\right), \\ &= \exp\left(-\int_0^{P_c(S_w)} M'(P) \frac{\hat{\lambda}_w(u)\hat{\lambda}_g(u)}{(\hat{\lambda}_w(u) + M(P)\hat{\lambda}_g(u))^2}\, du\right). \end{aligned} \tag{3.45}$$

A benefit of the formula (3.45), in contrast to (3.42), is its strict positivity. It is clear that the formula (3.42) gives only the first two terms in Taylor's expansion for the exponential function in (3.45) and these remarks allow us to conclude that (3.45) is a more consistent approximation than (3.42). Consequently, in numerical simulations with the simplified fractional flow model, ω given by (3.45) will be used.

Remark 3.4. *There is an another way of introducing a global pressure in compressible two-phase flow based on approximate calculation of mass densities. Namely, for the case* $P_c(1) = 0$*, one can use the global pressure definition from incompressible case [25]:*

$$P = P_g - \int_{S_w}^1 \frac{\lambda_w(s)}{\lambda_w(s) + \lambda_g(s)} P_c'(s)\, ds. \tag{3.46}$$

This change of variables permits to eliminate the saturation gradient from the total velocity, $\mathbf{q}_t = \mathbf{q}_w + \mathbf{q}_g$. *However, it will not eliminate it from the pressure equation (2.39), except* *in the case* $\rho_w(P) = \rho_g(P)$. *In that particular case, the global pressure (3.46) is the same as the global pressure in the simplified fractional flow formulation presented in this section. Further formulation based on (3.46) will not be considered in the scope of this thesis. Note that the existence of its weak solution was recently proved in [43, 44]*

3.4 Comparison of Fully Equivalent and Simplified Formulation

Note that the simplified assumption introduced in Section 3.3 leads to a fractional flow model in which the coefficients are calculated from the mass densities, the relative permeabilities and the capillary pressure, without solving a large number of the Cauchy problems for ordinary differential equation as in (3.23)–(3.25). This makes the simplified model (3.33)–(3.35) interesting and raises a question of error introduced by replacing systematically the phase pressures with the global pressure in the calculations of the mass densities. This question will be addressed by comparison of the coefficients of the two models. Also these two models are going to be compared by performing the simulation in Chapter 4. From now on, the model based on equations (3.23)–(3.25), and coefficients defined by (3.14) and (3.16)–(3.22), will be referred to as *the new model*. The model based on the equations (3.33)–(3.35), and coefficients defined by (3.36)–(3.41) and (3.45), will be referred to as *the simplified model*. It is assumed that $P_c(1) = 0$.

3.4.1 Comparison of the Coefficients

The difference in the coefficients of the two models is introduced by replacing the fluid phase pressures $P_g = \hat{P}_g(u, P)$ and $P_w = \hat{P}_g(u, P) - u$ with the global pressure P. The differences $P_g - P$ and $P - P_w$ will be estimated based on $P_w \le P \le P_g$ and the mass density being a non decreasing function for the corresponding phase pressure.

$$\frac{\rho_g(P_g)}{\rho_w(P_w)} \ge \frac{\rho_g(P)}{\rho_w(P)} = M(P), \tag{3.47}$$

where $M(P)$ is introduced in (3.43). From (3.12) it follows

$$0 \le P_g(S_w, P) - P = \int_0^{P_c(S_w)} \frac{\hat{\lambda}_w(u)}{\hat{\lambda}_w(u) + (\rho_g(P_g)/\rho_w(P_w))\hat{\lambda}_g(u)}\, du,$$

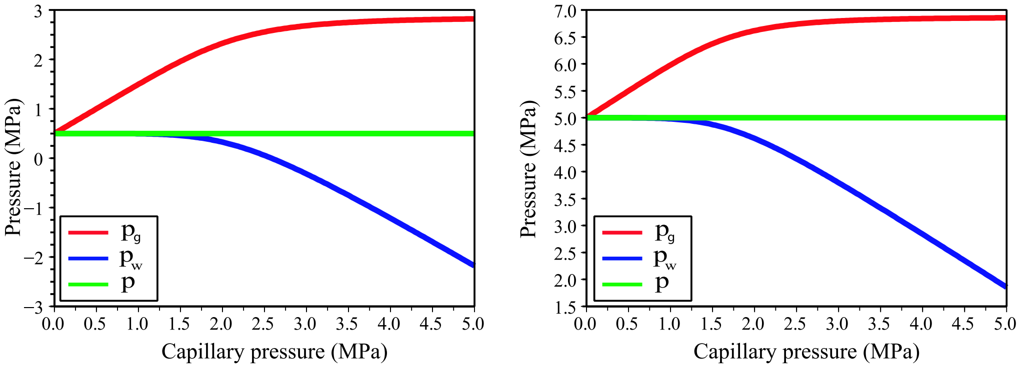


Figure 3.1: Phase pressures $P_g = \hat{P}_g(u,P)$ and $P_w = \hat{P}_g(u,P) - u$, for two fixed global pressures $P = 0.5$ and $P = 5$ MPa, as functions of capillary pressure u.

and using (3.47)

$$0 \le P_g(S_w, P) - P \le \int_0^{P_c(S_w)} \frac{\hat{\lambda}_w(u)}{\hat{\lambda}_w(u) + M(P)\hat{\lambda}_g(u)}\, du. \tag{3.48}$$

Note also that in general, the relative permeability functions depend on a dimensionless variable of the form $v = u/P_c^0$, where u is the capillary pressure and P_c^0 is some characteristic capillary pressure value. In that case a simple change of variables yields,

$$0 \le P_g(S_w, P) - P \le P_c^0 \int_0^{+\infty} \frac{\hat{\lambda}_w(v)}{\hat{\lambda}_w(v) + M(P)\hat{\lambda}_g(v)}\, dv, \tag{3.49}$$

where the integral on the right hand side is independent of the strength of the capillary pressure.

For the difference between the wetting fluid pressure and the global pressure one obtains,

$$P - P_w = \int_0^{P_c(S_w)} \frac{\hat{\lambda}_g(u)}{(\rho_w(P_w)/\rho_g(P_g))\hat{\lambda}_w(u) + \hat{\lambda}_g(u)}\, du, \tag{3.50}$$

and therefore

$$\int_0^{P_c(S_w)} \frac{M(P)\hat{\lambda}_g(u)}{\hat{\lambda}_w(u) + M(P)\hat{\lambda}_g(u)}\, du \le P - P_w \le P_c(S_w). \tag{3.51}$$

From these estimates a several conclusions can be drawn. To simplify discussion, only the most common case will be considered. This is the case where the nonwetting phase is more compressible than the wetting phase, i.e. the case in which $P \mapsto M(P)$ is increasing.

1. The global pressure will be uniformly close to the gas pressure if the characteristic capillary pressure P_c^0 is small. Following (3.49) one obtains that the difference between the global and the gas pressure is smaller for higher global pressures.

2. Considering (3.48) and (3.51) and for S_w close to one, the global pressure is closer to the wetting phase pressure than to the nonwetting one. However, for small S_w, the difference $P - P_w$ can be arbitrary large.

3. From the preceding conclusions it is visible that approximation errors are larger when the two fluids are equally compressible, and capillary pressure is large. There is also an influence of the pressure P that affects differently $P_g - P$ and $P - P_w$: when P increases difference $P_g - P$ decreases and $P - P_w$ increases.

For comparison of the coefficients, assume a set of data with incompressible wetting phase (water) and the ideal gas law $\rho_g(P) = c_g P$ for the nonwetting phase (hydrogen) and a set of van Genuchten's saturation-functions defined by (2.12)-(2.13).

The choice of incompressible wetting phase makes the approximation of coefficients independent of difference $P - P_w$. The error introduced by replacing P_g with P in density calculation depends now only on the characteristic capillary pressure P_c^0 and the global pressure P.

The fluid characteristics are given in Table 3.1, where n and Pr are van Genuchten's parameters.

μ_w Pa s	μ_g Pa s	ρ_w kg/m^3	c_g kg/(m^{3}MPa)	n -	Pr MPa
$0.86 \cdot 10^{-3}$	$9 \cdot 10^{-6}$	996.5	0.808	2	2

Table 3.1: Fluid properties

Water and gas residual saturation are assumed equal to zero.

In figure 3.1 $P_g = \hat{P}_g(u, P)$ and $P_w = \hat{P}_g(u, P) - u$ for a two fixed global pressures, $P = 0.5$ and 5 MPa. These figures show the global pressure is closer to the nonwetting phase pressure P_w for small to intermediate capillary pressure values. The difference $P - P_w$ grows unboundedly when capillary pressure augments. The difference $P_g - P$ tends to a constant when the capillary pressure grows.

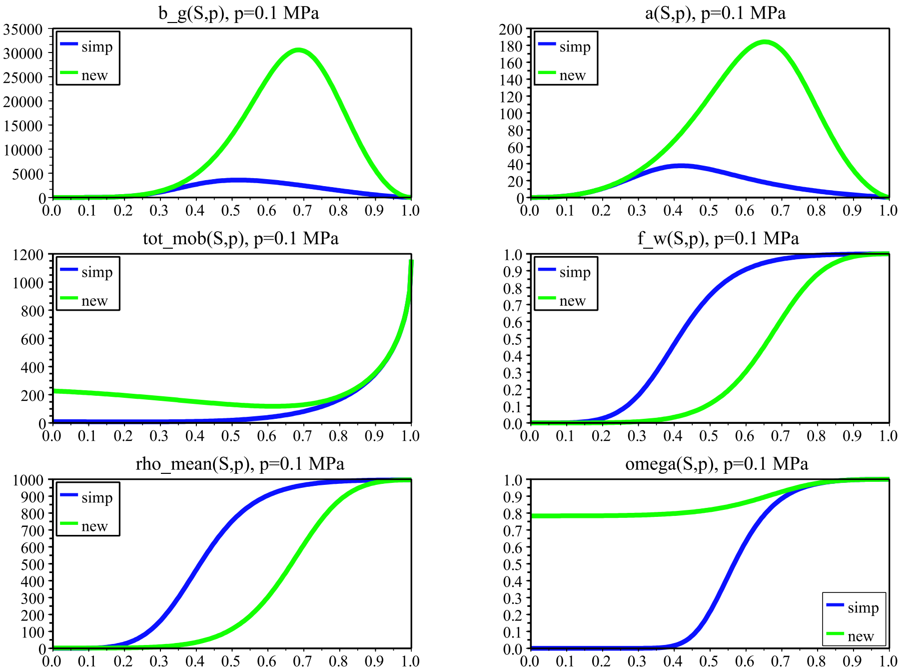


Figure 3.2: Comparison of the coefficients in the new and the simplified global pressure models at the global pressure of 0.1 MPa. The coefficients are presented as functions of the wetting phase saturation with fixed global pressure.

In figures 3.2 and 3.3 the coefficients in new and simplified models are compared: b_g and b_g^n (= `b_g` in the figure), a and a^n, λ and λ^n (= `tot_mob` in the figure), f_w and f_w^n (= `f_w` on the figure), and functions ω (= `omega` in the figure) given by formulae (3.22) and (3.45). The comparisons are given at the global pressure of $P = 0.1$ MPa in figure 3.2 and at $P = 5$ MPa in Figure 3.3. All functions are presented as functions of wetting fluid saturation, while the global pressure is a parameter.

These figures confirm that the difference in the coefficients diminishes when the global pressure augments, which is a consequence of the fact that ρ_w is constant and the approximation error depends only on $P_g - P$. Analogously, it could be demonstrated that the difference in the coefficients diminishes when the capillary pressure diminishes.

3.5 Treatment of Multiple Rock Types in the Global Pressure Formulation

In this section the conditions at the interface, in the case of fully equivalent global pressure model will be formulated. For the wetting phase variable in the situations where $P_d^{m1} \leq$

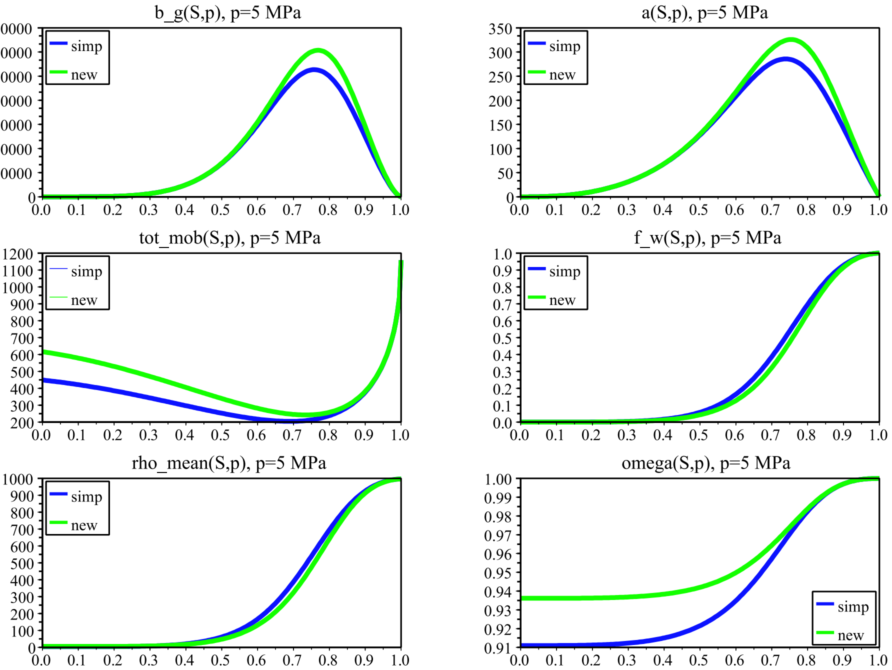


Figure 3.3: Comparison of the coefficients in the new and the simplified models at the global pressure of 5 MPa. The coefficients are presented as functions of the wetting phase saturation with fixed global pressure.

P_d^{m2} one observes the following:

$$S_w^{m2} = \begin{cases} 1 & \text{for } S_w^{m1} > S_w^* \\ (P_c^{m2})^{-1}(P_c^{m1}(S_w^{m1})) & \text{for } S_w^{m1} \leq S_w^*. \end{cases}$$

For the global pressure, the interface condition is derived from the transmission condition of one phase pressure. Given that porous media is denoted by $\Omega = \Omega^{m1} \cup \Omega^{m2}$. Similar to [17], where incompressible case was considered, one can have two different cases:

(C.1) $S_w^{m1} > S_w^*$, $S_w^{m2} = 1$; in this situation, the nonwetting pressure is not defined in the domain Ω^{m2} and P_w is continuous at the interface. Thus, one may use the derived representation for the wetting phase pressure (3.13). From $P_w^{m1}(1, P) = P$ and from the continuity of the wetting phase pressure the following condition is obtained

$$P_w^{m1}(S_w^{m1}, P^{m1}) = P^{m2} - \int_1^{S_w^{m2}} f_g^{m2}(s, P_g^{m2}(s, P^{m2})) \frac{dP_c^{m2}(s)}{ds}\, ds, \tag{3.52}$$

In this case transmission condition between two limiting values of the global pressure is described by the nonlinear equation (3.52). In fact, the following applies:

$$P^{m2} = P_w^{m1}(S_w^{m1}, P^{m1}). \tag{3.53}$$

From given P^{m1} and S_w^{m1} the P^{m2} can be calculated by (3.52)). In reverse, for given P^{m2} and S_w^{m1} one may calculate P^{m1} by solving the nonlinear equation (3.53), for which the solution is defined since the derivative of the wetting phase pressure over global pressure is strictly positive.

(C.2) $S_w^{m1} \leq S_w^*$, $P_c^{m1}(S_w^{m1}) = P_c^{m2}(S_w^{m2})$; here the phase pressures are continuous across the interface, and in the same way like described in [17] one can use the continuity of the nonwetting phase pressure to obtain

$$P_g^{m1}(S_w^{m1}, P^{m1}) = P_g^{m2}(S_w^{m2}, P^{m2}). \tag{3.54}$$

In this case, when S_w^{m1} and S_w^{m2} are given, one obtains P^{m2} from any given P^{m1} by solving the nonlinear equation

$$P_g^{m1} = P_g^{m2}(S_w^{m2}, P^{m2}), \tag{3.55}$$

whose solution is well defined since the partial derivative of the nonwetting pressure over global pressure is strictly positive. Also, for any given P^{m2} one may calculate P^{m1} from the nonlinear equation

$$P_g^{m1}(S_w^{m1}, P^{m1}) = P_g^{m2}.$$

Remark 3.5. *Note that in the case of the van Genuchten functions the case (C.2) always applies.*

Remark 3.6. *In the situation when the interface separates multiple rock types, the conditions described above are assumed for each pair of materials containing the same interface*

Remark 3.7. *The same transmission conditions can be applied in the case of simplified model, in the range of its validity.*

3.6 Conclusion

A new immiscible compressible two-phase flow model (3.23)–(3.25) is developed. The model is based on the global pressure concept which is fully equivalent to the original phase equation formulation (2.20), (2.21). This model is compared to the simplified fractional flow model presented in section 3.3. A comparison of the coefficients in the two models reveals that simplification based on replacing the phase pressures by the global pressure in calculations of mass densities can safely be used in applications when mean field pressure is high, capillary pressure is relatively small and if the wetting phase is not strongly compressible. This is the case in oil-gas systems. In hydro-geological applications, where capillary pressures may be elevated with respect to mean field pressure, this approximation can introduce unacceptably large errors, especially in predicting total mass of the nonwetting phase. These conclusions are confirmed by numerical simulation in the following chapter.

Chapter 4

Numerical Simulations

This chapter is devoted to the numerical simulations of the fully equivalent global pressure model. At first the numerical scheme is presented. Special attention is paid to the treatment of the heterogeneities and association of the numerical scheme and the transmission conditions. Furthermore, three monodimensional test cases are presented [52].

The first test case is related to the flow of gas and water in heterogeneous porous media with no discontinuities of the capillary pressure at the initial time. The second test case is the benchmark BO-BG, French acronym of Engineered Barrier Geological Barrier, which was proposed by the French research group MoMaS (http://www.gdrmomas.org/) to advance numerical methods used in the simulations concerning the gas migration through engineered and geological barriers for the deep repository of radioactive waste. In this test the initial capillary pressure is taken to be discontinuous. The third test case presents the situations that include the capillary pressure curves with nonzero entry pressure. During this chapter, most of the time the subscript w referring to the wetting phase saturation is omitted, and only S is used.

4.1 A Finite Volume Scheme

In this section, a vertex-centered finite volume method applied to the system of equations (3.23)-(3.25) for the one-dimensional case is presented.

4.1.1 Basic Notation

The equations (3.24)-(3.25) are solved on a finite time interval $J =]0, T[$, and in a finite spatial domain $I =]a, b[$. In order to present the discretization, the following notation is applied, similar to the one presented in [1, 2, 5]:

(N.1) Let $\left\{t^0 < t^1 < \ldots < t^{N_T}\right\}$ be the discretization of the time domain and by $J_k = [t^k, t^{k+1}[$ denote the k-level time interval. The time step is: $\triangle t^k = t^{k+1} - t^k$, $k = 0, 1, \ldots, N_T - 1$.

(N.2) Let $\{x_0 < x_1 < \ldots < x_{N_x}\}$ be the discretization of the spatial domain where: $E_{i+\frac{1}{2}} := [x_i, x_{i+1}]$, $i = 0, 1, \ldots, N_x - 1$, as shown in the figure 4.1 and set $\triangle x_i = |E_{i+\frac{1}{2}}| = x_{i+1} - x_i$, $i = 0, 1, \ldots, N_x - 1$.

(N.4) Control volumes are defined as follows: for each $i \in 0, 1, \ldots, N_x - 1$ denote the center of the element $E_{i+\frac{1}{2}}$ by $x_{i+\frac{1}{2}} := \frac{x_i + x_{i+1}}{2}$, and set $x_{-\frac{1}{2}} = x_0$ and $x_{N_x+\frac{1}{2}} = x_{N_x}$. For $i = 0, \ldots, N_x$, the control volume is defined as $V_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$. By setting $h_i = |V_i| = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}, \quad i = 0, 1, 2 \ldots, N_x$, one obtains $h_0 = \frac{\Delta x_0}{2}$, $h_{N_x} = \frac{\Delta x_{N_x - 1}}{2}$ and $h_i = \frac{\Delta x_{i-1} + \Delta x_i}{2}$, $i = 0, 1, \ldots, N_x - 1$.

(N.5) Let $\{\phi_j, j = 0, \ldots, N_x\}$ $(\phi_j(x_j) = 1)$ be the set of P_1 base functions. The approximations

$$S(x,t) = \sum_{j=0}^{N} S_j(t)\phi_j(x), \quad P(x,t) = \sum_{j=0}^{N} P_j(t)\phi_j(x)$$

are required. The approximations of $S(x_i, t_k)$ and $P(x_i, t_k)$, are denoted by S_i^k and P_i^k.

(N.6) For the porosity, $\Phi \in L^\infty(I)$ one sets: $\phi_i = \frac{1}{h_i} \int_{V_i} \Phi(x)\, dx$.

(N.7) The permeability is scalar function of the space and it is assumed to be constant on the element: $K_{i+\frac{1}{2}} = K\big|_{E_{i+\frac{1}{2}}}$

A special care has to be taken when spatial mesh creation is performed in the situations with multiple rock types. As explained in the previous chapters, in each rock type the rock properties differ. Relative permeability and the capillary pressure functions may be different for each rock type as well.

If the spatial domain in one dimension is divided into N_m parts, and each part of the domain is related to a certain rock type, there are $N_m - 1$ interfaces. Every interface point is set to be an element of the spatial mesh $\{x_0 < x_1 < \ldots < x_{N_x}\}$. The other nodes of the spatial mesh can be chosen arbitrarily.

For the sake of simplicity and without loss of generality, the numerical scheme will be presented for the situation of the two rock types. A higher number of materials does not influence the presentation of the treatment of heterogeneity employed in this thesis. In the case with higher dimensions, the situation complicates further. In the following, it is assumed that the spatial domain is divided into two parts, one related to the material $m1$ and the other related to the material $m2$, as is presented in the figure 4.1.

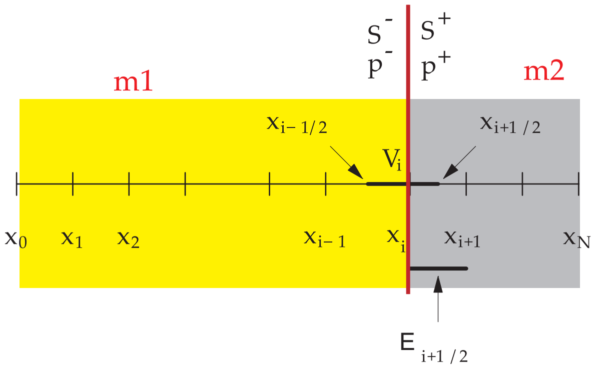


Figure 4.1: Spatial mesh in one-dimensional case

Let $I_{m1} \cup I_{m2} = I$ and the interface node is set to be $\{x_\delta\} = I_{m1} \cap I_{m2}$, for an index $\delta \in \{0, 1, \ldots, N_x\}$

The superscript n in the definition of the coefficients (3.16)-(3.20) is omitted to further simplify notation. Also the subscript t used previously in the notation of the total flux, is omitted. For the same reason the following functions are introduced (either $m = m1$ or $m = m2$):

$$M^m := M^m(S,P) := \rho_w(P_w^m(S,P))S + \rho_g(P_g^m(S,P))(1-S)$$

$$N^m := N(S,p) := \rho_w(P_w^m(S,p))S.$$

$$\chi^m(S,P) := \lambda^m(S,P)\omega^m(S,P)$$

$$\gamma(S,P) := -\alpha(S,P), \text{ so that } a(S,P) = \gamma(S,P)P_c'(S).$$

The equations (3.23)-(3.25) (with neglected gravity term) rewritten in one-dimensional case are:

$$\Phi\frac{\partial}{\partial t}\left(M^m(S,P)\right)\right) - \frac{\partial}{\partial x}\left(\chi^m(S,P)K\frac{\partial P}{\partial x}\right) = \mathcal{F}_w + \mathcal{F}_g \tag{4.1}$$

$$Q^m = -\chi^m(S,P)K\frac{\partial P}{\partial x} \tag{4.2}$$

$$\Phi\frac{\partial}{\partial t}(N^m(S,P)) + \frac{\partial}{\partial x}\left(Q^m f_w^m(S,p)\right) - \frac{\partial}{\partial x}\left(\gamma^m(S,P)K\frac{\partial P_c^m(S)}{\partial x}\right) = \mathcal{F}_w \tag{4.3}$$

At initial time, either the global pressure, the saturation or the phase pressures are given. A set of boundary conditions of diverse types can be given.

As already mentioned, in the chapter 3, the saturation and the global pressure are generally discontinuous at the interface point. Therefore, it is worthwhile to explain the meaning and use of the global unknowns S_δ^k and P_δ^k, at the interface node x_δ.

4.1.2 Interface Conditions

The values S_δ^k and P_δ^k are solutions of the nonlinear problem for each time step. These are considered to be the representative values of the true limit values defined by the elements. The index k is omitted below to simplify the notation.

There are several ways of defining these global unknowns. At first consider the saturation variable and recall that at the interface point the following equality has to be satisfied:

$$P_c^{m1}(S_\delta^{m1}) = P_c^{m2}(S_\delta^{m2}), \tag{4.4}$$

if one assumes that $P_c^{m1}(1) = P_c^{m2}(1) = 0$, otherwise *extended capillary pressure condition* needs to be satisfied. Here P_c^{m1} (P_c^{m2}) is the capillary pressure defined for the material $m1$ (material $m2$), and $S_\delta^{m1}(S_\delta^{m2})$ are respective limiting saturations. When the wetting phase saturation is the primary unknown of the system, in the computation by the elements the true limit values of the saturation need to be used. This also guarantees that during calculation one actually always works with the correct capillary pressure at the interface node x_δ.

The unknown value S_δ at the interface node x_δ can be chosen in several ways. For instance, it can be taken as $S_\delta = f(S_\delta^{m1}, S_\delta^{m2})$, where f an invertible function in every variable. The simplest approach, however, is to choose $S_\delta = S_\delta^{m1}$ or $S_\delta = S_\delta^{m2}$.

The situation with the global pressure is similar. The global pressure will generally be discontinuous at the interface point. The choice of P_δ can be done in several ways, and the simplest approach is to choose $P_\delta = P_\delta^{m1}$ or $P_\delta = P_\delta^{m2}$, and then use the continuity of the nonwetting phase pressure:

$$P_g^{m1}(S_\delta^{m1}, P_\delta^{m1}) = P_g^{m2}(S_\delta^{m2}, P_\delta^{m2}) \tag{4.5}$$

at the interface, in order to obtain the other limiting value, depending on which part of the domain the calculation is done.

This is applicable if the nonwetting phase is mobile at the interface, otherwise one needs to use the continuity of the wetting phase pressure.

Remark 4.1. *In the simulations where the entry pressure is present (e.g. Brooks and Corey capillary pressure), the choice of the unknown S_δ is more restrictive. It has to be taken equal to the limiting saturation of the material which is related to the smaller "entry pressure" [17, 56]. If this is the region I_{m1}, the extended capillary pressure condition (2.50) to calculate the saturation S_δ^{m2} is used.*

4.1.3 Numerical Scheme Presentation

For any function $f(S, P)$ we define:

$$f_{i+\frac{1}{2}}^{m,k} = f^m(S_{i+\frac{1}{2}}^k, P_{i+\frac{1}{2}}^k).$$

The following notation is used:

$$S_{i+\frac{1}{2}}^k = \frac{S_i^k + S_{i+1}^k}{2}, \quad P_{i+\frac{1}{2}}^k = \frac{P_i^k + P_{i+1}^k}{2}.$$

At first, the system (4.1)-(4.3) is integrated over the set $V_i \times J_k$ to obtain:

$$
\begin{aligned}
\int_{V_i} \Phi \left(M^m(S^{k+1}, P^{k+1}) - M^m(S^k, P^k)) \right) dx - \int_{J_k} \sum_{j=\pm\frac{1}{2}} (2j)\chi^m_{i+j} K_{i+j} \left(\frac{\partial P}{\partial x} \right)_{i+j} dt \\
= |V_i|(\mathcal{F}_{w,i} + \mathcal{F}_{g,i}) \\
\int_{V_i} \Phi \left(N^m(S^{k+1}, P^{k+1}) - N^m(S^k, P^k)) \right) dx + \int_{J_k} \sum_{j=\pm\frac{1}{2}} (2j) Q^m_{i+j} f^{m,up}_{w,i+j}\, dt \\
= \int_{J_k} \sum_{j=\pm\frac{1}{2}} (2j)\gamma^m_{i+j} K_{i+j} \left(\frac{\partial P^m_c(S)}{\partial x} \right)_{i+j} dt \\
+ |V_i| \mathcal{F}_{w,i}
\end{aligned}
$$

Now, various approximations can be used:

$$
\left(\frac{\partial P}{\partial x} \right)_{i+\frac{1}{2}} = \frac{P_{i+1} - P_i}{\Delta x_i}, \quad \left(\frac{\partial P^m_c(S)}{\partial x} \right)_{i+\frac{1}{2}} = \frac{P^m_c(S_{i+1}) - P^m_c(S_i)}{\Delta x_i}.
$$

On the left side of the equations the mass lumping is applied. The following equations are obtained:

$$
\Phi_i h_i \frac{M^{m,k+1}_i - M^{m,k}_i}{\Delta t^k} = R^{k+1}_{p,i} \tag{4.6}
$$

$$
\Phi_i h_i \frac{N^{m,k+1}_i - N^{m,k}_i}{\Delta t^k} = R^{k+1}_{S,i}. \tag{4.7}
$$

The following notation is introduced:

$$
T_{i+1/2} := \frac{K_{i+1/2}}{\triangle x_i}, \quad i = 0, 1, 2 \dots, N_x - 1.
$$

For $i = 1, 2, \dots, N_x - 1$, the right hand side of the (4.6) is

$$
R^{k+1}_{p,i} = \sum_{j=\pm\frac{1}{2}} \chi^{m,k+1}_{i+j} T_{i+j} (P^{k+1}_{i+2j} - P^i_i) + |V_i|(\mathcal{F}_{g,i} + \mathcal{F}_{w,i}). \tag{4.8}
$$

The total velocity for $j = \pm\frac{1}{2}$ is

$$
Q^{m,k+1}_{i+j} = -\chi^{m,k+1}_{i+j} T_{i+j} (P^{k+1}_{i+2j} - P^{k+1}_i)
$$

where $m = m1$ or $m = m2$.
For $i = 1, 2, \dots N_x - 1$

$$R_{S,i}^{k+1} = \sum_{j=\pm\frac{1}{2}} \gamma_{i+j}^{m,k+1} T_{i+j} (P_c^m(S_{i+2j}^{k+1}) - P_c^m(S_i^{k+1})) \tag{4.9}$$

$$- \sum_{j=\pm\frac{1}{2}} (2j) Q_{i+j}^{m,k+1} (f_w^m)_{i+j}^{m,up,k+1} + |V_i|(\mathcal{F}_{w,i}), \tag{4.10}$$

where, if the type of problem requires, the following **upwind** procedure is applied:

$$f_{w,i+\frac{1}{2}}^{m,up,k+1} = \begin{cases} f_w^m(S_i^{k+1}, P_i^{k+1}) & \text{for } Q_{i+\frac{1}{2}}^{k+1} \geq 0 \\ f_w^m(S_{i+1}^{k+1}, P_{i+1}^{k+1}) & \text{for } Q_{i+\frac{1}{2}}^{k+1} < 0 \end{cases}.$$

Otherwise, the standard expression for $R_{S,i}^{k+1}$ is used:

$$R_{S,i}^{k+1} = \sum_{j=\pm\frac{1}{2}} \gamma_{i+j}^{m,k+1} T_{i+j} (P_c^m(S_{i+2j}^{k+1}) - P_c^m(S_i^{k+1})) \tag{4.11}$$

$$- \sum_{j=\pm\frac{1}{2}} Q_{i+j}^{m,k+1} (f_w^m)_{i+j}^{m,k+1} + |V_i|(\mathcal{F}_{w,i}). \tag{4.12}$$

The terms $R_{S,0}^{k+1}, R_{p,0}^{k+1}, R_{p,N_x}^{k+1}, R_{S,N_x}^{k+1}$ depend on the imposed boundary conditions.

Notes on the Discretization of Boundary Conditions

For simplicity it is assumed $\mathcal{F}_w = 0$ $\mathcal{F}_g = 0$. If setting the total flux $Q = Q_{in}$, and flux of wetting phase $Q_w = Q_{w,in}$ on the left boundary, one obtains:

$$R_{p,0}^{k+1} = \chi_{\frac{1}{2}}^{m1,k+1} T_{\frac{1}{2}} (P_1^{k+1} - P_0^{k+1}) + Q_{in}$$

$$R_{S,0}^{k+1} = \gamma_{\frac{1}{2}}^{m,k+1} T_{\frac{1}{2}} (P_c^m(S_1^{k+1}) - P_c^m(S_0^{k+1})) - Q_{\frac{1}{2}}^{m,k+1} (f_w)_{\frac{1}{2}}^{m,up,k+1} + Q_{w,in}.$$

If setting the total flux $Q = Q_{out}$, and $Q_w = Q_{w,out}$ on the right boundary, one obtains:

$$R_{p,N_x}^{k+1} = -\chi_{N_x-\frac{1}{2}}^{m2,k+1} T_{N_x-\frac{1}{2}} (P_{N_x}^{k+1} - P_{N_x-1}^{k+1}) - Q_{out}$$

$$R^{k+1}_{S,N_x} = -\gamma^{m,k+1}_{N_x-\frac{1}{2}} T_{N_x-\frac{1}{2}} (P^m_c(S^{k+1}_{N_x}) - P^m_c(S^{k+1}_{N_x-1})) + Q^{m,k+1}_{N_x-\frac{1}{2}} (f_w)^{m,up,k+1}_{N_x-\frac{1}{2}} - Q_{w,out}$$

Remark 4.2. *If fluxes are set to be zero at the boundary* ($Q = 0, Q_w = 0$) *the expressions (4.8) and (4.10) can also be used for* $i = 0$ *and for* $i = N_x$ *if:*

$$P^k_{-1} = P^k_0 \quad Q^k_{-\frac{1}{2}} := Q^k_{N_x+\frac{1}{2}} = 0$$

$$P^{m1}_c(S^k_{-1}) = P^{m1}_c(S^k_0) \quad P^{m2}_c(S^k_{N_x+1}) = P^{m2}_c(S^k_{N_x}).$$

For Dirichlet boundary conditions $S = S_{in}$ and $P = P_{in}$ on the left part of the boundary one obtains:

$$R^{k+1}_{p,0} = P - P_{in}, \quad M^{m,k+1}_0 - M^{m,k}_0 \equiv 0.$$

$$R^{k+1}_{S,0} = S^{k+1}_0 - S_{in}, \quad N^{m,k+1}_0 - N^{m,k}_0 \equiv 0.$$

Similar expressions, are obtained for setting Dirichlet boundary conditions on the right part of the boundary.

Commonly, Neumann boundary condition for the saturation is used. A case when at the right boundary it is taken $\frac{\partial S}{\partial x}\big|_{x=x_{N_x}} = 0$ is discussed in the following.

Note that for x_{N_x} one obtains

$$\Phi_{N_x} h_{N_x} \frac{M^{m2,k+1}_{N_x} - M^{m2,k}_{N_x}}{\Delta t} = -Q^{m2,k+1}_{out} - \chi^{k+1}_{i-\frac{N_x}{2}} T_{N_x-\frac{1}{2}} (P^{k+1}_{N_x} - P^{k+1}_{N_x-1}),$$

which provides a way to calculate Q^{n+1}_{out}:

$$Q^{m2,n+1}_{out} = -\Phi_{N_x} h_{N_x} \frac{M^{m2,k+1}_{N_x} - M^{m2,k}_{N_x}}{\Delta t} - \chi^{m2,k+1}_{i-\frac{N_x}{2}} T_{i-\frac{1}{2}} (P^{k+1}_{N_x} - P^{k+1}_{N_x-1})$$

One can set an upwind value at the node x_{N_x} as follows:

$$f^{up,n+1}_{w,out} = \begin{cases} f\left(\left(\frac{S^{k+1}_{N_x-1}+S^{n+1}_{N_x})}{2}, \frac{(P^{k+1}_{N_x-1}+P_{out})}{2}\right) & \text{for } Q^{k+1}_{out} \geq 0 \\ f(S^{n+1}_{N_x}, P_{out}) & \text{for } Q^{n+1}_{out} < 0 \end{cases}$$

and in that case equation (4.10) for R^{k+1}_{S,N_x} can be used.

Nonlinear Equations

Notice that at each time step a nonlinear problem is obtained. This type of problem may be solved by the Picard iterations or by the Newton method. In order to use the Newton method, one needs to know how to form a residual and a Jacobian at the previous iteration. While those calculations are done, special attention needs to be paid to the interface node. Considering that all the calculations are performed locally at the element E, it is worthwhile to have an insight into the local calculations. A brief explanation is given in the following subsection.

4.1.4 Local Calculations

All the functions used in the discretization belong to the material where the current element is positioned. Therefore, material index will be omitted in this section. Considering that the time index is constant in the scope of this discussion, it is omitted as well. The local calculations are presented for the situation when phase fluxes are set to be zero at the boundary. For the simplicity, it is assumed that $P_c(1) = 0$.

Local Residuals

Denote the local element by $E = [x_0, x_1]$. The global unknowns are: P_0, P_1, S_0, S_1. In general, assume that local values S_0^+, S_1^- depend on the values S_0 and S_1 respectively. Assume, as well, that P_0^+ depends on S_0 and P_0, and P_1^- depends on P_1 and S_1.

In the local calculation, the local values $S_0^+, P_0^+, S_1^-, P_1^-$ will be used. As discussed in the previous section, if calculations are performed at the interface node, one needs to know the limit values of saturation and global pressure. These are obtained from the global unknown value from the previous iteration. Consider the simplest example:

- If the global unknown at the node x_δ is set to be equal to the left limiting saturation, then $S_1^- = S_1$ is always valid. However, at the point x_0 the calculations have to be performed more carefully. the following is set:

$$S_0^+ = \begin{cases} S_0 & \text{if } x_0 \neq x_\delta \\ (P_c^{m2})^{-1}(P_c^{m1}(S_0)) & \text{for } x_0 = x_\delta \end{cases}.$$

- If the global unknown at the node x_δ is set to be equal to the left limiting pressure, then $P_1^- = P_1$ and at x_0 calculation have to be performed more carefully. Assuming

S_0^+ is already calculated, the following is set:

$$P_0^+ = \begin{cases} P_0 & \text{if } x_0 \neq x_\delta \\ \text{solution of } P_g^{m1}(S_0, P_0) = P_g^{m2}(S_0^+, P_0^+) & \text{if } x_0 = x_\delta \end{cases}.$$

The permeability K is constant on the element. One sets:

$$P_{\frac{1}{2}} = \frac{P_0^+ + P_1^-}{2}, \quad S_{\frac{1}{2}} = \frac{S_0^+ + S_1^-}{2}, \quad dx = x_1 - x_0, \quad T = \frac{K}{dx},$$

and now follows:

$$\begin{aligned} R_{p,0} &= \chi(S_{\frac{1}{2}}, P_{\frac{1}{2}})T(P_1^- - P_0^+) \\ R_{p,1} &= -\chi(S_{\frac{1}{2}}, P_{\frac{1}{2}})T(P_1^- - P_0^+). \end{aligned}$$

Also, the following equalities are obtained:

$$\begin{aligned} R_{S,0} &= \gamma(S_{\frac{1}{2}}, P_{\frac{1}{2}})T(P_c(S_1^-) - P_c(S_0^+)) - Q_{\frac{1}{2}} f_w^{up} \\ R_{S,1} &= -\gamma(S_{\frac{1}{2}}, p_{\frac{1}{2}})T(P_c(S_1^-) - P_c(S_0^+)) + Q_{\frac{1}{2}} f_w^{up} \end{aligned}$$

where

$$Q_{\frac{1}{2}} = -\chi(S_{\frac{1}{2}}, P_{\frac{1}{2}})T(P_1^- - P_0^+), \quad f_w^{up} = \begin{cases} f_w(S_0^+, P_0^+) & \text{for } Q_{\frac{1}{2}} \geq 0 \\ f_w(S_1^-, P_1^-) & \text{for } Q_{\frac{1}{2}} < 0 \end{cases}.$$

Local Jacobian

To form the Jacobian, one needs to know the derivatives

$$\frac{dS_0^+}{dS_0}(S_0), \frac{dS_1^-}{dS_1}(S_1), \frac{\partial P_0^+}{\partial S_0}(S_0, P_0), \frac{\partial P_0^+}{\partial P_0}(S_0, P_0), \frac{\partial P_1^-}{\partial S_1}(S_1, P_1), \frac{\partial P_1^-}{\partial P_1}(S_1, P_1).$$

If x_0 is not the interface node these values are calculated as usual. The following applies:

$$S_0^+ = S_0, \ \frac{dS_0^+}{dS_0} = 1, \ P_0^+ = P_0, \ \frac{\partial P_0^+}{\partial S_0} = 0, \ \frac{\partial P_0^+}{\partial P_0} = 1.$$

The same situation is when x_1 is not the interface node.

Remark 4.3. *To further simplify the notation, the function arguments will be omitted. By setting the global unknown at the interface equal to the left limiting saturation (pressure), one obtains:*

$$S_1^- = S_1,\ \frac{\partial S_1^-}{\partial S_1} = 1,\ P_1^- = P_1,\ \frac{\partial P_1^-}{\partial S_1} = 0,\ \frac{\partial P_1^-}{\partial P_1} = 1.$$

From the transmission conditions (4.4) and (4.5) one obtains the following:

$$\frac{\partial S_0^+}{\partial S_0} = \begin{cases} 1 & \textit{if } x_0 \neq x_\delta \\ \left(\frac{dP_c^{m1}(S_0)}{dS}\right) / \left(\frac{dP_c^{m2}(S_0^+)}{dS}\right) & \textit{for } x_0 = x_\delta \end{cases}$$

$$\frac{\partial P_0^+}{\partial S_0} = \begin{cases} 0 & \textit{if } x_0 \neq x_\delta \\ \frac{\frac{\partial P_g^{m1}(S_0,P_0)}{\partial S_0} - \frac{\partial P_g^{m2}(S_0^+,P_0^+)}{\partial S}\frac{\partial S_0^+}{\partial S}}{\omega^{m2}(S_0^+,P_0^+)} & \textit{for } x_0 = x_\delta \end{cases}$$

$$\frac{\partial P_0^+}{\partial P_0} = \begin{cases} 1 & \textit{if } x_0 \neq x_\delta \\ \frac{\omega^{m1}(S_0,P_0)}{\omega^{m2}(S_0^+,P_0^+)} & \textit{for } x_0 = x_\delta \end{cases}.$$

Note that when the unknowns at the interface node are selected differently, the above derivatives have to be calculated accordingly.

It follows:

$$D_P R_P = \begin{bmatrix} \partial_{P_0} R_{P,0} & \partial_{P_1} R_{P,0} \\ \partial_{P_0} R_{p,1} & \partial_{P_1} R_{P,1} \end{bmatrix} = T \begin{bmatrix} \alpha_1 & \beta_1 \\ -\alpha_1 & -\beta_1 \end{bmatrix}$$

where

$$\alpha_1 = \frac{1}{2}\partial_P \chi(S_{\frac{1}{2}}, P_{\frac{1}{2}}) \frac{\partial P_0^+}{\partial P_0}(P_1^- - P_0^+) - \chi(S_{\frac{1}{2}}, P_{\frac{1}{2}}) \frac{\partial P_0^+}{\partial P_0}$$
$$\beta_1 = \frac{1}{2}\partial_P \chi(S_{\frac{1}{2}}, P_{\frac{1}{2}}) \frac{\partial P_1^-}{\partial P_1}(P_1^- - P_0^+) + \chi(S_{\frac{1}{2}}, P_{\frac{1}{2}}) \frac{\partial P_1^-}{\partial P_1}.$$

One obtains

$$D_S R_p = \begin{bmatrix} \partial_{S_0} R_{P,0} & \partial_{S_1} R_{P,0} \\ \partial_{S_0} R_{P,1} & \partial_{S_1} R_{P,1} \end{bmatrix} = T \begin{bmatrix} \alpha_2 & \beta_2 \\ -\alpha_2 & -\beta_2 \end{bmatrix}$$

where

$$\alpha_2 = \frac{1}{2}\left(\partial_S \chi(S_{\frac{1}{2}}, P_{\frac{1}{2}})\frac{\partial S_0^+}{\partial S_0} + \partial_P \chi(S_{\frac{1}{2}}, p_{\frac{1}{2}})\frac{\partial P_0^+}{\partial S_0}\right)(P_1^- - P_0^+) - \chi(S_{\frac{1}{2}}, P_{\frac{1}{2}})\frac{\partial P_0^+}{\partial S_0}$$

$$\beta_2 = \frac{1}{2}\left(\partial_S \chi(S_{\frac{1}{2}}, P_{\frac{1}{2}})\frac{\partial S_1^-}{\partial S_1} + \partial_P \chi(S_{\frac{1}{2}}, P_{\frac{1}{2}})\frac{\partial P_1^-}{\partial S_1}\right)(P_1^- - P_0^+) + \chi(S_{\frac{1}{2}}, P_{\frac{1}{2}})\frac{\partial P_1^-}{\partial S_1}.$$

Total velocity derivatives are

$$\frac{\partial Q_{\frac{1}{2}}}{\partial S_0} = -T\alpha_2 \quad \frac{\partial Q_{\frac{1}{2}}}{\partial S_1} = -T\beta_2 \quad \frac{\partial Q_{\frac{1}{2}}}{\partial P_0} = -T\alpha_1 \quad \frac{\partial Q_{\frac{1}{2}}}{\partial P_1} = -T\beta_1.$$

Upwind flux derivatives are

$$\partial_{S_0} f_w^{up} = \begin{cases} \partial_S f_w(S_0^+, P_0^+)\frac{\partial S_0^+}{\partial S_0} + \partial_P f_w(S_0^+, P_0^+)\frac{\partial P_0^+}{\partial S_0} & \text{for } Q_{\frac{1}{2}} \geq 0 \\ 0 & \text{for } Q_{\frac{1}{2}} < 0 \end{cases}$$

$$\partial_{P_0} f_w^{up} = \begin{cases} \partial_P f_w(S_0^+, P_0^+)\frac{\partial P_0^+}{\partial P_0} & \text{for } Q_{\frac{1}{2}} \geq 0 \\ 0 & \text{for } Q_{\frac{1}{2}} < 0 \end{cases}$$

$$\partial_{S_1} f_w^{up} = \begin{cases} 0 & \text{for } Q_{\frac{1}{2}} \geq 0 \\ \partial_S f_w(S_1^-, P_1^-)\frac{\partial S_1^-}{\partial S_1} + \partial_P f(S_1^-, P_1^-)\frac{\partial P_1^-}{\partial S_1} & \text{for } Q_{\frac{1}{2}} < 0 \end{cases}$$

$$\partial_{P_1} f_w^{up} = \begin{cases} 0 & \text{for } Q_{\frac{1}{2}} \geq 0 \\ \partial_p f(S_1^-, P_1^-)\frac{\partial P_1^-}{\partial P_1} & \text{for } Q_{\frac{1}{2}} < 0 \end{cases}.$$

Convective flux derivatives are

$$\frac{\partial}{\partial S_0}(Q_{\frac{1}{2}} f_w^{up}) = \frac{\partial Q_{\frac{1}{2}}}{\partial S_0} f_w^{up} + Q_{\frac{1}{2}}\frac{\partial f_w^{up}}{\partial S_0} = -T\alpha_2 f_w^{up} + \max(Q_{\frac{1}{2}}, 0)\partial_{S_0} f_w^{up}$$

$$\frac{\partial}{\partial S_1}(Q_{\frac{1}{2}} f_w^{up}) = \frac{\partial Q_{\frac{1}{2}}}{\partial S_1} f_w^{up} + Q_{\frac{1}{2}}\frac{\partial f_w^{up}}{\partial S_1} = -T\beta_2 f_w^{up} + \min(Q_{\frac{1}{2}}, 0)\partial_{S_1} f_w^{up}$$

$$\frac{\partial}{\partial P_0}(Q_{\frac{1}{2}} f_w^{up}) = \frac{\partial Q_{\frac{1}{2}}}{\partial P_0} f_w^{up} + Q_{\frac{1}{2}}\frac{\partial f_w^{up}}{\partial P_0} = -T\alpha_1 f_w^{up} + \max(Q_{\frac{1}{2}}, 0)\partial_{P_0} f_w^{up}$$

$$\frac{\partial}{\partial P_1}(Q_{\frac{1}{2}} f_w^{up}) = \frac{\partial Q_{\frac{1}{2}}}{\partial P_1} f_w^{up} + Q_{\frac{1}{2}}\frac{\partial f_w^{up}}{\partial p_1} = -T\beta_1 f_w^{up} + \min(Q_{\frac{1}{2}}, 0)\partial_{P_1} f_w^{up}.$$

The residual is decomposed as follows:

$$R_{S,0} = R^{dif}_{S,0} + R^{con}_{S,0}, \quad R_{S,1} = R^{dif}_{S,1} + R^{con}_{S,1}$$

where

$$\begin{aligned} R^{dif}_{S,0} &= \gamma(S_{\frac{1}{2}}, P_{\frac{1}{2}})T(P_c(S^-_1) - P_c(S^+_0)), \quad & R^{con}_{S,0} &= -Q_{\frac{1}{2}} f^{up}_w \\ R^{dif}_{S,1} &= -\gamma(S_{\frac{1}{2}}, P_{\frac{1}{2}})T(P_c(S^-_1) - P_c(S^+_0)), \quad & R^{con}_{S,1} &= Q_{\frac{1}{2}} f^{up}_w, \end{aligned}$$

so it follows

$$D_S R_S = \begin{bmatrix} \partial_{S_0} R_{S,0} & \partial_{S_1} R_{S,0} \\ \partial_{S_0} R_{S,1} & \partial_{S_1} R_{S,1} \end{bmatrix} = D_S R^{dif}_S + D_S R^{con}_S$$

$$D_p R_S = \begin{bmatrix} \partial_{P_0} R_{S,0} & \partial_{P_1} R_{S,0} \\ \partial_{P_0} R_{S,1} & \partial_{P_1} R_{S,1} \end{bmatrix} = D_P R^{dif}_S + D_P R^{con}_S.$$

Using the notation $\gamma_{\frac{1}{2}} = \gamma(S_{\frac{1}{2}}, P_{\frac{1}{2}})$ and $\partial_P \gamma_{\frac{1}{2}} = \partial_P \gamma(S_{\frac{1}{2}}, P_{\frac{1}{2}})$ one obtains:

$$D_S R^{dif}_S = \begin{bmatrix} \partial_{S_0} R^{dif}_{S,0} & \partial_{S_1} R^{dif}_{S,0} \\ \partial_{S_0} R^{dif}_{S,1} & \partial_{S_1} R^{dif}_{S,1} \end{bmatrix} = T \begin{bmatrix} \alpha_3 & \beta_3 \\ -\alpha_3 & -\beta_3 \end{bmatrix},$$

where

$$\begin{aligned} \alpha_3 &= \left(\frac{1}{2} \partial_S \gamma_{\frac{1}{2}} \frac{\partial S^+_0}{\partial S_0} + \frac{1}{2} \partial_P \gamma_{\frac{1}{2}} \frac{\partial P^+_0}{\partial S_0} \right) (P_c(S^-_1) - P_c(S^+_0)) - \gamma_{\frac{1}{2}} P'_c(S^+_0) \frac{\partial S^+_0}{\partial S_0} \\ \beta_3 &= \left(\frac{1}{2} \partial_S \gamma_{\frac{1}{2}} \frac{\partial S^-_1}{\partial S_1} + \frac{1}{2} \partial_P \gamma_{\frac{1}{2}} \frac{\partial P^-_1}{\partial S_1} \right) (P_c(S^-_1) - P_c(S^+_0)) + \gamma_{\frac{1}{2}} P'_c(S^-_1) \frac{\partial S^-_1}{\partial S_1}. \end{aligned}$$

It follows:

$$D_P R^{dif}_S = \begin{bmatrix} \partial_{P_0} R^{dif}_{S,0} & \partial_{P_1} R^{dif}_{S,0} \\ \partial_{P_0} R^{dif}_{S,1} & \partial_{P_1} R^{dif}_{S,1} \end{bmatrix} = T \begin{bmatrix} \alpha_4 & \beta_4 \\ -\alpha_4 & -\beta_4 \end{bmatrix}$$

where

$$\alpha_4 = \frac{1}{2}\partial_P \gamma_{\frac{1}{2}} \frac{\partial P_0^+}{\partial P_0}(P_c(S_1^-) - P_c(S_0^+))$$
$$\beta_4 = \frac{1}{2}\partial_P \gamma_{\frac{1}{2}} \frac{\partial P_1^-}{\partial P_1}(P_c(S_1^-) - P_c(S_0^+)).$$

For the convective part of the Jacobian is valid:

$$D_S R_S^{con} = \begin{bmatrix} -\partial_{S_0}(Q_{\frac{1}{2}} f_w^{up}) & -\partial_{S_1}(Q_{\frac{1}{2}} f_w^{up}) \\ \partial_{S_0}(Q_{\frac{1}{2}} f_w^{up}) & \partial_{S_1}(Q_{\frac{1}{2}} f_w^{up}) \end{bmatrix}, \quad D_P R_S^{con} = \begin{bmatrix} -\partial_{P_0}(Q_{\frac{1}{2}} f_w^{up}) & -\partial_{P_1}(Q_{\frac{1}{2}} f_w^{up}) \\ \partial_{P_0}(Q_{\frac{1}{2}} f_w^{up}) & \partial_{P_1}(Q_{\frac{1}{2}} f_w^{up}) \end{bmatrix}.$$

Mass Residual and Jacobian

In calculations by elements one has to calculate

$$M_0 = \rho_w(S_0^+, P_0^+)S_0^+ + \rho_g(S_0^+, P_0^+)(1 - S_0^+)$$
$$N_0 = \rho_w(S_0^+, P_0^+)S_0^+,$$

$$M_1 = \rho_w(S_1^-, P_1^-)S_1^- + \rho_g(S_1^-, P_1^-)(1 - S_1^-)$$
$$N_1 = \rho_w(S_1^-, P_1^-)S_1^-.$$

To form the Jacobian, one requires derivatives of the functions M and N:

$$\frac{\partial M(S_0^+, P_0^+)}{\partial P_0} = \partial_p M(S_0^+, P_0^+)\frac{\partial P_0^+}{\partial P_0}$$

$$\frac{\partial M(S_1^-, P_1^-)}{\partial P_1} = \partial_p M(S_1^-, P_1^-)\frac{\partial P_1^-}{\partial P_1}$$

$$\frac{\partial M(S_0^+, P_0^+)}{\partial S_0} = \partial_S M(S_0^+, P_0^+)\frac{\partial S_0^+}{\partial S_0} + \partial_p M(S_0^+, P_0^+)\frac{\partial P_0^+}{\partial S_0}$$
$$\frac{\partial M(S_1^-, P_1^-)}{\partial S_1} = \partial_S M(S_1^-, P_1^-)\frac{\partial S_1^-}{\partial S_1} + \partial_p M(S_1^-, P_1^-)\frac{\partial P_1^-}{\partial S_1}.$$

For the function N, the calculation is analogous.

4.2 Numerical Simulations

In the following subsections three test cases are presented. These test cases [52] are developed within MoMaS, a federation of French research groups. Test case 3 is slightly modified in order to present the effect of the entry pressure. In all test cases the flow of incompressible water and compressible gas is observed.

4.2.1 Test Case 1

In the first test case, the results obtained for the fully equivalent and the simplified fractional flow formulation are presented and discussed. The porous domain $I =]0, 200[\subset \mathbb{R}$ is taken to be 200 m long. The domain is assumed to be composed of two materials such that $I = I_{m1} \cup I_{m2}$ where is $I_{m1} =]0, 20]$ and $I_{m2} =]20, 200[$, so that the point $x = 20$ is an interface between the two materials. In this test, the source terms are equal to zero, which means that $\mathcal{F}_\alpha = 0,\ \alpha = w, g$. The duration of the simulation is $T = 10^6$ years.

The boundary conditions are set to be Dirichlet at the right boundary point:

$$P_{w,out} = 1.0 \text{ MPa} \qquad P_{g,out} = 1.5 \text{ MPa}.$$

Phase fluxes conditions are set on the left boundary:

$$Q_w = 0 \quad \text{and} \quad Q_g = 5.57 \cdot 10^{-6} \text{ kg/m}^2\text{/years}.$$

The initial conditions are equal to Dirichlet conditions on the right part of the boundary. Therefore, the following is set:

$$P_{w,t=0} = 1.0 \text{ MPa} \qquad P_{g,t=0} = 1.5 \text{ MPa}.$$

In this test case the van Genuchten capillary pressure and the van Genuchten Mualem relative permeabilities (2.12)-(2.13) are used. It is assumed that $K = cte$ in each subset of the domain. The same is valid for the porosity. The parameters for the relative permeabilities and capillary pressures are different on each subdomain. Temperature is taken to be fixed, $T = 303$ K. The parameters for each subdomain are presented in the table 4.1. The following fluid properties are considered: $\mu_w = 1$ cP, $\mu_g = 0.009$ cP, $\rho_w = 1000$ kg/m^3, $c_g = 0.794$ kg/m^{3}MPa. The gas density is modeled by the ideal gas law.

In this simulation, an equidistant grid of the space domain with $\Delta x = 200$ cm is used.

	n	P_e	S_{wr}	S_{gr}	ϕ	K
	-	MPa	-	-	-	m^2
I_{m1}	1.54	2	0.01	0.0	0.3	10^{-18}
I_{m2}	1.49	15	0.4	0.0	0.15	$5 \cdot 10^{-20}$

Table 4.1: Test 1. Function parameters and rock properties

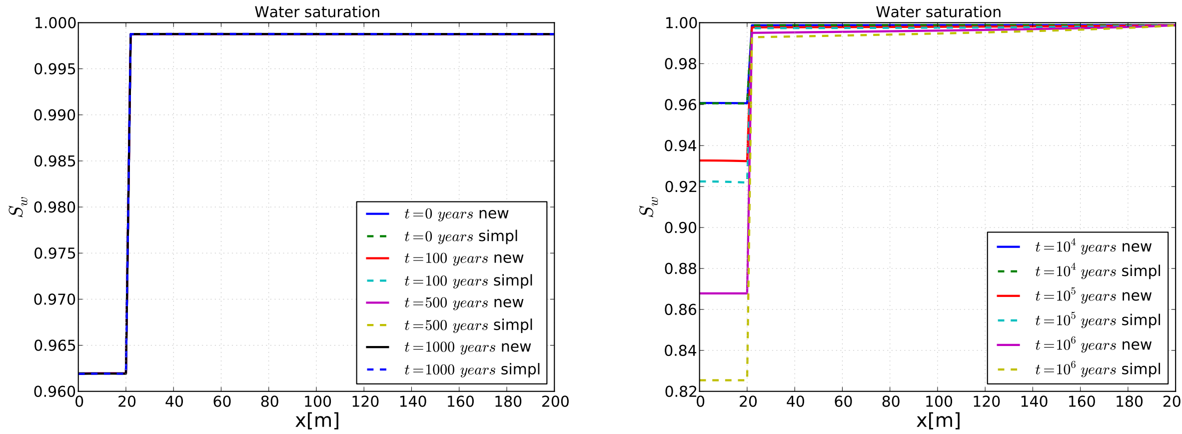


Figure 4.2: Test 1. Water saturation at different times

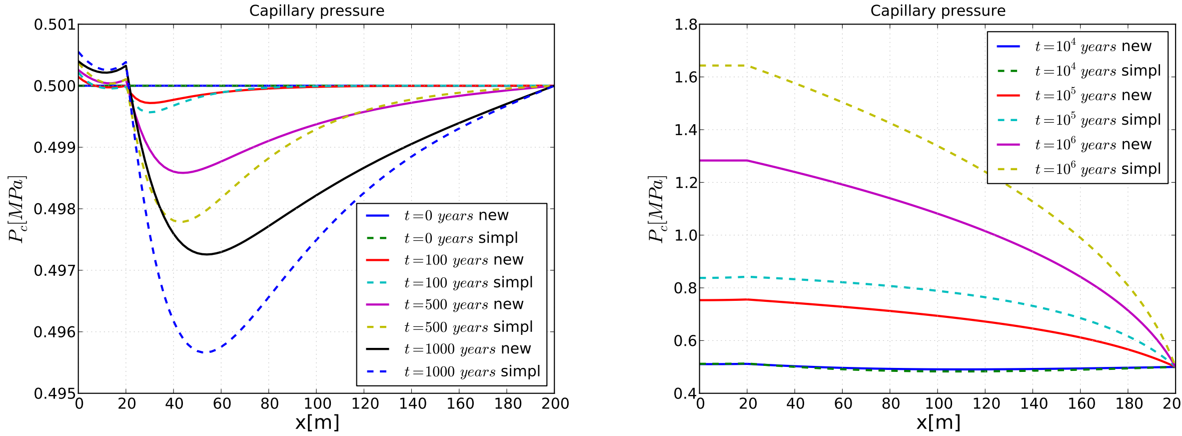


Figure 4.3: Test 1. Capillary pressure at different times

For the time domain, a non-equidistant mesh is used, starting with $\Delta t = 10$ years at the beginning to $\Delta t = 250$ years at the end of the simulation. The obtained results are presented in the figures 4.2-4.7 for the fully equivalent fractional flow formulation, for which the term “new” is used, and for simplified fractional flow formulation for which the term “simpl” is used.

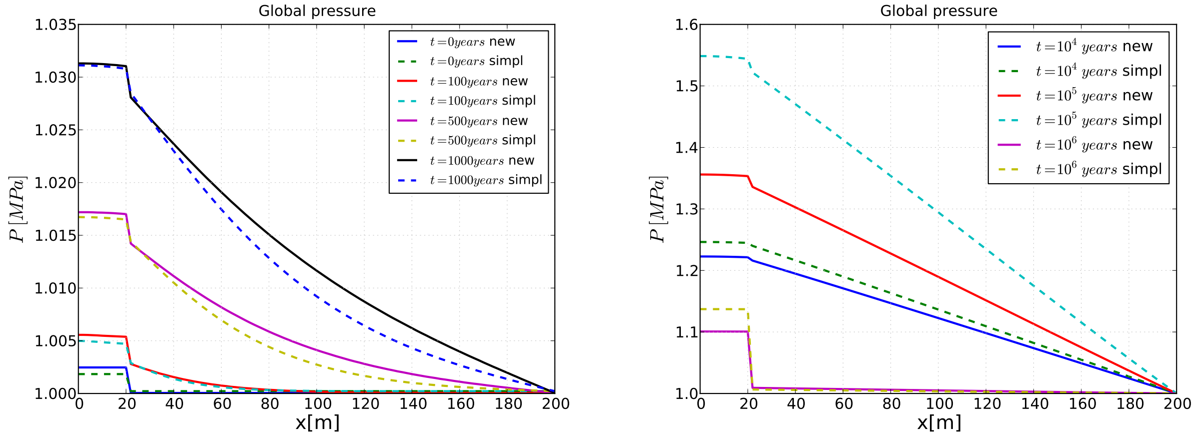


Figure 4.4: Test 1. Global pressure at different times

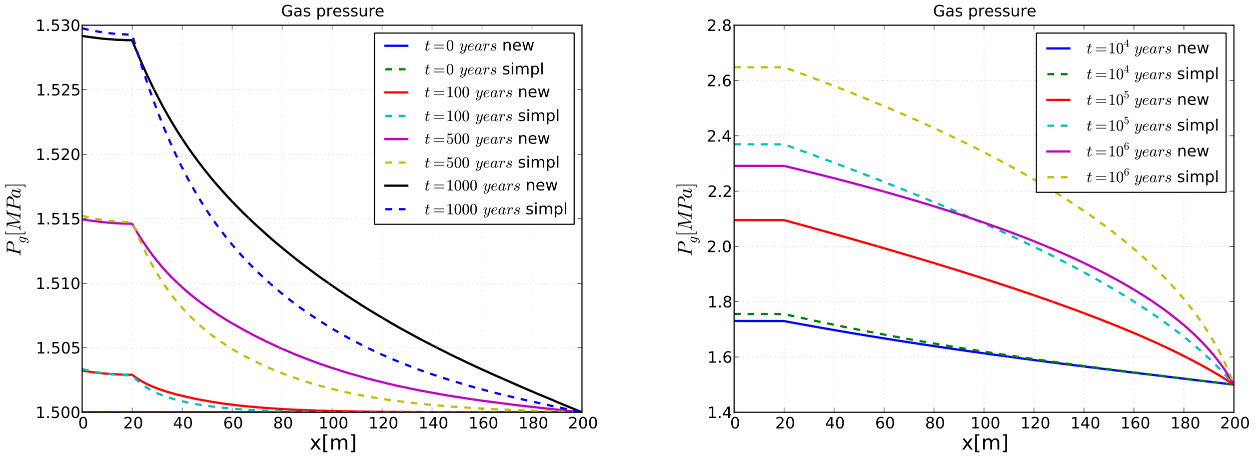


Figure 4.5: Test 1. Gas pressure at different times

One can observe that first 1000 years, due to the small amount of gas (hydrogen) injected, the changes in the saturation are very small. Also, the changes in the water pressure presented in the figure 4.6 are not significant at the first 1000 years. The water pressure is increasing at the beginning and as one may observe in the figure 4.7, around the time of $5 \cdot 10^4$ years it starts to decrease. At the end of the simulation, it tends to its initial value 1.0 MPa. During the whole simulation the gas pressure (presented in the figure 4.5) is increasing attaining the values in the range of 1.5 MPa to 2.3 MPa for the new model, and the values of 1.5 MPa to 2.65 MPa for the simplified model. The global pressure is presented in the figure 4.4, and its behavior is similar to the water pressure, since as commented in chapter 3, the difference between the water and global pressure is

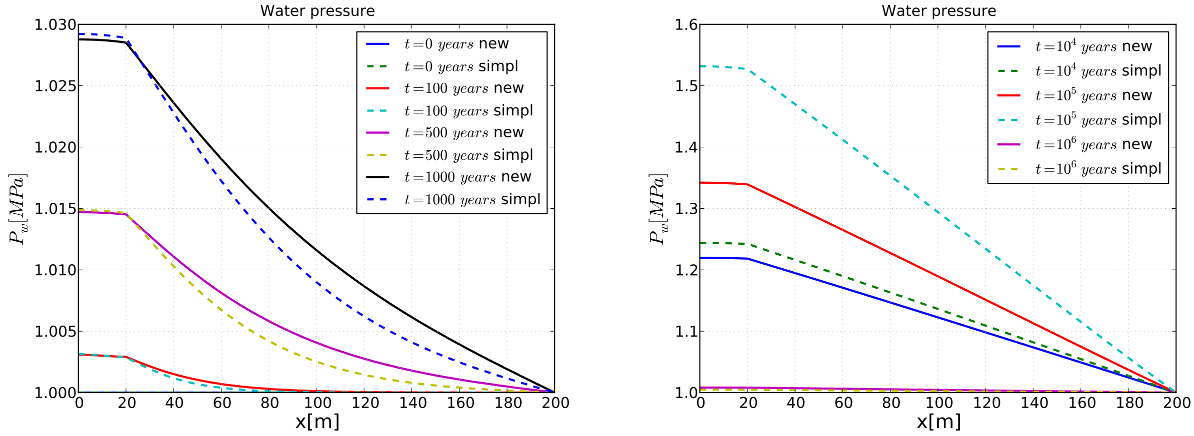


Figure 4.6: Test 1. Water pressure at different times

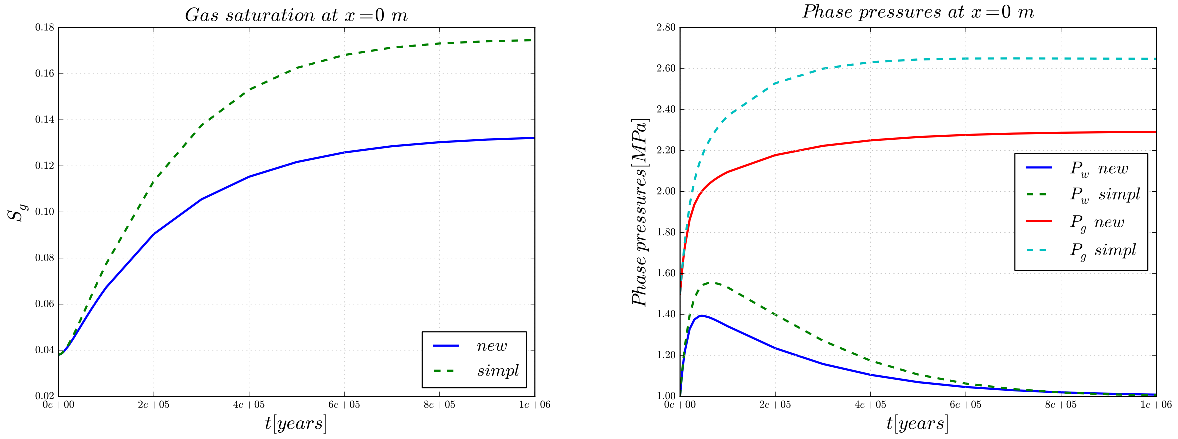


Figure 4.7: Test 1. Phase pressures and saturation on the left end

very small for relatively small capillary pressures, and because of the high value of the wetting phase density compared to the gas density. From the formula (3.50) one can also observe that if $\rho_w \geq \rho_g$ the global pressure would be in general closer to the wetting phase pressure. The continuity condition for the gas pressure is used in this example, and also for the capillary pressure. They are assumed to be continuous at the interface point. This produces a discontinuity of the saturation and the global pressure at the interface.

One can see that the difference in the gas pressure in the simplified model and the new model in this test case, is more visible at the end of the simulation. The reason for this is, that at the beginning of the simulation the effective saturation is nearly equal to 1, and the capillary pressure is low, compared to the one at the end of the simulation. The global pressure does not have significant variations, it stays during the whole simulation in the range of 1.0 MPa to 1.40 MPa in the case of the new model, and in the simplified model it attains values between 1.0 MPa and 1.55 MPa. The difference in the global pressure in the simplified and the new model is significant in the period from 10^4 years to $6 \cdot 10^5$ years. The water pressure behaves similarly. From these observations, one can see that the difference in the phase pressures obtained by the simplified and by the new model may be significant.

4.2.2 Test Case 2

The second test case is a BO-BG test case [52]. This test was numerically solved by other authors [5, 14]. The porous domain $I =]-0.5, 0.5[\subset \mathbb{R}$ is taken to be 1 m long. The porous domain is assumed to be composed of two materials such that $I = I_{m1} \cup I_{m2}$ where is $I_{m1} =]-0.5, 0]$ and $I_{m2} =]0, 0.5[$, so that the point $x = 0$ is interface between the two materials. In this test the source terms are equal to zero, which means $\mathcal{F}_\alpha = 0,\ \alpha = w, g$.

Phase fluxes are set to be zero at the boundary points, both on the left and the right end for each phase, which means that a total flux is also set to be zero.

$$Q_w = Q_g = 0 \text{ kg/m}^2\text{/s}.$$

Initially, the capillary pressure is discontinuous, and the following initial condition for the water saturation is given

$$S_w(x,0) = \begin{cases} 0.77 & \text{for } x \leq 0.0 \\ 1 & \text{for } x > 0.0 \end{cases}, \quad x \in I.$$

Regarding to the initial conditions for the gas pressure two cases are considered:

Test case 2.1

$$P_g(x,0) = 0.1 \text{ MPa},\ x \in I.$$

From these initial conditions one obtains initial condition for the global pressure $P = -88.8449$ MPa in I_{m1}, and $P = 0.0$ MPa in I_{m2}.

Test case 2.2

$$P_g(x,0)=\begin{cases}0.1 \text{ MPa} & \text{for } x \le 0.0\\ 0.0 \text{ MPa} & \text{for } x > 0.0\end{cases}, \quad x \in \ I.$$

From these initial conditions one obtains initial condition for the global pressure $P = -88.8449$ MPa in I_{m1}, and $P = 0.1$ MPa in I_{m2}.

In this test case the van Genuchten capillary pressure is used. Relative permeabilities are given by the following formulae:

$$kr_g(S) = (1-S)^2(1-S^{\frac{5}{3}}) \quad kr_w(S) = (1 + A(S^{-B}-1)^C)^{-D}$$

$$S_w(P_c) = \left(1 + \left(\frac{P_C}{Pr}\right)^{\frac{1}{1-m}}\right)^{-m}.$$

It is assumed that $K = cte$ in each subset of the domain. The same is valid for the porosity. The parameters for the relative permeabilities and capillary pressures are different on each subdomain. The parameters for each subdomain are presented in the table 4.2. Temperature is taken to be fixed, $T = 300$ K.

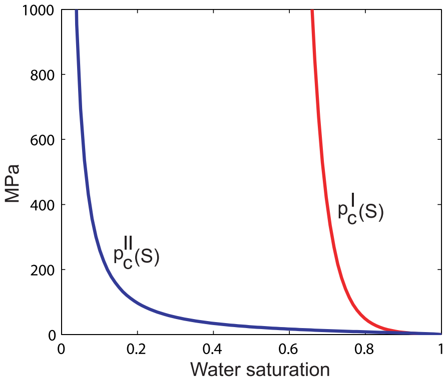


Figure 4.8: Test 2. Capillary pressures in the different domains

The following fluid properties are taken $\rho_w = 1000$ kg/m^3 $\mu_w = 1$ cP, $\mu_g = 0.009$ cP, $\rho_w = 1000$ kg/m^3, $M_g = 0.02896$ kgmol^{-1}. In numerical results presented here in the test case 2.1, the density of gas is scaled so it is actually taken that $c_g = 1.0$ kg/m^{3}MPa. In the spatial domain, an equidistant mesh is taken with the step size $\Delta x = 0.01$ m. The obtained results are presented in the figures 4.9-4.13.

As shown at the figures the results for the test case 2.1 and 2.2 differ visibly only in

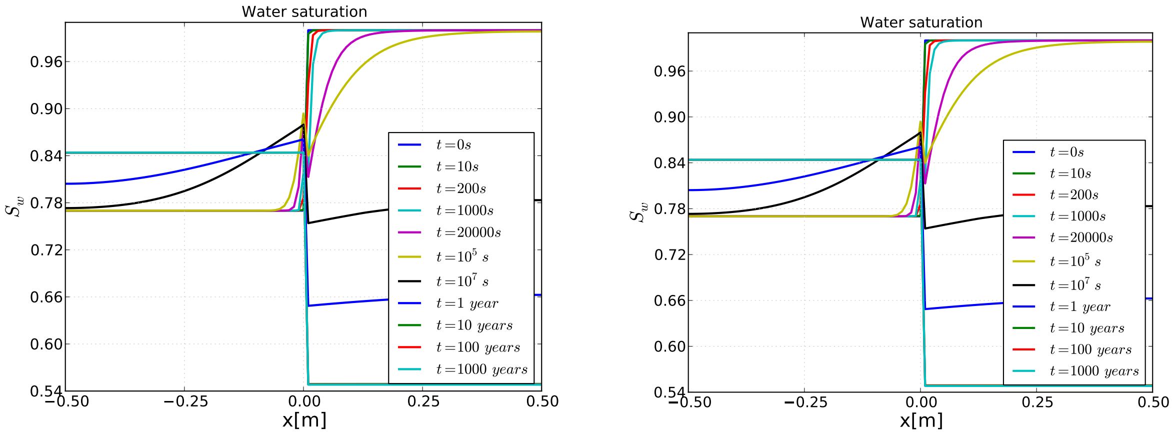


Figure 4.9: Test 2. Water saturation at different times for the test case 2.1 (left) and test case 2.2 (right)

	Pr MPa	m -	A -	B -	C -	D -	ϕ -	K m^2
I_{m1}	1.5	0.06	0.25	16.67	1.88	0.5	0.3	10^{-20}
I_{m2}	10	0.412	1.0	2.429	1.176	1.0	0.05	10^{-19}

Table 4.2: Test 2. Function parameters and rock properties

the gas pressures obtained at first 10^5 s. The right part of the domain is initially fully saturated by the water. At first, the changes of saturation are very small, the water starts to flow from the domain I_{m2} to the domain I_{m1}. After a certain time a change in the saturation in the region I_{m2} becomes more visible, when the gas starts to flow to the right part of the domain. The gas pressure is increasing near the interface, since the gas is expected to enter the domain fully saturated by the water. At the time of 10^5 s in the test case 2.1 the gas pressure becomes zero on the subdomain I_{m2}, while in the test case 2.2 it obtains the values close to the initial value. After the time of 10^5s in both cases the gas pressure starts to decrease from its maximum value near interface in the region I_{m1}, an behaves similarly in both of the cases. In both cases, at the later times the water pressure attains value of around -20.0 MPa and the difference between the global pressure and the water pressure is small compared to its difference from the gas pressure. This observation is valid during the whole simulation. This follows from the fact that when one calculates the difference by the formula (3.50), the small value compared to the range of pressures is obtained. From the continuity condition of the capillary pressure one obtains discontinuous saturation. The initial discontinuity of the capillary pressure is treated as follows: the left

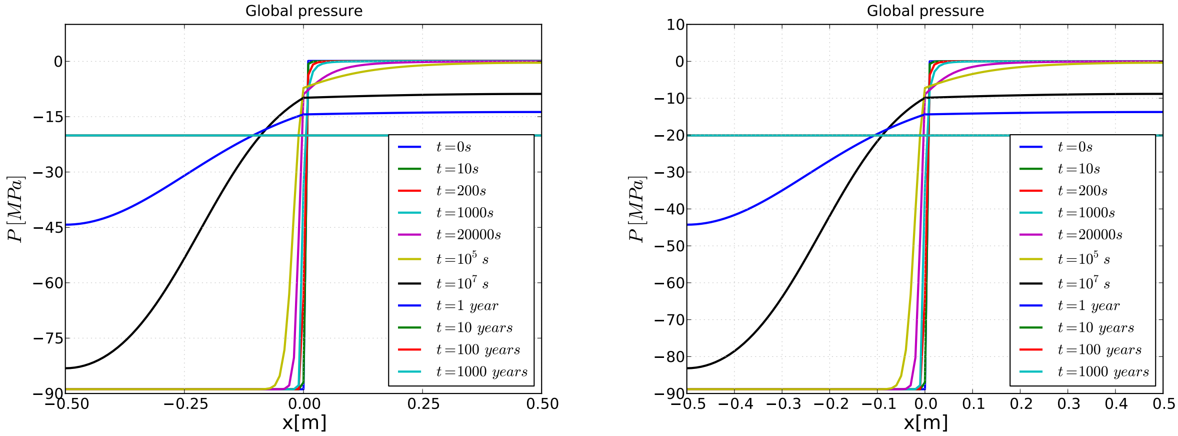


Figure 4.10: Test 2. Global pressure at different times for the test case 2.1 (left) and test case 2.2 (right)

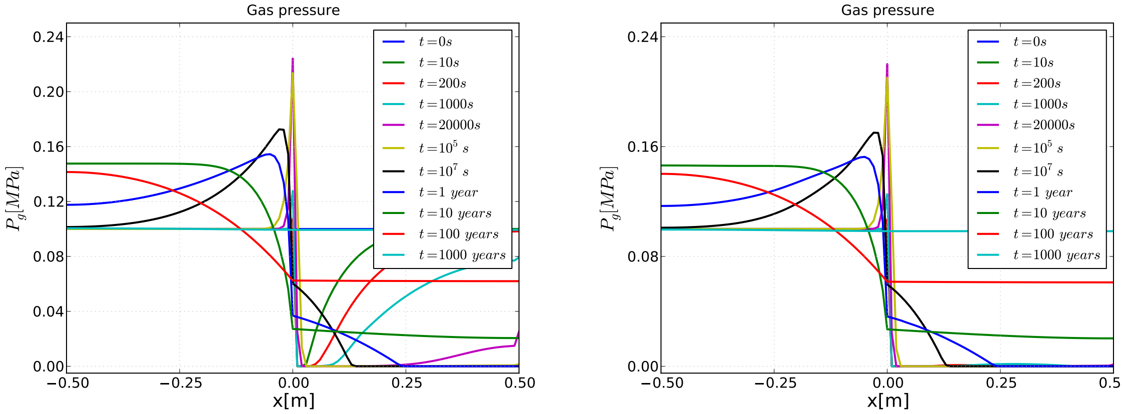


Figure 4.11: Test 2. Gas pressure at different times for the test case 2.1 (left) and test case 2.2 (right)

limiting saturation is taken to be global unknown in the simulation, so when calculation is performed on the interface element in domain I_{m2}, the left limiting value of the capillary pressure is used. In the both cases, the wetting saturation attains the values $S_w = 0.844$ on the left part of the domain, and $S_w = 0.548$ on the right part of the domain by the end of the simulation. In both cases after the time of 10^8 s, the changes in saturation are not significant, while the gas pressure tends to the value of 0.1 MPa which is the initial value that was set in the case 2.1. The time steps used during the simulation are from 10^{-5} s at the beginning to the $2 \cdot 10^6$ s at the end of the simulation.

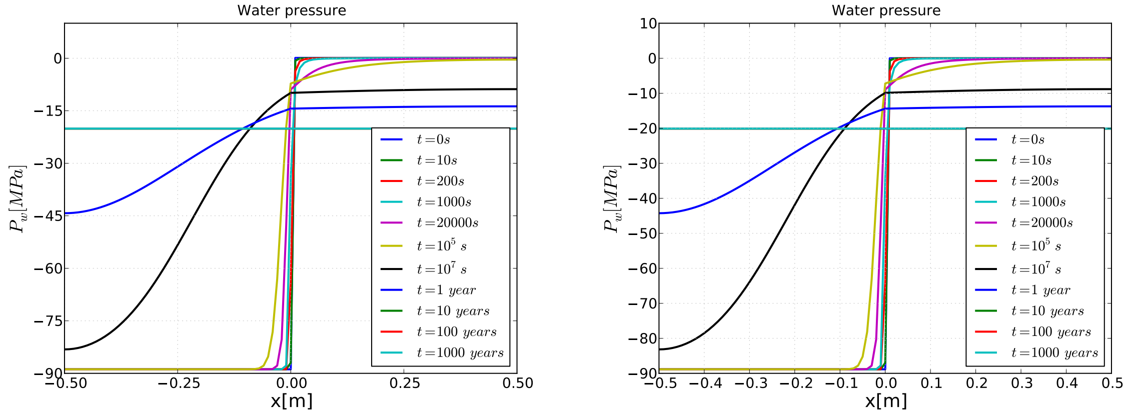


Figure 4.12: Test 2. Water pressure at different times for the test case 2.1 (left) and test case 2.2 (right)

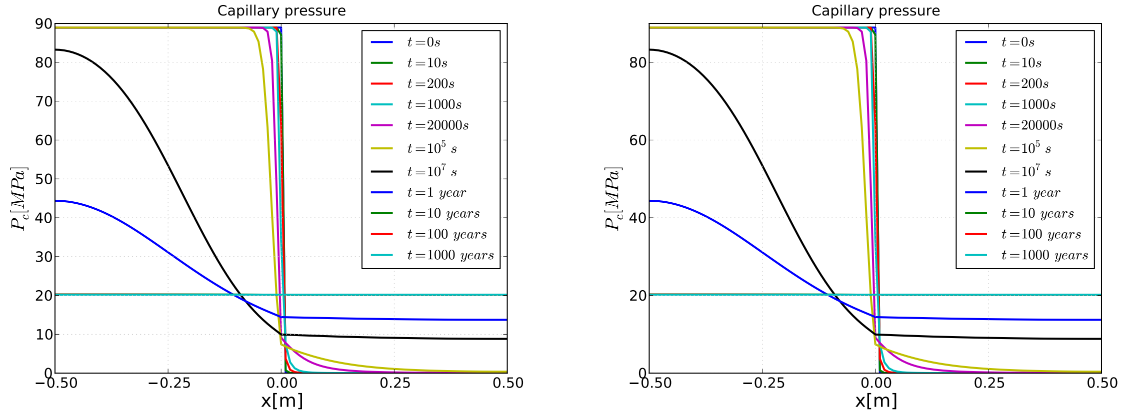


Figure 4.13: Test 2. Capillary pressure at different times for the test case 2.1 (left) and test case 2.2 (right)

4.2.3 Test Case 3

The third test case is considered in order to simulate the effect of the entry pressure. The porous domain $I =]0, 200[\subset \mathbb{R}$ is taken to be 200 m long. The domain is assumed to be composed of the two materials such that $I = I_{m1} \cup I_{m2}$ where $I_{m1} =]0, 100]$ and $I_{m2} =]100, 200[$, so that the point $x = 100$ is the interface between the two materials. In this test, the source terms are equal to zero, which means that $\mathcal{F}_\alpha = 0,\ \alpha = w, g$.

The boundary conditions are set to be Dirichlet on the right boundary point, and it is set

$$S_{w,out} = 1.0 \qquad P_{w,out} = 1.0 \text{ MPa}.$$

On the left boundary, phase fluxes conditions (total flux) are set:

$$Q_w = 0 \quad \text{and} \quad Q_g = 500 \text{ mg/m}^2\text{/years.}$$

The initial conditions are equal to Dirichlet conditions on the right part of the boundary. Therefore,

$$S_{w,t=0} = 1.0 \qquad P_{w,t=0} = 1.0 \text{ MPa.}$$

It is assumed that the porous medium is fully saturated by the water, and that the gas is injected. In this numerical test, Brooks and Corey capillary pressure and Brooks and Corey Burdine relative permeabilities (2.14)-(2.15) are used. It is assumed that all parameters are the same for each part of the domain: only the entry pressures differ. Temperature is assumed to be fixed, $T = 303$ K.

	λ	P_d	S_{wr}	S_{gr}	ϕ	K
	-	MPa	-	-	-	m^2
I_{m1}	0.5	1.9	0.0	0.0	0.3	10^{-16}
I_{m2}	0.5	2.1	0.0	0.0	0.3	10^{-16}

Table 4.3: Test 3. Function parameters and rock properties

The following fluid properties are considered: $\mu_w = 1$ cP, $\mu_g = 0.009$ cP, $\rho_w = 1000$ kg/m^3, $c_g = 0.794$ kg/m^{3}MPa. The density of gas is modeled by the ideal gas law $\rho_g(P_g) = c_g P_g$. In this example *extended capillary pressure condition* (2.50) is applied. This means that the capillary pressure is discontinuous until the threshold saturation $S^* = 0.95119$ at the interface is reached.

In this simulation, an equidistant mesh of the space domain with $\Delta x = 200$ cm is used. For the time domain, a non-equidistant, mesh is used, starting with $\Delta t = 10^{-2}$ s at the beginning to $\Delta t = 1$ year at the end of the simulation. Also, since only the water is mobile across the interface and consequently continuous, the continuity condition is applied to the water pressure (and extended capillary pressure condition is used). Therefore, until the threshold saturation is reached, the capillary pressure and the gas pressure would be discontinuous at the interface point. The gas will not enter right part of the domain until the threshold saturation is reached.

The obtained results are presented in the figures 4.14-4.18.

In the figure 4.14 the water saturation is presented. As the extended capillary pressure condition is used, the saturation is equal to 1 in the subdomain I_{m2}, until the threshold saturation is reached, which is about 7685 years. One can observe the visible changes in

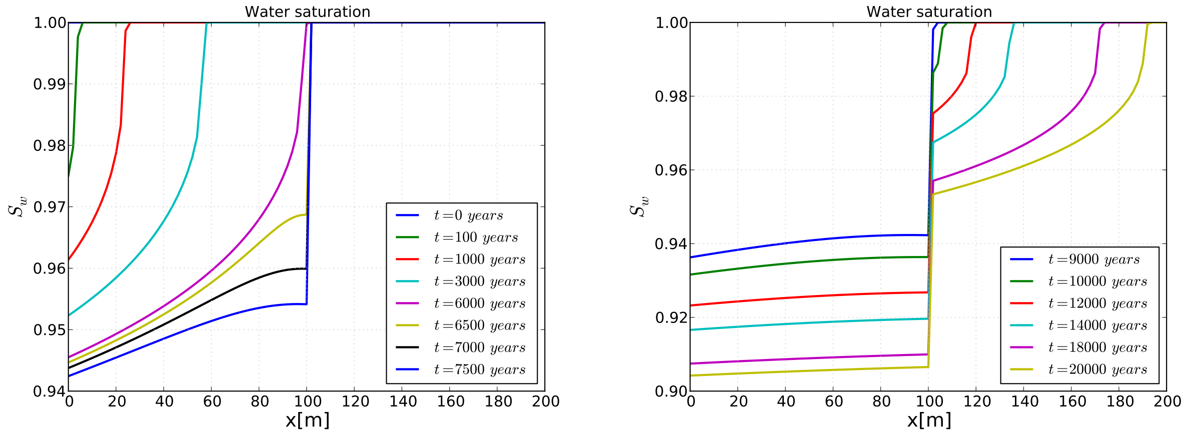


Figure 4.14: Test 3. Water saturation at different times

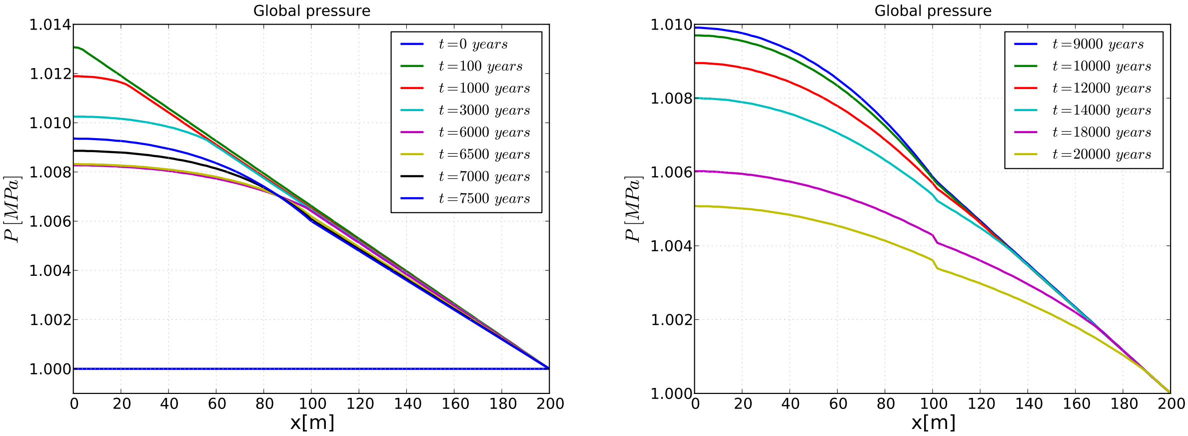


Figure 4.15: Test 3. Global pressure at different times

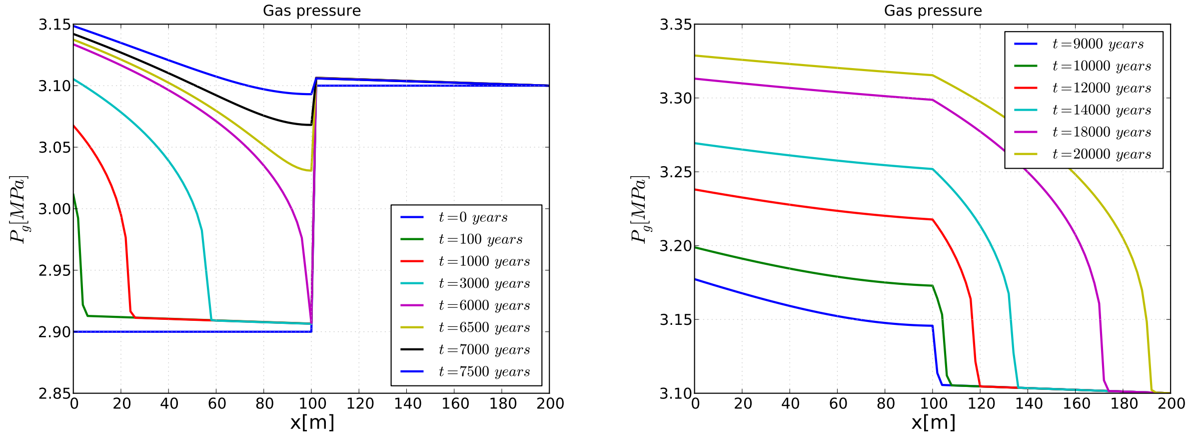


Figure 4.16: Test 3. Gas pressure at different times

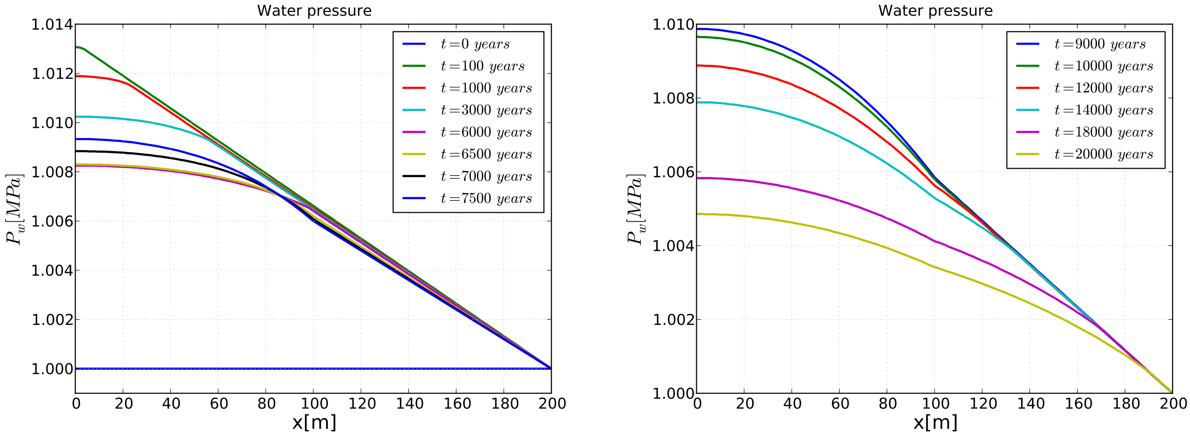


Figure 4.17: Test 3. Water pressure at different times

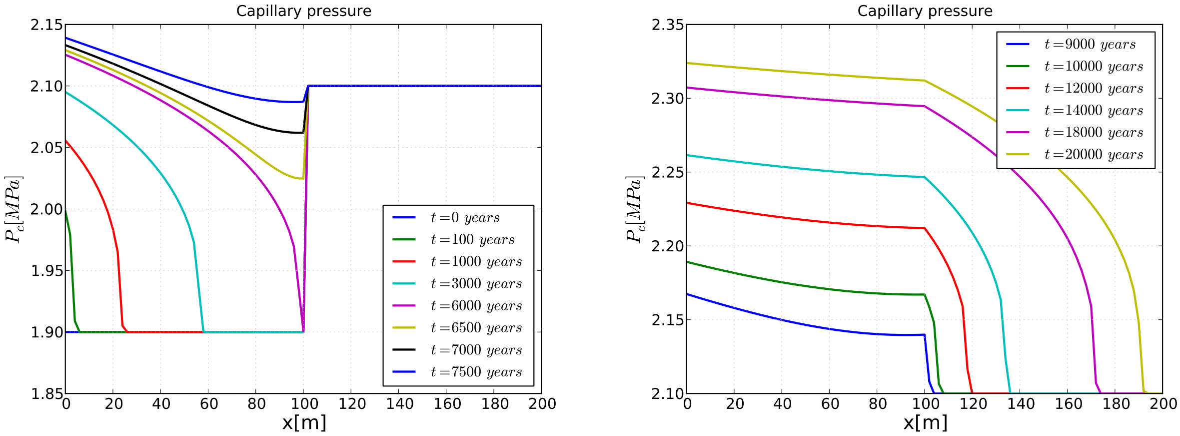


Figure 4.18: Test 3. Capillary pressure at different times

the saturation on the right part of the domain around 9000 years. During all the time water and global pressure do not change significantly, since the water saturation is very high. The global pressure has a visible discontinuity at the interface, during the time of the simulation. The capillary pressure, and the gas pressure are discontinuous until the threshold saturation is reached at the interface. The capillary pressure is increasing, which also has an effect on the behavior on the gas pressure, since the changes of water pressure are relatively small.

4.3 Conclusion

By comparing the simplified and fully equivalent formulation it has been shown by means of the numerical simulation, that the difference between the solutions obtained in the new and simplified model may be significant, especially in the area of higher capillary pressures. The results obtained for the test case 2, are similar to those obtained in [5, 14], and show model applicability in the simulations with highly heterogeneous porous media. The third example shows that the model is applicable in the simulations with initially fully saturated porous media by the wetting phase, and demonstrates the significance of the entry pressure.

Chapter 5

Existence Theory for the Two-phase Immiscible, Compressible Flow Model in Global Pressure Formulation

The aim of this chapter is to establish existence of weak solutions for a new formulation for immiscible, compressible, two-phase flows under realistic assumptions. The main difficulties related to the mathematical analysis of such equations are the coupling, the degeneracy of the diffusion term in the saturation equation and the degeneracy of the temporal term in the global pressure equation. In the following section a short description of the mathematical and physical model used in this study is given. Afterwards the assumptions on data are formulated. The existence is shown with the help of a regularized system, a time discretization, a priori estimates and compactness arguments. This chapter contains results from [9] In section 5.2 the regularized problem is defined with a parameter $\eta > 0$, some auxiliary results are established and the existence of weak solutions of the problem in the non-degenerate case which will be proved in section 5.3 is formulated. The proof will be done in three main steps. In subsection 5.3.1, a small parameter $h > 0$ is used and approximate solutions are constructed with a time discretization. The existence of the weak solutions for the corresponding system and a maximum principle for the saturation is proved. In subsection 5.3.2, suitable test functions introduced in [44] are used to get uniform estimates with respect to h. These estimates permit passing to the limit when h tends to zero and obtaining the existence of weak solutions for the regularized problem which is carried out in subsection 5.3.3. Section 5.5 is devoted to the presentation of the result for the degenerate case.

5.1 Main Results

Recall that the mass balance equations and the Darcy law for each phase $\alpha \in \{w, g\}$ can be written as

$$\Phi \frac{\partial}{\partial t}(\rho_\alpha(P_\alpha)S_\alpha) + \operatorname{div}(\rho_\alpha(P_\alpha)\mathbf{q}_\alpha) = \mathcal{F}_\alpha, \quad \mathbf{q}_\alpha = -\lambda_\alpha(S_\alpha)\mathbb{K}(\nabla P_\alpha - \rho_\alpha(P_\alpha)\mathbf{g}), \tag{5.1}$$

where Φ and $\mathbb{K}$ are the porosity and the absolute permeability of the porous medium, and $\mathbf{g}$ is the gravitational, downward-pointing, constant vector. The source terms $\mathcal{F}_\alpha$ will be precised in the sequel.

Here, the governing equations are rewritten firstly by choosing the nonwetting saturation S_g and the global pressure P as primary unknowns. All the coefficients are considered to be functions of S_g and P, as written in remark 3.2. The superscript n used in the same remark 3.2 is omitted for the simplicity of the notation from now on. The following functions are introduced:

$$\Lambda_\alpha(S_g, P) = \lambda_\alpha(S_\alpha)\rho_\alpha(S_g, P)\omega(S_g, P), \alpha = w, g.$$

From the definitions of nonwetting, and wetting pressure (3.27) and (3.28), it follows that the mass fluxes can be rewritten as

$$\begin{aligned}
\rho_w(P_w)\mathbf{q}_w &= -\Lambda_w(S_g, P)\mathbb{K}\nabla P + a(S_g, P)\mathbb{K}\nabla S_g + \lambda_w(S_g)\rho_w(S_g, P)^2\mathbb{K}\mathbf{g}, \\
\rho_g(P_g)\mathbf{q}_g &= -\Lambda_g(S_g, P)\mathbb{K}\nabla P - a(S_g, P)\mathbb{K}\nabla S_g + \lambda_g(S_g)\rho_g(S_g, P)^2\mathbb{K}\mathbf{g},
\end{aligned}$$

and consequently the differential equations of the two-phase, compressible, immiscible flow (5.1) can now be written as (cf. [7,8]):

$$\begin{aligned}
&\Phi \frac{\partial}{\partial t}(\rho_w(S_g, P)S_w) - \operatorname{div}(\Lambda_w(S_g, P)\mathbb{K}\nabla P) + \operatorname{div}(a(S_g, P)\mathbb{K}\nabla S_g) \\
&\qquad + \operatorname{div}(\lambda_w(S_g)\rho_w(S_g, P)^2\mathbb{K}\mathbf{g}) + \rho_w(S_g, P)f_w(S_g, P)F_P = \rho_w(S_g, P)S_w^* F_I,
\end{aligned} \tag{5.2}$$

$$
\begin{aligned}
&\Phi\frac{\partial}{\partial t}(\rho_g(S_g,P)S_g) - \operatorname{div}(\Lambda_g(S_g,P)\mathbb{K}\nabla P) - \operatorname{div}(a(S_g,P)\mathbb{K}\nabla S_g)\\
&\qquad + \operatorname{div}(\lambda_g(S_g)\rho_g(S_g,P)^2\mathbb{K}\mathbf{g}) + \rho_g(S_g,P)f_g(S_g,P)F_P = \rho_g(S_g,P)S_g^*F_I,
\end{aligned}
\tag{5.3}
$$

where $S_w = 1 - S_g$, $F_I, F_P \geq 0$ are given injection and production rates and S_α^* is known saturation determining the composition of the injected fluid. Note that the choice of $S = S_g$ as primary saturation variable is motivated by the fact that $S_g \mapsto P_c(S_g)$ is an increasing function. A priori estimates that will be used in the sequel are based on the integrability of the quadratic terms $\lambda_\alpha(S_g)\mathbb{K}\nabla P_\alpha \cdot \nabla P_\alpha$. In presence of unbounded capillary pressure function P_c, the non-wetting phase saturation S_g will be replaced by a new variable θ (as in [6]),

$$
\theta = \beta(S) = \int_0^S \sqrt{\lambda_g(s)\lambda_w(s)}P_c'(s)\,ds,
\tag{5.4}
$$

which is well defined since β is strictly increasing. Finally, introducing the function

$$
A(S_g,P) = \rho_w(S_g,P)\rho_g(S_g,P)\frac{\sqrt{\lambda_w(S_w)\lambda_g(S_g)}}{\lambda(S_g,P)}
\tag{5.5}
$$

the system (5.2), (5.3) can be rewritten as

$$
\begin{aligned}
&\Phi\frac{\partial}{\partial t}(\rho_w(S_g,P)S_w) - \operatorname{div}(\Lambda_w(S_g,P)\mathbb{K}\nabla P) + \operatorname{div}(A(S_g,P)\mathbb{K}\nabla\theta)\\
&\qquad + \operatorname{div}(\lambda_w(S_g)\rho_w(S_g,P)^2\mathbb{K}\mathbf{g}) + \rho_w(S_g,P)f_w(S_g,P)F_P = \rho_w(S_g,P)S_w^*F_I,
\end{aligned}
\tag{5.6}
$$

$$
\begin{aligned}
&\Phi\frac{\partial}{\partial t}(\rho_g(S_g,P)S_g) - \operatorname{div}(\Lambda_g(S_g,P)\mathbb{K}\nabla P) - \operatorname{div}(A(S_g,P)\mathbb{K}\nabla\theta)\\
&\qquad + \operatorname{div}(\lambda_g(S_g)\rho_g(S_g,P)^2\mathbb{K}\mathbf{g}) + \rho_g(S_g,P)f_g(S_g,P)F_P = \rho_g(S_g,P)S_g^*F_I,
\end{aligned}
\tag{5.7}
$$

where $S_g = \mathcal{S}(\theta)$ and $S_w = 1 - S_g$ and the phase mass fluxes are:

$$
\begin{aligned}
\mathbf{Q}_w &= \rho_w(P_w)\mathbf{q}_w = -\Lambda_w(S_g,P)\mathbb{K}\nabla P + A(S_g,P)\mathbb{K}\nabla\theta + \lambda_w(S_g)\rho_w(S_g,P)^2\mathbb{K}\mathbf{g},\\
\mathbf{Q}_g &= \rho_g(P_g)\mathbf{q}_g = -\Lambda_g(S_g,P)\mathbb{K}\nabla P - A(S_g,P)\mathbb{K}\nabla\theta + \lambda_g(S_g)\rho_g(S_g,P)^2\mathbb{K}\mathbf{g}.
\end{aligned}
$$

Boundary conditions: let $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, be a bounded, Lipschitz domain with its boundary divided in two parts, $\partial\Omega = \Gamma_{inj} \cup \Gamma_{imp}$, where Γ_{inj} denotes the injection boundary, and Γ_{imp} denotes the impervious one. Let $]0,T[$ be the time interval of interest and $Q_T = \Omega\times]0,T[$. Setting

$$\theta = 0, \quad P = 0 \quad \text{on } \Gamma_{inj}\times]0,T[\tag{5.8}$$

$$\mathbf{q}_w \cdot \mathbf{n} = \mathbf{q}_g \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_{imp}\times]0,T[, \tag{5.9}$$

where $\mathbf{n}$ is the outward pointing unit normal on $\partial\Omega$ and $\mathbf{q}_\alpha$ being the volumetric velocity of the α-phase, $\alpha = w, g$.

Initial conditions are given by

$$\theta(x,0) = \theta_0(x), \quad P(x,0) = p_0(x) \quad \text{in } \Omega. \tag{5.10}$$

The assumptions needed to prove an existence result for the coupled system (5.6), (5.7) with boundary and initial conditions (5.8), (5.9) and (5.10) are:

(A.1) The porosity Φ belongs to $L^\infty(\Omega)$, and there exist constants, $\phi_M \geq \phi_m > 0$, such that $0 < \phi_m \leq \Phi(x) \leq \phi_M$ a.e. in Ω.

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

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

(A.3) Relative mobilities satisfy $\lambda_w, \lambda_g \in C([0,1];\mathbb{R}^+)$, $\lambda_w(S_w = 0) = 0$ and $\lambda_g(S_g = 0) = 0$; λ_j is a non decreasing function of S_j. Moreover, there exist constants $\lambda_M \geq \lambda_m > 0$ such that for all $S_g \in [0,1]$

$$0 < \lambda_m \leq \lambda_w(S_g) + \lambda_g(S_g) \leq \lambda_M.$$

(A.4) There exist constants $p_{c,min} > 0$ and $M > 0$ such that the capillary pressure function $S_g \mapsto P_c(S_g)$, $P_c \in C([0,1[;\mathbb{R}^+) \cap C^1(]0,1[;\mathbb{R}^+)$, for all $S_g \in]0,1[$ satisfy

$$P_c'(S_g) \geq p_{c,min} > 0, \tag{5.11}$$

$$P_c(S_g)(1-S_g) + \int_0^1 P_c(s)\,ds + \sqrt{\lambda_g(S_g)\lambda_w(S_g)}P_c'(S_g) \leq M. \tag{5.12}$$

(A.5) There exist $S^{\#} \in]0,1[$, $0 < \gamma$ and $M > 0$ such that for all $S \in]0, S^{\#}]$

$$S^{-\gamma}\lambda_g(S)(P_c(S) - P_c(0)) + S^{2-\gamma}P_c'(S) \leq M, \tag{5.13}$$

and for all $S \in [S^{\#}, 1[$

$$(1-S)^{2-\gamma}P_c'(S) \leq M. \tag{5.14}$$

(A.6) ρ_w and ρ_g are $C^1(\mathbb{R})$ non decreasing functions, and there exist $\rho_m, \rho_M > 0$ such that for all $p \in \mathbb{R}$ it holds

$$\rho_m \leq \rho_w(p), \rho_g(p) \leq \rho_M, \quad 0 < \rho_w'(p), \rho_g'(p) \leq \rho_M.$$

(A.7) $F_I, F_P \in L^2(Q_T)$, $F_I, F_P \geq 0$, and $0 \leq S_w^* \leq 1$ a.e. in Q_T.

(A.8) There exist $0 < \tau < 1$ and $C > 0$ such that for all $S_1, S_2 \in [0,1]$

$$C \left| \int_{S_1}^{S_2} \sqrt{\lambda_g(s)\lambda_w(s)}\, ds \right|^{\tau} \geq |S_1 - S_2|.$$

(A.9) $S_g^* = 1$.

The assumptions (A.1)–(A.3) and (A.7)–(A.8) are classical for two-phase flow in porous media. The assumptions (A.4) and (A.5) control the strength of singularities in the capillary pressure and its derivative at the end points $S = 0, 1$, and it will be commented further on. The assumption (A.6) is satisfied by mass densities given by a physical law, such as the ideal gas law, by correcting the density function for extremely small and large pressure values. Such correction does not influence the system behavior in physically admissible range of pressures, and therefore (A6) does not limit the applicability of our result.

Remark 5.1. *Under assumptions (A.3), (A.4) and (A.6), it is easy to see that (3.27) has a unique solution $P_g \in C([0,1] \times \mathbb{R}) \cap C^1(]0,1] \times \mathbb{R})$ and consequently $P_w \in C^1([0,1[\times\mathbb{R})$. Using the boundedness of $P_c(S_g)(1-S_g)$ in (A.4), it is easy to see that there exists a constant M such that for all $S_g \in [0,1]$,*

$$P \leq P_g(S_g, P) \leq P + M, \quad P(1-S_g) - M \leq P_w(S_g, P)(1-S_g) \leq P(1-S_g).$$

The wetting phase pressure P_w, in contrast to P_g, is unbounded when $S_g \to 1$. From (A.3) and (A.6) it also follows that ω is smooth, strictly positive and bounded function. There exist constants ω_m, ω_M, such that for all $S_g \in [0,1]$ and $P \in \mathbb{R}$,

$$0 < \omega_m \leq \omega(S_g, P) \leq \omega_M < +\infty,$$

and also

$$0 < \rho_m \lambda_m \omega_m \leq \Lambda(S_g, P) = \Lambda_w(S_g, P) + \Lambda_g(S_g, P) \leq \rho_M \lambda_M \omega_M.$$

Remark 5.2. *From (A.5) it follows that there exists a constant $C > 0$ such that for all $S_1, S_2 \in]0, S^{\#}]$*

$$|P_c(S_1) - P_c(S_2)| \min(S_1, S_2) \leq C|S_1 - S_2|^{\gamma}, \tag{5.15}$$

and for all $S_1, S_2 \in [S^{\#}, 1[$

$$|P_c(S_1) - P_c(S_2)|(1 - \max(S_1, S_2)) \leq C|S_1 - S_2|^{\gamma}. \tag{5.16}$$

For example, for $S_1 < S_2 < S^{\#}$

$$\begin{aligned} |P_c(S_1) - P_c(S_2)| \min(S_1, S_2) = S_1(P_c(S_2) - P_c(S_1)) &\leq \int_{S_1}^{S_2} sP_c'(s)\, ds \\ = \int_{S_1}^{S_2} s^{2-\gamma} P_c'(s) s^{\gamma-1}\, ds \leq C \int_{S_1}^{S_2} s^{\gamma-1}\, ds &\leq \frac{C}{\gamma}|S_1 - S_2|^{\gamma}, \end{aligned}$$

and analogously for $S_1 > S_2$. The estimate (5.16) can be proved in a similar way. For $S^{\#} < S_1 < S_2$

$$\begin{aligned} |P_c(S_1) - P_c(S_2)|(1 - \max(S_1, S_2)) = (1 - S_2)(P_c(S_2) - P_c(S_1)) &\leq \int_{S_1}^{S_2} (1-s)P_c'(s)\, ds \\ &= \int_{S_1}^{S_2} (1-s)^{2-\gamma} P_c'(s)(1-s)^{\gamma-1}\, ds \leq C \int_{S_1}^{S_2} (1-s)^{\gamma-1} \\ &= \frac{C}{\gamma}((1-S_1)^{\gamma} - (1-S_2)^{\gamma}) \leq \frac{C}{\gamma}|S_1 - S_2|^{\gamma} \end{aligned}$$

where the last inequality follows from the fact that the function $(1-S)^{\gamma}$ is Hölder continuous with exponent γ, when $0 < \gamma \leq 1$. The case $S_1 > S_2$ can be shown analogously.

Remark 5.3. *Note that (A.8) is satisfied if the function* $\alpha(S) = \sqrt{\lambda_g(S)\lambda_w(S)}$ *has the following asymptotic behavior at* $S = 0, 1$*:*

$$\alpha(S) \geq C_0 \begin{cases} S^{\gamma_1} & \text{for } S \leq S_0 \\ (1-S)^{\gamma_2} & \text{for } S \geq S_0 \end{cases}$$

Then (A.8) is fulfilled for $\tau = \min(1/(1+\gamma_1), 1/(1+\gamma_2))$*. Furthermore, (A.4) and (A.8) imply that* $S \mapsto \beta(S)$ *is a monotone increasing function satisfying* $\beta(1) < +\infty$ *and thus there exists an inverse function* $\mathcal{S} = \beta^{-1} \colon [0, \beta(1)] \to [0, 1]$*. From (A.8) it follows*

$$|\beta(S_2) - \beta(S_1)|^\tau \geq \frac{p^\tau_{c,min}}{C} |S_2 - S_1|, \tag{5.17}$$

and $\mathcal{S}$ *is Hölder continuous with exponent* τ*.*

Remark 5.4. *Conditions (A.4) and (A.5) are satisfied for many relative permeability-capillary pressure models in suitable range of theirs parameters. A calculation can show, that Brooks and Corey model satisfy (A.4) and (A.5) for parameter* $\lambda > 1$ *and any* $\gamma \leq 1 - \frac{1}{\lambda}$*. For van Genuchten's functions these conditions are satisfied for* $n > 2$ *and any* $\gamma \leq \frac{n-2}{n-1}$*.*

In order to take into account the Dirichlet boundary condition the following space is introduced:

$$V = \{\varphi \in H^1(\Omega) \colon \varphi|_{\Gamma_{inj}} = 0\}.$$

Throughout the rest of the chapter the notation $S = S_g$ is used. Now the existence result of weak solutions of the system (5.6), (5.7), (5.8), (5.9) and (5.10) in variables P and θ is presented.

Theorem 5.1. *Let (A.1)-(A.8) hold and assume* $(\theta_0, p_0) \in L^2(\Omega) \times L^2(\Omega)$*,* $0 \leq \theta_0 \leq \beta(1)$ *a.e. in* Ω*. Then there exists* (P, θ) *satisfying*

$$P \in L^2(0, T; V),\ \theta \in L^2(0, T; V),\ 0 \leq \theta \leq \beta(1) \ \textit{a.e. in } Q_T,\ S = \mathcal{S}(\theta),$$
$$\Phi \partial_t(\rho_w(S, P)(1 - S)) \in L^2(0, T; V'), \quad \Phi \partial_t(\rho_g(S, P)S) \in L^2(0, T; V'),$$

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

$$\int_0^T \langle \Phi \partial_t(\rho_w(S,P)(1-S)), \varphi \rangle dt + \int_{Q_T} [\Lambda_w(S,P)\mathbb{K}\nabla P \cdot \nabla \varphi - A(S,P)\mathbb{K}\nabla\theta \cdot \nabla\varphi] dxdt$$
$$- \int_{Q_T} [\lambda_w(S)\rho_w(S,P)^2 \mathbb{K}\mathbf{g} \cdot \nabla\varphi - \rho_w(S,P) f_w(S,P) F_P \varphi] dxdt = 0, \tag{5.18}$$

$$\int_0^T \langle \Phi \partial_t(\rho_g(S,P)S), \psi \rangle dt + \int_{Q_T} [\Lambda_g(S,P)\mathbb{K}\nabla P \cdot \nabla \psi + A(S,P)\mathbb{K}\nabla\theta \cdot \nabla\psi] dxdt$$
$$- \int_{Q_T} [\lambda_g(S)\rho_g(S,P)^2 \mathbb{K}\mathbf{g} \cdot \nabla\psi - \rho_g(S,P) f_g(S,P) F_P \psi] dxdt \tag{5.19}$$
$$= \int_{Q_T} \rho_g(S,P) F_I \psi dxdt.$$

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

$$t \mapsto \int_\Omega \Phi \rho_w(P_w(S,P))(1-S)\psi dx, \quad t \mapsto \int_\Omega \Phi \rho_g(P_g(S,P)) S \psi dx$$

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

$$\left(\int_\Omega \Phi \rho_w(P_w(S,P))(1-S)\psi dx \right)(0) = \int_\Omega \Phi \rho_w(P_w(s_0,p_0))(1-s_0)\psi dx,$$

$$\left(\int_\Omega \Phi \rho_g(P_g(S,P)) S \psi dx \right)(0) = \int_\Omega \Phi \rho_g(P_g(s_0,p_0)) s_0 \psi dx,$$

where $s_0 = \mathcal{S}(\theta_0)$.

Compared to [44, 48], this existence result permits to consider unbounded capillary pressure functions and can be applied to physically relevant situations. In contrast to [42–44] and [48], no additional regularity of porosity and permeability fields apart from boundedness and positivity are demanded. This is achieved by a modification of a standard compactness result in [60]. By considering this new model for immiscible compressible two-phase flow in porous media by the concept of global pressure, the proof of the existence of weak solutions greatly simplifies compared to the one presented in [42–44, 48].

5.2 Regularised Problem and Auxiliary Results

In the proof of Theorem 5.1 a crucial role is played by the fact that the change of variables $(u, v) = G(S, P)$ given by

$$u = \rho_w(P_w(S, P))(1 - S), \quad v = \rho_g(P_g(S, P))S \tag{5.20}$$

$(S = S_g)$ is a diffeomorphism. This is proved in the next two lemmas.

Lemma 5.1. *Assume (A.4) and (A.6) hold. Then the map* $(u, v) = G(S, P)$, $G\colon [0, 1] \times \mathbb{R} \to [0, \rho_M] \times [0, \rho_M]$ *defined by (5.20) is injective.*

Proof. Assume that there exist $(S_1, P_1) \neq (S_2, P_2)$ such that

$$\rho_w(P_w(S_1, P_1))(1 - S_1) = \rho_w(P_w(S_2, P_2))(1 - S_2),$$
$$\rho_g(P_g(S_1, p_1))S_1 = \rho_g(P_g(S_2, P_2))S_2.$$

First the case $S_1 = S_2$ is considered. If $S_1 = S_2 (= S) > 0$ then the strict monotonicity of ρ_g gives $P_g(S, P_1) = P_g(S, P_2)$. The nonwetting pressure P_g is strictly monotone function of the global pressure, leading to $P_1 = P_2$. The argument is also valid in the case $S = 1$ since $P_g(1, P)$ is finite. If $S_1 = S_2 = 0$ then $\rho_w(P_w(0, P_1)) = \rho_w(P_w(0, P_2))$ or $\rho_w(P_1) = \rho_w(P_2)$ which leads again to $P_1 = P_2$.

Consider the case $S_1 > S_2$. Then

$$\frac{S_2}{S_1} < 1 \quad \text{and} \quad \frac{1 - S_1}{1 - S_2} < 1.$$

From

$$\rho_w(P_w(S_1, P_1))\frac{1 - S_1}{1 - S_2} = \rho_w(P_w(S_2, P_2)), \quad \rho_g(P_g(S_1, P_1)) = \rho_g(P_g(S_2, P_2))\frac{S_2}{S_1}.$$

it follows that

$$\rho_w(P_w(S_1, P_1)) > \rho_w(P_w(S_2, P_2)), \quad \rho_g(P_g(S_1, P_1)) < \rho_g(P_g(S_2, P_2)).$$

The density functions are strictly increasing and therefore

$$P_w(S_1, P_1) > P_w(S_2, P_2), \quad P_g(S_1, P_1) < P_g(S_2, P_2).$$

By subtraction one obtains

$$P_c(S_1) = P_g(S_1, P_1) - P_w(S_1, P_1) < P_c(S_2) = P_g(S_2, P_2) - P_w(S_2, P_2)$$

which leads to $S_1 < S_2$ since $S = S_g \to P_c(S)$ is strictly increasing function. This is in contradiction with starting assumption, $S_1 > S_2$. In the same way, one may prove that the case $S_1 < S_2$ is not possible and the conclusion follows. $\square$

In order to study the map G, given by (5.20), it is decomposed as $G = G_2 \circ G_1$,

$$(S, P) \mapsto (S, P_g(S, P)) \mapsto (\rho_w(P_g - P_c(S))(1 - S), \rho_g(P_g)S).$$

Mapping $G_1(S, P) = (S, P_g(S, P))$ is a homeomorphism from $[0, 1] \times \mathbb{R}$ to $[0, 1] \times \mathbb{R}$, and a diffeomorphism in $]0, 1[\times\mathbb{R}$.

Next, consider the mapping $G_2(S, P_g) = (\rho_w(P_g - P_c(S))(1 - S), \rho_g(P_g)S)$. A simple analysis shows that G_2 maps $[0, 1] \times \mathbb{R}$ into lower triangle of $[0, \rho_{w,max}] \times [0, \rho_{g,max}]$. Indeed, if one sets

$$u = \rho_w(P_g - P_c(S))(1 - S), \quad v = \rho_g(P_g)S,$$

then, for a fixed $v \in [0, \rho_{g,max}]$, S is allowed to vary in the interval

$$\frac{v}{\rho_{g,max}} \le S \le \min(1, \frac{v}{\rho_{g,min}}).$$

u is expressed as a function of S (and v which is fixed) as

$$u = \rho_w(\rho_g^{-1}(\frac{v}{S}) - P_c(S))(1 - S).$$

This function is strictly decreasing since

$$\frac{du}{dS} = -\rho_w(\rho_g^{-1}(\frac{v}{S}) - P_c(S)) + \rho_w'(\rho_g^{-1}(\frac{v}{S}) - P_c(S))(1 - S)(D\rho_g^{-1}(\frac{v}{S})(-\frac{v}{S^2}) - P_c'(S)) < 0.$$

One easily see that (u, v) covers all of shadowed region on Figure 5.2, which will be denoted by $\mathcal{R}$. Note that $\mathcal{R}$ contains open segments BC and DA, but it does not contain closed segments $\overline{AB}$ and $\overline{CD}$ which correspond, respectively, to $P_g = +\infty$ and $P_g = -\infty$.

Lemma 5.2. *The mappings G and G_2 are homeomorphisms from $[0, 1] \times \mathbb{R}$ to $\mathcal{R}$ and diffeomorphisms from $]0, 1[\times\mathbb{R}$ to Int($\mathcal{R}$).*

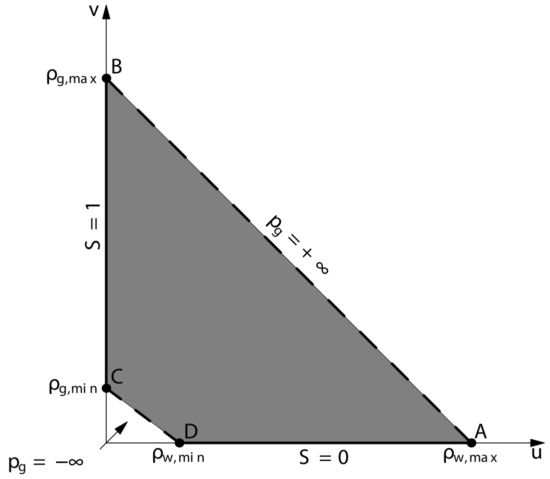


Figure 5.1: Range of the mapping G_2.

Proof. Injectivity of the map G is proved in Lemma 5.2 and thus G_2 is also injective. Surjectivity of the map G_2 from $[0,1] \times \mathbb{R}$ to $\mathcal{R}$ and surjectivity of G_1 on $[0,1] \times \mathbb{R}$ proves that G is a surjection form $[0,1] \times \mathbb{R}$ to $\mathcal{R}$. Thus, $H_2 = G_2^{-1}$ exists. Calculating the jacobian of G_2 gives

$$\begin{vmatrix} \frac{\partial u}{\partial P_g} & \frac{\partial u}{\partial S} \\ \frac{\partial v}{\partial P_g} & \frac{\partial v}{\partial S} \end{vmatrix} = [\rho_w'(P_w)(1-S)]\rho_g(P_g) + \rho_g'(P_g)S[\rho_w'(P_w)(1-S)P_c'(S) + \rho_w(P_w)] > 0,$$

where $P_w = P_g - P_c(S)$. Therefore, G_2 is a diffeomorphism from $]0,1[\times\mathbb{R}$ onto $\mathrm{Int}(\mathcal{R})$. To show the continuity of G_2^{-1} on BC and DA, consider a sequence

$$(u^k, v^k) \to (u, 0) \quad \text{as } k \to \infty, \quad \text{for } \rho_{w,min} < u < \rho_{w,max}.$$

Then, obviously, $S^k \to 0$, and $\rho_w(P_g^k - P_c(S^k)) \to u$. From the continuity of ρ_w and P_c and since $u \neq \rho_{w,min}, \rho_{w,max}$, $P_g^k \to \rho_w^{-1}(u) + P_c(0)$. The continuity on BC is shown analogously. □

Unboundedness of the capillary pressure function is the reason why the gas saturation S cannot be taken as the primary variable. To avoid integrability problems, capillary pressure curve will be corrected in order to make it bounded. Also, a small constant is added to the diffusivity coefficient in order to achieve uniform ellipticity of discretized system. therefore, a small parameter $\eta > 0$ is introduced into the coefficients. The limit when $\eta \to 0$ is analysed.

The capillary pressure derivative may be unbounded at $S = 0$ and $S = 1$. The derivative will be limited by applying an operator R_η, $0 < \eta < 1$, to the capillary pressure derivative in the following way:

$$R_\eta(P_c'(S)) = \begin{cases} 2(1 - \frac{S}{\eta})\frac{P_c(\eta)-P_c(0)}{\eta} + (2\frac{S}{\eta} - 1)P_c'(\eta) & \text{for } S \leq \eta \\ P_c'(S) & \text{for } \eta \leq S \leq 1-\eta \\ P_c'(1-\eta) & \text{for } 1-\eta \leq S \leq 1, \end{cases} \tag{5.21}$$

and let

$$P_c^\eta(S) = P_c(0) + \int_0^S R_\eta(P_c'(s))\,ds. \tag{5.22}$$

Obviously, if the derivative $P_c'(S)$ is bounded at $S = 0$ or $S = 1$, then the correction at that end in $R_\eta(P_c'(S))$ is not needed. It is easy to see that, for any $\eta > 0$, $P_c^\eta(S)$ is a bounded, monotone, $C^1([0,1])$ function, and that $P_c^\eta(S) = P_c(S)$ for $S \in [\eta, 1-\eta]$. From (A.4) it follows that for sufficiently small η it holds

$$\frac{d}{dS}P_c^\eta(S) \geq p_{c,min}/2 > 0. \tag{5.23}$$

Also, the operator R_η satisfies

$$|R_\eta(P_c'(S))| \leq p_{c,max}^\eta < +\infty,$$

for some constant $p_{c,max}^\eta$ such that, generally, $p_{c,max}^\eta \to \infty$ when $\eta \to 0$. Note also that one can assume that $R_\eta(P_c'(S))$ satisfies

$$R_\eta(P_c'(S)) \leq P_c'(S), \quad \text{for } S \geq \eta, \tag{5.24}$$

since if it does not one can modify the definition of $R_\eta(P_c'(S))$ for $S > 1-\eta$ by replacing the constant value $P_c'(1-\eta)$ by suitable continuous curve, staying below $P_c'(S)$ for $S > 1-\eta$. Define:

$$P_g^\eta(S,P) = P + P_c(0) + \int_0^S f_w(s,P)R_\eta(P_c'(s))\,ds, \tag{5.25}$$

$$P_w^\eta(S,P) = P - \int_0^S f_g(s,P)R_\eta(P_c'(s))\,ds. \tag{5.26}$$

Obviously,

$$P_g^\eta(S,P) - P_w^\eta(S,P) = P_c^\eta(S). \tag{5.27}$$

The derivatives of regularized phase pressures are given as

$$\frac{\partial P_g^\eta}{\partial P} = \frac{\partial P_w^\eta}{\partial P} = \omega^\eta(S,P),$$

where, from Remark 5.1

$$\omega^\eta(S,P) = \\ \exp\left(-\int_0^S (\nu_g(s,P) - \nu_w(s,P)) \frac{\rho_w(s,P)\rho_g(s,P)\lambda_w(s)\lambda_g(s)R_\eta(P_c'(s))}{(\rho_w(s,P)\lambda_w(s) + \rho_g(s,P)\lambda_g(s))^2}\, ds\right).$$

Now it follows that

$$\nabla P_g^\eta = \omega^\eta(S,P)\nabla P + f_w(S,P)R_\eta(P_c'(S))\nabla S, \tag{5.28}$$

$$\nabla P_w^\eta = \omega^\eta(S,P)\nabla P - f_g(S,P)R_\eta(P_c'(S))\nabla S, \tag{5.29}$$

and for given $P, S \in L^2(0,T;H^1(\Omega))$ it follows that $P_g^\eta, P_w^\eta \in L^2(0,T;H^1(\Omega))$.

In the regularized version of the system (5.6), (5.7) the functions P_α^η instead of P_α are used in calculations of the mass densities. That means, $\rho_\alpha(S,P)$ is replaced with

$$\rho_\alpha^\eta(S,P) = \rho_\alpha(P_\alpha^\eta(S,P)). \tag{5.30}$$

The function $A(S,P)$ is replaced with $A^\eta(S,P)$, for $\eta > 0$, defined as

$$A^\eta(S,P) = \frac{\rho_w(S,P)\rho_g(S,P)}{\lambda(S,P)}\lambda_w(S)\lambda_g(S)R_\eta(P_c'(S)) + \eta. \tag{5.31}$$

Obviously, $A^\eta(S,P) \geq \eta > 0$. *The regularized system* now takes the form

$$\begin{aligned}\Phi\frac{\partial}{\partial t}(\rho_w^\eta(S,P)(1-S)) - \operatorname{div}(\Lambda_w^\eta(S,P)\mathbb{K}\nabla P) + \operatorname{div}(A^\eta(S,P)\mathbb{K}\nabla S)\\ + \operatorname{div}(\lambda_w(S)\rho_w^\eta(S,P)^2\mathbb{K}\mathbf{g}) + \rho_w^\eta(S,P)f_w(S,P)F_P = \rho_w^\eta(S,P)S_w^*F_I,\end{aligned} \tag{5.32}$$

$$\begin{aligned}\Phi\frac{\partial}{\partial t}(\rho_g^\eta(S,P)S) - \operatorname{div}(\Lambda_g^\eta(S,P)\mathbb{K}\nabla P) - \operatorname{div}(A^\eta(S,P)\mathbb{K}\nabla S)\\ + \operatorname{div}(\lambda_g(S)\rho_g^\eta(S,P)^2\mathbb{K}\mathbf{g}) + \rho_g^\eta(S,P)f_g(S_w,P)F_P = \rho_g^\eta(S,P)S_g^*F_I,\end{aligned} \tag{5.33}$$

where $S = S_g$ and for $\alpha \in \{w, g\}$

$$\Lambda_\alpha^\eta(S,P) = \lambda_\alpha(S)\rho_\alpha(S,P)\omega^\eta(S,P). \tag{5.34}$$

The regularized total mobility is introduced:

$$\Lambda^\eta(S,P) = \Lambda_w^\eta(S,P) + \Lambda_g^\eta(S,P), \tag{5.35}$$

and the regularized β function:

$$\beta^\eta(S) = \int_0^S \sqrt{\lambda_w(s)\lambda_g(s)}R_\eta(P_c'(s))\,ds. \tag{5.36}$$

Remark 5.5. *The regularized wetting phase flux (without gravity term) can be written as:*

$$\Lambda_w^\eta(S,P)\mathbb{K}\nabla P - A^\eta(S,P)\mathbb{K}\nabla S = \lambda_w(S)\rho_w(S,P)\mathbb{K}\nabla P_w^\eta - \eta\mathbb{K}\nabla S, \tag{5.37}$$

and similarly for the regularized non wetting flux:

$$\Lambda_g^\eta(S,P)\mathbb{K}\nabla P + A^\eta(S,P)\mathbb{K}\nabla S = \lambda_g(S)\rho_g(S,P)\mathbb{K}\nabla P_g^\eta + \eta\mathbb{K}\nabla S. \tag{5.38}$$

Remark 5.6. *A priori estimates that will be used in the proof of Theorem 5.1 are based on the following equality,*

$$\begin{aligned}\rho_g(S,P)\lambda_g(S)\mathbb{K}\nabla P_g^\eta \cdot \nabla P_g^\eta + \rho_w(S,P)\lambda_w(S)\mathbb{K}\nabla P_w^\eta \cdot \nabla P_w^\eta\\ = \Lambda^\eta(S,p)\omega^\eta(S,p)\mathbb{K}\nabla P\cdot\nabla P + \frac{\rho_g(S,P)\rho_w(S,P)}{\lambda(S,P)}\mathbb{K}\nabla\beta^\eta(S)\cdot\nabla\beta^\eta(S).\end{aligned} \tag{5.39}$$

From (3.27) and similarly from (3.28) one obtains

$$\begin{aligned}\nabla P_g^\eta\cdot\nabla P_g^\eta = \omega^\eta(S,P)^2\nabla P\cdot\nabla P + 2\omega^\eta(S,P)f_w(S_P)R_\eta(P_c'(S))\nabla S\cdot\nabla P\\ + f_w(S,P)^2R_\eta(P_c'(S))^2\nabla S\cdot\nabla S.\end{aligned}$$

Then by setting $\mathcal{U} = \rho_g(S,P)\lambda_g(S)\mathbb{K}\nabla P_g^\eta \cdot \nabla P_g^\eta + \rho_w(S,P)\lambda_w(S)\mathbb{K}\nabla P_w^\eta \cdot \nabla P_w^\eta$*, one obtains*

$$\begin{aligned}\mathcal{U} = \omega^\eta(S,P)^2(\rho_g(S,P)\lambda_g(S) + \rho_w(S,P)\lambda_w(S))\mathbb{K}\nabla P \cdot \nabla P&\\ + (\rho_g(S,P)\lambda_g(S) f_w(S,P)^2 R_\eta(P_c'(s))^2&\\ + \rho_w(S,P)\lambda_w(S) f_g(S,P)^2 R_\eta(P_c'(s))^2)\mathbb{K}\nabla S \cdot \nabla S&\\ + 2\frac{\rho_g(S,P)\lambda_g(S)\rho_w(S,P)\lambda_w(S)}{\lambda(S,P)}\omega^\eta(S,P)R_\eta(P_c'(S))\mathbb{K}\nabla S \cdot \nabla P&\\ - 2\frac{\rho_w(S,P)\lambda_w(S)\rho_g(S,P)\lambda_g(S)}{\lambda(S,P)}\omega^\eta(S,P)R_\eta(P_c'(S))\mathbb{K}\nabla S \cdot \nabla P&\end{aligned}$$

which gives

$$\begin{aligned}\mathcal{U} = \omega^\eta(S,P)\Lambda^\eta(S,P)\mathbb{K}\nabla P \cdot \nabla P + (\rho_g(S,P)\lambda_g(S) f_w(S,P)^2 R_\eta(P_c'(s))^2&\\ + \rho_w(S,P)\lambda_w(S) f_g(S,P)^2 R_\eta(P_c'(s))^2)\mathbb{K}\nabla S \cdot \nabla S.&\end{aligned}$$

Using the following equality $(\rho_g = \rho_g(S,P), \rho_w = \rho_w(S,P))$

$$\frac{\rho_g\lambda_g(S)\rho_w^2\lambda_w(S)^2 + \rho_w\lambda_w(S)\rho_g)^2\lambda_g(S)^2}{\lambda(S,P)^2} = \frac{\rho_g\lambda_g(S)\rho_w\lambda_w(S)}{\lambda(S,P)},$$

it can be obtained

$$\begin{aligned}\mathcal{U} = \omega^\eta(S,P)\Lambda^\eta(S,P)\mathbb{K}\nabla P \cdot \nabla P&\\ + \frac{\rho_g(S,P)\rho_w(S,P)}{\lambda(S,P)}\left(\sqrt{\lambda_g(S)\lambda_w(S)}R_\eta(P_c'(S))\right)^2 \mathbb{K}\nabla S \cdot \nabla S,&\end{aligned}$$

which gives

$$\mathcal{U} = \omega^\eta(S,P)\Lambda^\eta(S,P)\mathbb{K}\nabla P \cdot \nabla P + \frac{\rho_g(S,P)\rho_w(S,P)}{\lambda(S,P)}\mathbb{K}\nabla\beta^\eta(S) \cdot \nabla\beta^\eta(S).$$

From the equality (5.39) the estimate follows

$$\begin{aligned}\rho_g(S,P)\lambda_g(S)\mathbb{K}\nabla P_g^\eta \cdot \nabla P_g^\eta + \rho_w(S,P)\lambda_w(S)\mathbb{K}\nabla P_w^\eta \cdot \nabla P_w^\eta&\\ \geq \lambda_m\rho_m\omega_m^2 k_m|\nabla P|^2 + \frac{\rho_m^2}{\lambda_M\rho_M}k_m|\nabla\beta^\eta(S)|^2.&\end{aligned} \tag{5.40}$$

Remark 5.7. *From (5.23), as in Remark 5.3, that* β^η *has Hölder continuous inverse*

$\mathcal{S}^\eta = (\beta^\eta)^{-1}$, *with the same exponent* τ. *Indeed,*

$$\begin{aligned}|\beta^\eta(S_1) - \beta^\eta(S_2)|^\tau = |\int_{S_1}^{S_2} \sqrt{\lambda_w(s)\lambda_g(s)} R_\eta(P_c'(s))\, ds|^\tau \geq P_{c,min}| \int_{S_1}^{S_2} \sqrt{\lambda_w(s)\lambda_g(s)}\, ds|^\tau \\ \geq C|S_1 - S_2|.\end{aligned}$$

Remark 5.8. *Lemma 5.2 is equally applicable to the mapping* $(u, v) = G^\eta(S, P)$, $G^\eta\colon [0,1]\times \mathbb{R} \to \mathcal{R}$ *defined by*

$$u = \rho_w(P_w^\eta(S, P))(1 - S), \quad v = \rho_g(P_g^\eta(S, P))S, \tag{5.41}$$

which is therefore homeomorphism from $[0, 1] \times \mathbb{R}$ *onto* $\mathcal{R}$.

Now the convergence properties of the regularized coefficients will be investigated when $\eta \to 0$.

Lemma 5.3. *Assume that (A.4)-(A.6) are fulfilled. Then there exist constants* $M > 0$, ω_m *and* ω_M *such that*

$$\begin{aligned}P \leq & P_g^\eta(S, P) \leq P + M, && (5.42)\\ (1 - S)P - M \leq & (1 - S)P_w^\eta(S, P) \leq (1 - S)P, && (5.43)\\ \lambda_w(S)P - M \leq & \lambda_w(S)P_w^\eta(S, P) \leq \lambda_w(S)P, && (5.44)\\ 0 < \omega_m \leq & \omega^\eta(S, P) \leq \omega_M, && (5.45)\end{aligned}$$

and the following uniform convergences in $[0, 1] \times \mathbb{R}$ *hold:*

$$\begin{aligned}P_g^\eta(S, P) &\to P_g(S, P) \quad \text{as } \eta \to 0, && (5.46)\\ (1 - S)P_w^\eta(S, P) &\to (1 - S)P_w(S, P) \quad \text{as } \eta \to 0, && (5.47)\\ \lambda_w(S)P_w^\eta(S, P) &\to \lambda_w(S)P_w(S, P) \quad \text{as } \eta \to 0, && (5.48)\\ \omega^\eta(S, P) &\to \omega(S, P) \quad \text{as } \eta \to 0, && (5.49)\\ \beta^\eta(S) &\to \beta(S) \quad \text{as } \eta \to 0 \ \text{ uniformly in } [0, 1]. && (5.50)\end{aligned}$$

Proof. The estimates (5.42) and (5.43) follow easily as in Remark 5.1, by using (A.4) which gives the boundedness of $\lambda_w(S)P_c'(S)$ in $[S^\#, 1[$ and the boundedness of $(1 - S)P_c(S)$ in $[0, 1]$. Similarly (5.44), and (5.45) are obtained as in Remark 5.1. For the convergence

(5.46), using (A.4) which implies that $\lambda_w(S)P_c'(S)$ is bounded in vicinity of $S=1$, the estimate is:

$$
\begin{aligned}
|P_g^\eta(S,P)-P_g(S,P)| &\le \int_0^S f_w(s,p)|R_\eta(P_c'(s))-P_c'(s)|\,ds\\
&\le \frac{\rho_M}{\lambda_m\rho_m}\left(\lambda_M\int_0^\eta (R_\eta(P_c'(s))+P_c'(s))\,ds+\int_{1-\eta}^1 \lambda_w(s)(P_c'(1-\eta)+P_c'(s))\,ds\right)\\
&\le \frac{\rho_M}{\lambda_m\rho_m}\left(\lambda_M\int_0^\eta (R_\eta(P_c'(s))\,ds+\lambda_M\int_0^\eta P_c'(s)\,ds+\int_{1-\eta}^1 \lambda_w(1-\eta)P_c'(1-\eta)\,ds+\right.\\
&\left.+\int_{1-\eta}^1 \lambda_w(s)P_c'(s)\,ds\right)\le \frac{\rho_M}{\lambda_m\rho_m}(2\lambda_M(P_c(\eta)-P_c(0))+C\eta).
\end{aligned}
$$

This gives (5.46), and (5.50) is obtained in a similar way.

$$
\begin{aligned}
|\beta^\eta(S)-\beta(S)| &\le \int_0^S \sqrt{\lambda_w(s)\lambda_g(s)}|R_\eta(P_c'(s))-p_c'(s)|\,ds\\
&\le \int_0^\eta \sqrt{\lambda_w(S)\lambda_g(S)}R_\eta(P_c'(s))\,ds+\int_{1-\eta}^1 \sqrt{\lambda_w(s)\lambda_g(s)}P_c'(s)\,ds\\
&\le \lambda_M\int_0^\eta R_\eta(P_c'(s))\,ds+C\eta\\
&=\lambda_m(P_c(\eta)-P_c(0))+C\eta.
\end{aligned}
$$

For (5.47), for sufficiently small η it follows:

$$
\begin{aligned}
|(P_w^\eta(S,P)-P_w(S,P))(1-S)| &\le \frac{\rho_M}{\lambda_m\rho_m}|1-S|\int_0^S \lambda_g(s)|R_\eta(P_c'(s))-P_c'(s)|\,ds\\
&\le \frac{\rho_M\lambda_M}{\lambda_m\rho_m}(\int_0^\eta (R_\eta(P_c'(s))+P_c'(s))\;ds+|1-S|\int_{1-\eta}^{\max(1-\eta,S)} P_c'(s)\,ds)\\
&\le \frac{\rho_M\lambda_M}{\lambda_m\rho_m}(2(P_c(\eta)-P_c(0))+(1-S)\,[P_c(\max(1-\eta,S))-P_c(1-\eta)]).
\end{aligned}
$$

Applying (5.16) in Remark 5.2 one gets

$$
|(P_w^\eta(S,P)-P_w(S,P))(1-S)|\le C(P_c(\eta)-P_c(0)+\eta^\gamma)
$$

which gives (5.47).

The convergence (5.48) is obtained in a similar way as in (5.46) and (5.47) by using the monotonicity of $\lambda_w(S)$ and the fact that, due to (A.4), $\lambda_w(S)P_c'(S)$ is bounded in $[S^\#,1[$.

Therefore,

$$\begin{aligned}
|(P_w^\eta(S,P) - P_w(S,P))\lambda_w(S)| &\leq \frac{\rho_M}{\lambda_m\rho_m}\lambda_w(S)\int_0^S \lambda_g(s)|R_\eta(P_c'(s)) - P_c'(s)|\,ds \\
&\leq \frac{\rho_M}{\lambda_m\rho_m}(\int_0^\eta \lambda_w(s)\lambda_g(s)\,(R_\eta(P_c'(s)) + P_c'(s))\,ds + \int_{1-\eta}^1 2\lambda_w(s)\lambda_g(s)P_c'(s)\,ds) \\
&\leq \frac{\rho_M\lambda_M^2}{\lambda_m\rho_m}(2(P_c(\eta) - P_c(0)) + C\eta).
\end{aligned}$$

The convergence (5.49) is obtained similarly, using the fact that the exponential function is continuously differentiable. □

Corollary 5.1. *Assume that* $S^\eta, P^\eta, S, P \in L^2(\Omega_T)$ *are such that* $0 \leq S^\eta, S \leq 1$ *and*

$$P^\eta \to P, \quad S^\eta \to S \quad \text{a.e. in } Q_T \text{ when } \eta \to 0.$$

Then

$$P_g^\eta(S^\eta,P^\eta) \to P_g(S,P) \quad \omega^\eta(S^\eta,P^\eta) \to \omega(S,P), \quad \text{a.e. in } Q_T \text{ when } \eta \to 0, \tag{5.51}$$

$$(1-S^\eta)\rho_w(P_w^\eta(S^\eta,P^\eta)) \to (1-S)\rho_w(P_w(S,P)), \quad \text{a.e. in } Q_T \text{ when } \eta \to 0, \tag{5.52}$$

$$\lambda_w(S^\eta)\rho_w(P_w^\eta(S^\eta,P^\eta)) \to \lambda_w(S)\rho_w(P_w(S,P)), \quad \text{a.e. in } Q_T \text{ when } \eta \to 0. \tag{5.53}$$

Proof. This is a consequence of the uniform convergence in Lemma 5.3 and the continuity of functions P_α, ω and ρ_α. □

The weak formulation of the regularized problem is defined in the following theorem.

Theorem 5.2. *(Regularized problem) Let (A.1)-(A.7) hold and assume that* $(s_0, p_0) \in V \times V$, $0 \leq s_0 \leq 1$ *a.e. in* Ω. *For all* $\eta > 0$ *sufficiently small there exists* (P^η, S^η) *satisfying*

$$\begin{gathered}
P^\eta,\ S^\eta \in L^2(0,T;V),\ 0 \leq S^\eta \leq 1 \text{ a.e. in } Q_T, \\
\Phi\partial_t(\rho_w^\eta(S^\eta,P^\eta)(1-S^\eta)), \Phi\partial_t(\rho_g^\eta(S^\eta,P^\eta)S^\eta) \in L^2(0,T;V'), \\
\rho_w^\eta(S^\eta,P^\eta)(1-S^\eta), \rho_g^\eta(S^\eta,P^\eta)S^\eta \in L^2(0,T;V) \cap C([0,T];L^2(\Omega)),
\end{gathered}$$

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

$$\begin{aligned}&\int_0^T \langle \Phi\partial_t(\rho_w^\eta(S^\eta,P^\eta)(1-S^\eta)),\varphi\rangle dt\\&\quad+\int_{Q_T}[\Lambda_w^\eta(S^\eta,P^\eta)\mathbb{K}\nabla P^\eta\cdot\nabla\varphi - A^\eta(S^\eta,P^\eta)\mathbb{K}\nabla S^\eta\cdot\nabla\varphi]dxdt\\&\quad-\int_{Q_T}[\lambda_w(S^\eta)\rho_w^\eta(S^\eta,P^\eta)^2\mathbb{K}\mathbf{g}\cdot\nabla\varphi - \rho_w^\eta(S^\eta,P^\eta)f_w(S^\eta,P^\eta)F_P\varphi]dxdt\\&\quad=\int_{Q_T}\rho_w^\eta(S^\eta,P^\eta)(1-S^*)F_I\varphi dxdt,\end{aligned} \tag{5.54}$$

$$\begin{aligned}&\int_0^T \langle \Phi\partial_t(\rho_g^\eta(S^\eta,P^\eta)S^\eta),\psi\rangle dt\\&\quad+\int_{Q_T}[\Lambda_g^\eta(S^\eta,P^\eta)\mathbb{K}\nabla P^\eta\cdot\nabla\psi + A^\eta(S^\eta,P^\eta)\mathbb{K}\nabla S^\eta\cdot\nabla\psi]dxdt\\&\quad-\int_{Q_T}[\lambda_g(S^\eta)\rho_g^\eta(S^\eta,P^\eta)^2\mathbb{K}\mathbf{g}\cdot\nabla\psi - \rho_g^\eta(S^\eta,P^\eta)f_g(S^\eta,P^\eta)F_P\psi]dxdt\\&\quad=\int_{Q_T}\rho_g^\eta(S^\eta,P^\eta)S^*F_I\psi dxdt.\end{aligned} \tag{5.55}$$

Furthermore, $\rho_w^\eta(S^\eta,P^\eta)(1-S^\eta) = \rho_w^\eta(s_0,p_0)(1-s_0)$ *and* $\rho_g^\eta(S^\eta,P^\eta)S^\eta = \rho_g^\eta(s_0,p_0)s_0$ *a.e. in* Ω*, for* $t=0$*.*

The regularization of the capillary pressure (5.21) is not needed for problem (5.54), (5.55). The fact that the regularized function A^η is strictly positive (see (5.31)) and (A.4) are sufficient to obtain a regularized problem, i.e. a non-degenerate one. The need for regularization comes from the choice of the test function used in Section 5.3.2. Namely, $P_w(S,P)$ is not a good test function with $P,S\in L^2(0,T;V)$ since $\nabla P_w(S,P)$ is not in $L^2(Q_T)$ due to the singularity of $\partial P_w(S,P)/\partial S$ at $S=1$. This singularity is removed by correcting the capillary pressure curve.

5.3 Proof of Theorem 5.2

5.3.1 Step 1. Time Discretization

In this section a discretization of the time derivative for the regularized system (5.54)–(5.55) is introduced. In order to simplify the notation, the dependence of the saturation and the global pressure on the small parameter η will be omitted until the passage to the limit $\eta \to 0$.

The time derivatives in the variational formulation given in Theorem 5.2 are discretized in the following way: For each positive integer N interval $[0, T]$ is divided into N subintervals of equal length $h = T/N$. One sets $t_n = nh$ and $J_n =]t_{n-1}, t_n]$ for $1 \leq n \leq N$, and denote the time difference operator by

$$\partial^h v(t) = \frac{v(t+h) - v(t)}{h},$$

for any $h > 0$. Also, for any Hilbert space $\mathcal{H}$ one denotes

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

For $v^h \in l_h(\mathcal{H})$ is set $v^n = (v^h)^n = v^h|_{J_n}$ and, therefore, it can be written

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

To each function $v^h \in l_h(\mathcal{H})$ one can assign a piecewise linear in time function

$$\tilde{v}^h = \sum_{n=1}^{N} \left(\frac{t_n - t}{h} v^{n-1} + \frac{t - t_{n-1}}{h} v^n \right) \chi_{]t_{n-1}, t_n]}(t), \quad \tilde{v}^h(0) = v^0. \tag{5.56}$$

Then it follows that

$$\partial_t \tilde{v}^h(t) = \sum_{n=1}^{N} \frac{1}{h}(v^n - v^{n-1}) \chi_{]t_{n-1}, t_n[}(t) = \partial^{-h} v^h(t), \quad \text{for } t \neq nh, n = 0, 1, \ldots, N.$$

Finally, for any function $f \in L^1(0, T; \mathcal{H})$ is defined $f^h \in l_h(\mathcal{H})$ with,

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

The discrete system is defined as follows: Find $P^h \in l_h(V)$ and $S^h \in l_h(V)$ satisfying

$$\begin{aligned}
&\int_{Q_T} \Phi\partial^{-h}(\rho_w^\eta(S^h, P^h)(1-S^h))\varphi dxdt \\
&\quad + \int_{Q_T} [\Lambda_w^\eta(S^h, P^h)\mathbb{K}\nabla P^h \cdot \nabla\varphi - A^\eta(S^h, P^h)\mathbb{K}\nabla S^h \cdot \nabla\varphi] dxdt \\
&\quad - \int_{Q_T} [\lambda_w(S^h)\rho_w^\eta(S^h, P^h)^2\mathbb{K}\mathbf{g} \cdot \nabla\varphi - \rho_w^\eta(S^h, P^h) f_w(S^h, P^h) F_P^h \varphi] dxdt \qquad (5.57)\\
&\quad = \int_{Q_T} \rho_w^\eta(S^h, P^h)(1 - S^{*,h}) F_I^h \varphi dxdt,
\end{aligned}$$

for all $\varphi \in l_h(V)$;

$$\begin{aligned}
&\int_{Q_T} \Phi\partial^{-h}(\rho_g^\eta(S^h, P^h)S^h)\psi dxdt \\
&\quad + \int_{Q_T} [\Lambda_g^\eta(S^h, P^h)\mathbb{K}\nabla P^h \cdot \nabla\psi + A^\eta(S^h, P^h)\mathbb{K}\nabla S^h \cdot \nabla\psi] dxdt \qquad (5.58)\\
&\quad - \int_{Q_T} [\lambda_g(S^h)\rho_g(S^h, P^h)^2\mathbb{K}\mathbf{g} \cdot \nabla\psi - \rho_g^\eta(S^h, P^h) f_g(S^h, P^h) F_P^h \psi] dxdt \\
&\quad = \int_{Q_T} \rho_g^\eta(S^h, P^h) S^{*,h} F_I^h \psi dxdt,
\end{aligned}$$

for all $\psi \in l_h(V)$. For $t \leq 0$ $S^h = s_0$, $P^h = p_0$.

Proposition 5.1. *Assume (A.1)–(A.7), $0 \leq S^* \leq 1$, $0 \leq s_0 \leq 1$ and $p_0 \in V$. Then there exists a solution $P^h, S^h \in l_h(V)$ of (5.57), (5.58), such that*

$$0 \leq S^h \leq 1 \quad a.e. \text{ in } Q_T.$$

Proof. The proof is based on the Schauder fixed point theorem. Fix $1 \leq k \leq N$. It is enough to prove that for given $P^{k-1}, S^{k-1} \in V$, with $0 \leq S^{k-1} \leq 1$, problem

$$\begin{aligned}
&\frac{1}{h}\int_\Omega \Phi(\rho_w^\eta(S^k, P^k)(1-S^k) - \rho_w^\eta(S^{k-1}, P^{k-1})(1-S^{k-1}))\varphi dx \\
&\quad + \int_\Omega [\Lambda_w^\eta(S^k, P^k)\mathbb{K}\nabla P^k \cdot \nabla\varphi - A^\eta(S^k, P^k)\mathbb{K}\nabla S^k \cdot \nabla\varphi] dx \qquad (5.59)\\
&\quad - \int_\Omega [\lambda_w(S^k)\rho_w^\eta(S^k, P^k)^2\mathbb{K}\mathbf{g} \cdot \nabla\varphi - \rho_w^\eta(S^k, P^k) f_w(S^k, P^k) F_P^k \varphi] dx \\
&\quad = \int_\Omega \rho_w^\eta(S^k, P^k)(1 - S^{*,k}) F_I^k \varphi dx,
\end{aligned}$$

for all $\varphi \in V$ and

$$\begin{aligned}
&\frac{1}{h}\int_\Omega \Phi(\rho_g^\eta(S^k,P^k)S^k - \rho_g^\eta(S^{k-1},P^{k-1})S^{k-1})\psi dx \\
&\quad + \int_\Omega [\Lambda_g^\eta(S^k,P^k)\mathbb{K}\nabla P^k\cdot\nabla\psi + A^\eta(S^k,P^k)\mathbb{K}\nabla S^k\cdot\nabla\psi]dx \\
&\quad - \int_\Omega [\lambda_g(S^k)\rho_g^\eta(S^k,P^k)^2\mathbb{K}\mathbf{g}\cdot\nabla\psi - \rho_g^\eta(S^k,P^k)f_g(S^k,P^k)F_P^k\psi]dx \\
&\quad = \int_\Omega \rho_g^\eta(S^k,P^k)S^{*,k}F_I^k\psi dx,
\end{aligned} \tag{5.60}$$

for all $\psi \in V$, has a unique solution $P^k, S^k \in V$. By summing (5.59) and (5.60) one gets

$$\begin{aligned}
&\frac{1}{h}\int_\Omega \Phi(H^\eta(S^k,P^k) - H^\eta(S^{k-1},P^{k-1}))\varphi dx + \int_\Omega \Lambda^\eta(S^k,P^k)\mathbb{K}\nabla P^k\cdot\nabla\varphi dx \\
&\quad - \int_\Omega [H_1^\eta(S^k,P^k)\mathbb{K}\mathbf{g}\cdot\nabla\varphi - H_2^\eta(S^k,P^k)F_P^k\varphi]dx \\
&\quad = \int_\Omega (\rho_w^\eta(S^k,P^k)(1-S^{*,k}) + \rho_g^\eta(S^k,P^k)S^{*,k})F_I^k\varphi dx,
\end{aligned} \tag{5.61}$$

for all $\varphi \in V$, where the functions have been introduced.

$$\begin{aligned}
H^\eta(S,P) &= \rho_w^\eta(S,P)(1-S) + \rho_g^\eta(S,P)S, \\
H_1^\eta(S,P) &= \lambda_w(S)\rho_w^\eta(S,P)^2 + \lambda_g(S)\rho_g^\eta(S,P)^2, \\
H_2^\eta(S,P) &= \rho_w^\eta(S,P)f_w(S,P) + \rho_g^\eta(S,P)f_g(S,P).
\end{aligned}$$

Note that the system (5.60), (5.61) is equivalent to the system (5.59), (5.60). Therefore, the existence of a solution to (5.60), (5.61) will be proven.

Let $\mathcal{T}\colon L^2(\Omega)\times L^2(\Omega) \to L^2(\Omega)\times L^2(\Omega)$ be a mapping defined by $\mathcal{T}(\overline{S},\overline{P}) = (S,P)$, where (S,P) is a solution of the following linear system:

$$\begin{aligned}
&\frac{1}{h}\int_\Omega \Phi(H^\eta(Z(\overline{S}),\overline{P}) - H^\eta(S^{k-1},P^{k-1}))\varphi dx + \int_\Omega \Lambda^\eta(Z(\overline{S}),\overline{P})\mathbb{K}\nabla P\cdot\nabla\varphi dx \\
&\quad - \int_\Omega [H_1^\eta(Z(\overline{S}),\overline{P})\mathbb{K}\mathbf{g}\cdot\nabla\varphi - H_2^\eta(Z(\overline{S}),\overline{P})F_P^k\varphi]dx \\
&\quad = \int_\Omega (\rho_w^\eta(Z(\overline{S}),\overline{P})(1-S^{*,k}) + \rho_g^\eta(Z(\overline{S}),\overline{P})S^{*,k})F_I^k\varphi dx,
\end{aligned} \tag{5.62}$$

for all $\varphi \in V$,

$$\begin{aligned}
&\frac{1}{h}\int_\Omega \Phi(\rho_g^\eta(Z(\overline{S}), P)Z(\overline{S}) - \rho_g^\eta(S^{k-1}, P^{k-1})S^{k-1})\psi dx \\
&\qquad + \int_\Omega [\Lambda_g^\eta(Z(\overline{S}), P)\mathbb{K}\nabla P \cdot \nabla\psi + A^\eta(Z(\overline{S}), P)\mathbb{K}\nabla S \cdot \nabla\psi] dx \\
&\qquad - \int_\Omega [\lambda_g(Z(\overline{S}))\rho_g^\eta(Z(\overline{S}), P)^2\mathbb{K}\mathbf{g} \cdot \nabla\psi - \rho_g^\eta(Z(\overline{S}), P) f_g(Z(\overline{S}), P) F_P^k\psi] dx \\
&\qquad = \int_\Omega \rho_g^\eta(Z(\overline{S}), P)S^{*,k}F_I^k\psi dx,
\end{aligned} \tag{5.63}$$

for all $\psi \in V$. Here the following function is intorduced:

$$Z(S) = \begin{cases} 0 & \text{if } S < 0 \\ S & \text{if } 0 \le S \le 1 \\ 1 & \text{if } S > 1. \end{cases}$$

Note that (5.62) is a linear elliptic equation for the pressure P which has a unique solution by the Lax-Milgram lemma. From (5.62) by setting $\varphi = P$ it follows

$$\begin{aligned}
\int_\Omega \Lambda^\eta(Z(\overline{S}), \overline{P})\mathbb{K}\nabla P \cdot \nabla P\, dx &\le \int_\Omega (\rho_w^\eta(Z(\overline{S}), \overline{P})(1 - S^{*,k}) + \rho_g^\eta(Z(\overline{S}), \overline{P})S^{*,k})F_I^k|P| dx \\
&+ \int_\Omega H_1^\eta(Z(\overline{S}), \overline{P})|\mathbb{K}\mathbf{g} \cdot \nabla P|\, dx + \int_\Omega H_2^\eta(Z(\overline{S}), \overline{P})F_P^k|P|\, dx \\
&+ \frac{1}{h}\int_\Omega \Phi(H^\eta(Z(\overline{S}), \overline{P}) + H^\eta(S^{k-1}, P^{k-1}))|P| dx \\
&\le \rho_M\|F_I^k\|_{L^2(\Omega)}\|P\|_{L^2(\Omega)} + \lambda_M\rho_M^2 C\|\nabla P\|_{L^2(\Omega)} + \\
&+ \rho_M\|F_P^k\|_{L^2(\Omega)}\|P\|_{L^2(\Omega)} + \frac{2\rho_M}{h}\|\Phi\|_{L^2(\Omega)}\|P\|_{L^2(\Omega)},
\end{aligned}$$

and then the estimate is obtained:

$$\begin{aligned}
\rho_m\lambda_m\omega_m k_m \int_\Omega |\nabla P|^2\, d\mathbf{x} &\le 2\rho_M(1 + \frac{1}{h})(\|\Phi\|_{L^2(\Omega)} + \|F_I^k\|_{L^2(\Omega)} + \|F_P^k\|_{L^2(\Omega)})\|P\|_{L^2(\Omega)} \\
&+ C\rho_M^2\lambda_M\|\nabla P\|_{L^2(\Omega)},
\end{aligned} \tag{5.64}$$

where $C = C(k_M, |\Omega|)$ is a constant. Therefore, by an application of the Poincaré inequality it follows that

$$\|P\|_{H^1(\Omega)} \le C \tag{5.65}$$

where C is independent of $\bar{S}, \bar{P}$. Now, since P is known, (5.63) is an elliptic equation for S whose solution exists by the Lax-Milgram lemma.
From (5.63) by setting $\psi = S$ one obtains

$$\begin{aligned}
\int_\Omega A^\eta \mathbb{K}\nabla S \cdot \nabla S dx \le{}& \int_\Omega \rho_g^\eta(Z(\overline{S}), P) S^{*,k} F_I^k |S| dx + \int_\Omega \rho_g^\eta(Z(\overline{S}), P) f_g(Z(\overline{S}), P) F_P^k |S| \, dx + \\
&+ \frac{1}{h}\int_\Omega \Phi(\rho_g^\eta(Z(\overline{S}), P) Z(\overline{S}) + \rho_g^\eta(S^{k-1}, P^{k-1}) S^{k-1}) |S| \, dx + \\
&+ \int_\Omega \lambda_g(Z(\overline{S})) \rho_g^\eta(Z(\overline{S}), P)^2 |\mathbb{K}\mathbf{g} \cdot \nabla S| \, dx + \int_\Omega \Lambda_g^\eta(Z(\overline{S}), P) |\mathbb{K}\nabla P \cdot \nabla S| \, dx \\
&\le \rho_M \int_\Omega F_I^k |S| \, dx + \rho_M \int_\Omega F_P^k |S| \, dx + \frac{2\rho_M}{h} \int_\Omega \Phi |S| \, dx \\
&+ \lambda_M \rho_M k_M g \int_\Omega |\nabla S| \, dx + \rho_M \lambda_M \omega_M k_M \int_\Omega |\nabla P \cdot \nabla S| \, dx
\end{aligned}$$

and then using inequality $A^\eta = A^\eta(Z(\overline{S}), P) \ge \eta$ the estimate follows:

$$\begin{aligned}
k_m \eta \int_\Omega |\nabla S|^2 \, d\mathbf{x} \le{}& 2\rho_M (1 + \frac{1}{h})(\|\Phi\|_{L^2(\Omega)} + \|F_I^k\|_{L^2(\Omega)} + \|F_P^k\|_{L^2(\Omega)}) \|S\|_{L^2(\Omega)} \\
&+ \rho_M \lambda_M k_M (g|\Omega|^{1/2} + \omega_M \|\nabla P\|_{L^2(\Omega)}) \|\nabla S\|_{L^2(\Omega)},
\end{aligned} \tag{5.66}$$

and therefore, using the Poincaré inequality,

$$\|S\|_{H^1(\Omega)} \le C \tag{5.67}$$

with C is independent of $\bar{S}, \bar{P}$.

The application $\mathcal{T}\colon L^2(\Omega) \times L^2(\Omega) \to L^2(\Omega) \times L^2(\Omega)$ is well defined and maps $L^2(\Omega) \times L^2(\Omega)$ to a bounded set in $H^1(\Omega) \times H^1(\Omega)$, which is relatively compact in $L^2(\Omega) \times L^2(\Omega)$. From the uniform estimates (5.65) and (5.67) one can find a ball in $L^2(\Omega) \times L^2(\Omega)$ which $\mathcal{T}$ maps to itself. In order to apply the Schauder theorem, it remains to show the continuity of the map $\mathcal{T}$. To this end, let $(\overline{S}_i, \overline{P}_i)$ be a sequence in $L^2(\Omega) \times L^2(\Omega)$ which converges strongly to $(\overline{S}, \overline{P})$. Let $(S_i, P_i) = \mathcal{T}(\overline{S}_i, \overline{P}_i)$, then, up to a subsequence, one has when

$i \to \infty$

$$S_i \rightharpoonup S \quad \text{weakly in } V, \text{ strongly in } L^2(\Omega) \text{ and a.e. in } \Omega, \tag{5.68}$$

$$P_i \rightharpoonup P \quad \text{weakly in } V, \text{ strongly in } L^2(\Omega) \text{ and a.e. in } \Omega, \tag{5.69}$$

$$Z(\overline{S}_i) \to Z(\overline{S}) \quad \text{strongly in } L^2(\Omega) \text{ and a.e. in } \Omega. \tag{5.70}$$

One can pass to the limit in (5.62) and (5.63) using boundedness of the coefficients and the Lebesgue theorem, giving $(S,P) = \mathcal{T}(\overline{S},\overline{P})$, which proves the continuity of the map since the limit (S,P) is unique. Schauder's theorem now can be applied, which gives the existence of a fixed point of $\mathcal{T}$. The existence of a solution to (5.57), (5.58) is then achieved if one proves that $0 \leq S \leq 1$ a.e. in Ω. In order to show the boundedness of S, put $\psi = S^- = \min(S,0) \in V$ in (5.63). Note that $\psi \neq 0$ only if $S < 0$. Therefore, all terms containing factors $Z(S)$, $\Lambda_g^\eta(Z(S),P)$, $\lambda_g(Z(S))$ and $f_g(Z(S),P)$ (which are zero for $S \leq 0$) cancel:

$$\begin{aligned}\int_\Omega A^\eta(0,P)\mathbb{K}\nabla S^- \cdot \nabla S^- dx = &\int_\Omega \rho_g^\eta(0,P) S^{*,k} F_I^k S^- dx \\ &+ \frac{1}{h}\int_\Omega \Phi \rho_g^\eta(S^{k-1},P^{k-1}) S^{k-1} S^- dx \leq 0.\end{aligned}$$

Therefore,

$$\int_\Omega |\nabla S^-|^2 \, dx \leq 0$$

and it follows that $S^- = 0$, that is $S \geq 0$.

In order to show the boundedness of $S \leq 1$ put $\phi = (S-1)^+ = \max(S-1,0) \in V$ in the equation for the water phase, obtained by subtracting (5.62) and (5.63). Note that $\phi \neq 0$ only if $S > 1$. Therefore, all terms containing factors $1 - Z(S)$, $\Lambda_w^\eta(Z(S),P)$, $\lambda_w(Z(S))$ and $f_w(Z(S),P)$ (which are zero for $S \geq 1$) cancel:

$$\begin{aligned}-\int_\Omega A^\eta(1,p)\mathbb{K}\nabla(S-1)^+ \cdot \nabla(S-1)^+ dx = &\int_\Omega \rho_w^\eta(1,P)(1-S^{*,k})F_I^k (S-1)^+ dx + \\ &+ \frac{1}{h}\int_\Omega \Phi \rho_w^\eta(S^{k-1},P^{k-1})(1-S^{k-1})(S-1)^+ dx \geq 0.\end{aligned}$$

Therefore,

$$\int_\Omega |\nabla(S-1)^+|^2 \, dx \leq 0$$

and it follows that $(S-1)^+$ is constant and since it is zero on Γ_{in} one obtains $(S-1)^+ = 0$, that is $S \leq 1$. $\square$

5.3.2 Step 2. Uniform Estimates with Respect to h

Uniform estimates will be obtained using the following test functions introduced in [44] and used in [48]:

$$\varphi = G_g(P_g^{\eta,k}) = \int_{P_c(0)}^{P_g^{\eta,k}} \frac{1}{\rho_g(z)} dz, \quad \psi = G_w(P_w^{\eta,k}) = \int_0^{P_w^{\eta,k}} \frac{1}{\rho_w(z)} dz, \tag{5.71}$$

where $P_g^{\eta,k} = P_g^\eta(S^k, P^k)$ and $P_w^{\eta,k} = P_w^\eta(S^k, P^k)$; P_g^η and P_w^η are defined in (5.25) and (5.26). A special care will be taken to make the dependence on η explicit.

Note that if $P = S = 0$, then $P_g^{\eta,k} = P_c(0)$, $P_w^{\eta,k} = 0$ and therefore $G_g(P_g^{\eta,k})$, $G_w(P_w^{\eta,k})$ are admissible test functions. After setting $\varphi = G_w(P_w^{\eta,k})$ in (5.59) and $\psi = G_g(P_g^{\eta,k})$ in (5.60) the two equations are summed. First the terms with discrete time derivative will be estimated, namely

$$\begin{aligned} &\int_\Omega \Phi\big[\rho_w(P_w^{\eta,k})(1-S^k) - \rho_w(P_w^{\eta,k-1})(1-S^{k-1})\big] G_w(P_w^{\eta,k}) dx \\ &+ \int_\Omega \Phi\big[\rho_g(P_g^{\eta,k})S^k - \rho_g(P_g^{\eta,k-1})S^{k-1}\big] G_g(P_g^{\eta,k}) dx. \end{aligned} \tag{5.72}$$

If the function under the integrals in (5.72) is denoted by ΦX one can write (the superscript η is dropped for simplicity of notation)

$$\begin{aligned} X =& \rho_w(P_w^k) G_w(P_w^k)(1-S^k) + \rho_g(P_g^k) G_g(P_g^k) S^k \\ &- \rho_w(P_w^{k-1}) G_w(P_w^{k-1})(1-S^{k-1}) - \rho_g(P_g^{k-1}) G_g(P_g^{k-1}) S^{k-1} \\ &+ \rho_w(P_w^{k-1})[G_w(P_w^{k-1}) - G_w(P_w^k)](1-S^{k-1}) + \rho_g(P_g^{k-1})[G_g(P_g^{k-1}) - G_g(P_g^k)] S^{k-1}. \end{aligned}$$

Using the fact that $z \mapsto \rho_\alpha(z)$, $\alpha = w, g$, are increasing functions, one obtains

$$G_w(P_w^{k-1}) - G_w(P_w^k) = \int_{P_w^k}^{P_w^{k-1}} \frac{1}{\rho_w(z)} dz \geq \frac{1}{\rho_w(P_w^{k-1})}(P_w^{k-1} - P_w^k),$$

and similarly for $G_g(P_g)$. Therefore,

$$\begin{aligned}X \geq &\rho_w(P_w^k)G_w(P_w^k)(1-S^k)+\rho_g(P_g^k)G_g(P_g^k)S^k-(1-S^k)P_w^k-S^kP_g^k\\&-\big[\rho_w(P_w^{k-1})G_w(P_w^{k-1})(1-S^{k-1})+\rho_g(P_g^{k-1})G_g(P_g^{k-1})S^{k-1}-(1-S^{k-1})P_w^{k-1}\\&-S^{k-1}P_g^{k-1}\big]+(S^k-S^{k-1})(P_g^k-P_w^k).\end{aligned}$$

Again, using the monotonicity of the capillary pressure,

$$(S^k-S^{k-1})(P_g^k-P_w^k)=(S^k-S^{k-1})P_c^\eta(S^k)\geq\int_0^{S^k}P_c^\eta(z)dz-\int_0^{S^{k-1}}P_c^\eta(z)dz.$$

it follows that

$$X\geq\mathcal{H}^\eta(S^k,P^k)-\mathcal{H}^\eta(S^{k-1},P^{k-1}) \tag{5.73}$$

where

$$\mathcal{H}^\eta(S,P)=\big[\rho_w(P_w^\eta)G_w(P_w^\eta)-P_w^\eta\big](1-S)+\big[\rho_g(P_g^\eta)G_g(P_g^\eta)-P_g^\eta\big]S+\int_0^S P_c^\eta(z)dz.$$

From the monotonicity of the mass densities one finds

$$\mathcal{H}^\eta(S,P)\geq 0. \tag{5.74}$$

With the estimate (5.73) the sum of equations (5.59) and (5.60) can be written, with test functions $\varphi=G_w(P_w^{\eta,k})$ and $\psi=G_g(P_g^{\eta,k})$, as

$$\begin{aligned}&\frac{1}{h}\int_\Omega\Phi(\mathcal{H}^\eta(S^k,P^k)-\mathcal{H}^\eta(S^{k-1},P^{k-1}))dx\\&\quad+\int_\Omega\frac{1}{\rho_w(P_w^{\eta,k})}[\Lambda_w^\eta(S^k,P^k)\mathbb{K}\nabla P^k-A^\eta(S^k,P^k)\mathbb{K}\nabla S^k]\cdot\nabla P_w^{\eta,k}dx\\&\quad+\int_\Omega\frac{1}{\rho_g(P_g^{\eta,k})}[\Lambda_g^\eta(S^k,P^k)\mathbb{K}\nabla P^k+A^\eta(S^k,P^k)\mathbb{K}\nabla S^k]\cdot\nabla P_g^{\eta,k}dx\\&\quad\leq\int_\Omega[\lambda_w(S^k)\rho_w(P_w^{\eta,k})\mathbb{K}\mathbf{g}\cdot\nabla P_w^{\eta,k}+\lambda_g(S^k)\rho_g(P_g^{\eta,k})\mathbb{K}\mathbf{g}\cdot\nabla P_g^{\eta,k}]dx\\&\quad-\int_\Omega[\rho_w(P_w^{\eta,k})f_w(S^k,P^k)F_P^kG_w(P_w^{\eta,k})+\rho_g(P_g^{\eta,k})f_g(S^k,P^k)F_P^kG_g(P_g^{\eta,k})]dx\\&\quad+\int_\Omega(\rho_w(P_w^{\eta,k})(1-S^{*,k})F_I^kG_w(P_w^{\eta,k})+\rho_g(P_g^{\eta,k})S^{*,k}F_I^kG_g(P_g^{\eta,k}))dx.\end{aligned} \tag{5.75}$$

The integrals in (5.75) are denoted by X_1, X_2,…,X_6 respectively. Using (5.37) in X_2 it follows

$$\begin{aligned}
X_2 &= \int_\Omega \frac{1}{\rho_w(P_w^{\eta,k})}[\lambda_w(S^k)\rho_w(S^k,P^k)\mathbb{K}\nabla P_w^{\eta,k} - \eta\mathbb{K}\nabla S^k]\cdot\nabla P_w^{\eta,k}dx \\
&= \int_\Omega \frac{1}{\rho_w(P_w^{\eta,k})}\big[\lambda_w(S^k)\rho_w(S^k,P^k)\mathbb{K}\nabla P_w^{\eta,k}\cdot\nabla P_w^{\eta,k} \\
&\quad + \eta f_g(S^k,P^k)R_\eta(P_c'(S^k))\mathbb{K}\nabla S^k\cdot\nabla S^k\big]dx - \eta\int_\Omega \frac{\omega^\eta(S^k,P^k)}{\rho_w(P_w^{\eta,k})}\mathbb{K}\nabla S^k\cdot\nabla P^k dx.
\end{aligned}$$

Using (A.2), (A.3), (A.4) and (A.6) the following estimate is obtained:

$$\begin{aligned}
X_2 \geq{}& \frac{1}{\rho_M}\int_\Omega \lambda_w(S^k)\rho_w(S^k,P^k)\mathbb{K}\nabla P_w^{\eta,k}\cdot\nabla P_w^{\eta,k}\,dx + \eta\frac{k_m p_{c,min}}{2\rho_M}\int_\Omega f_g(S^k,P^k)|\nabla S^k|^2dx \\
&- \eta\frac{\omega_M k_M}{\rho_m}\int_\Omega |\nabla P^k|\,|\nabla S^k|\,dx.
\end{aligned}$$

Using (5.38) the third integral X_3 is treated in the same way, leading to the estimate:

$$\begin{aligned}
X_3 \geq{}& \frac{1}{\rho_M}\int_\Omega \lambda_g(S^k)\rho_g(S^k,P^k)\mathbb{K}\nabla P_g^{\eta,k}\cdot\nabla P_g^{\eta,k}\,dx + \eta\frac{k_m p_{c,min}}{2\rho_M}\int_\Omega f_w(S^k,P^k)|\nabla S^k|^2dx \\
&- \eta\frac{\omega_M k_M}{\rho_m}\int_\Omega |\nabla P^k|\,|\nabla S^k|\,dx
\end{aligned}$$

After summing X_2 and X_3 and using (5.40) one gets

$$\begin{aligned}
X_2 + X_3 \geq{}& \frac{\lambda_m}{\rho_M}\rho_m\omega_m^2 k_m\int_\Omega |\nabla P^k|^2\,dx + \frac{\rho_m^2}{\lambda_M\rho_M^2}k_m\int_\Omega |\nabla\beta^\eta(S^k)|^2\,dx \\
&+ \eta\frac{k_m p_{c,min}}{2\rho_M}\int_\Omega |\nabla S^k|^2dx - 2\eta\frac{\omega_M k_M}{\rho_m}\int_\Omega |\nabla P^k|\,|\nabla S^k|\,dx,
\end{aligned}$$

and therefore one can find constant η_0 and C_1, C_2 independent of η, such that for all $0 < \eta \leq \eta_0$,

$$X_2 + X_3 \geq C_1(\int_\Omega |\nabla P^k|^2\,dx + \int_\Omega |\nabla\beta^\eta(S^k)|^2\,dx) + \eta C_2\int_\Omega |\nabla S^k|^2dx.$$

To estimate X_4, (5.28) and (5.29) are used to get

$$\begin{aligned}|X_4| = \Big| \int_\Omega &[\lambda_w(S^k)\rho_w(P_w^{\eta,k})\mathbb{K}\mathbf{g}\cdot(\omega^\eta(S^k,P^k)\nabla P^k - f_g(S^k,P^k)R_\eta(P_c'(S^k))\nabla S^k) \\ &+ \lambda_g(S^k)\rho_g(P_g^{\eta,k})\mathbb{K}\mathbf{g}\cdot(\omega^k(S^k,P^k)\nabla P^k + f_w(S^k,P^k)R_\eta(P_c'(S^k))\nabla S^k)]dx\Big| \\ \le \lambda_M\rho_M k_M|\mathbf{g}|\omega_M &\int_\Omega |\nabla P^k|dx + \frac{\rho_M^2\lambda_M}{\lambda_m\rho_m}k_M|\mathbf{g}|\int_\Omega |\nabla\beta^\eta(S^k)|dx.\end{aligned}$$

To estimate X_5 and X_6, the superlinearity of the function $P_\alpha^\eta \mapsto G_\alpha(P_\alpha^\eta)$ and Lemma 5.3 is used which give the following estimates, uniform with respect to η, for $\alpha \in \{w,g\}$,

$$\begin{aligned}|G_g(P_g^\eta)| \le \frac{C_4}{\rho_m}(|P|+1), \quad |G_w(P_w^\eta)| \le \frac{1}{\rho_m}(|P| + p_{c,max}^\eta) \\ |\lambda_w(S)P_w^\eta(S,P)| \le C_3(|P|+1), \quad |P_g^\eta(S,P)| \le M(|P|+1).\end{aligned} \tag{5.76}$$

It follows that

$$\begin{aligned}|X_5| + |X_6| \le& \frac{\rho_M^2}{\lambda_m\rho_m^2}\int_\Omega F_P^k(\lambda_w(S^k)|P_w^{\eta,k}| + \lambda_m|P_g^{\eta,k} - P_c(0)|)dx \\ &+ \frac{\rho_M}{\rho_m}\int_\Omega (\|1 - S^{*,k}\|_{L^\infty(\Omega)}F_I^k|P_w^{\eta,k}| + F_I^k|P_g^{\eta,k} - P_c(0)|)dx \\ \le& \frac{\rho_M^2}{\lambda_m\rho_m^2}(C_3 + \lambda_m C_4)\int_\Omega F_P^k(|P^k|+1)dx + \frac{\rho_M}{\rho_m}C_4\int_\Omega F_I^k(|P^k|+1)dx \\ &+ \frac{\rho_M}{\rho_m}\|1 - S^{*,k}\|_{L^\infty(\Omega)}\int_\Omega F_I^k(|P^k| + p_{c,max}^\eta)dx,\end{aligned}$$

which can be written as

$$|X_5| + |X_6| \le (C_5 + C_{6,\eta})\int_\Omega (|F_I^k| + |F_P^k|)(|P^k|+1)dx,$$

where $C_{6,\eta}$ depends on η through $p_{c,max}^\eta$. Using estimates of all terms $X_2,\ldots,X_6$, it is obtained

$$\begin{aligned}\frac{1}{h}\int_\Omega &\Phi(\mathcal{H}^\eta(S^k,P^k) - \mathcal{H}^\eta(S^{k-1},P^{k-1}))dx \\ &+ C_1\int_\Omega (|\nabla P^k|^2 + |\nabla\beta^\eta(S^k)|^2)\,dx + \eta C_2\int_\Omega |\nabla S^k|^2dx \\ &\le C_7\int_\Omega (|\nabla P^k| + |\nabla\beta^\eta(S^k)|)\,dx + (C_5 + C_{6,\eta})\int_\Omega (|F_I^k| + |F_P^k|)(|P^k|+1)dx\end{aligned}$$

where the coefficients C_1, C_2, C_5, C_7 and $C_{6,\eta}$ do not depend on h. All of them, except $C_{6,\eta}$, are also independent of η and it follows $C_{6,\eta} = 0$ if $S^* = 1$ is taken. Using the Hölder inequality, multiplying by h and summing from 1 to N one finally gets

$$\begin{aligned}\int_\Omega \Phi\mathcal{H}^\eta(S^h, P^h)(T)dx + \int_{Q_T} (|\nabla P^h|^2 + |\nabla\beta^\eta(S^h)|^2)\, dxdt + \eta \int_{Q_T} |\nabla S^h|^2 dxdt \\ \leq C \int_{Q_T} (|F_I|^2 + |F_P|^2 + 1) dxdt + \int_\Omega \Phi\mathcal{H}^\eta(s^0, p^0)dx,\end{aligned} \tag{5.77}$$

where again the constant C is independent of h, and independent of η if $S^* = 1$. Using the estimates (5.76) and (5.43), it is easy to see that the last term in (5.77) is uniformly bounded with respect to η. The following result has been proved:

Proposition 5.2. *Under the assumptions of Proposition 5.1 the sequences $(P^h)_h$ and $(S^h)_h$ of solutions to problem (5.57), (5.58) satisfy the following uniform bounds with respect to h:*

$$(P^h)_h \text{ is uniformly bounded in } L^2(0, T; V), \tag{5.78}$$

$$(S^h)_h \text{ is uniformly bounded in } L^2(0, T; V), \tag{5.79}$$

$$(\beta^\eta(S^h))_h \text{ is uniformly bounded in } L^2(0, T; V). \tag{5.80}$$

The following funtions are introduced:

$$r_w^k = \rho_w(P_w^\eta(P^k, S^k))(1 - S^k), \quad r_g^k = \rho_g(P_g^\eta(P^k, S^k))S^k,$$

and corresponding piecewise constant time dependent functions which will be denoted by r_w^h and r_g^h, respectively. By $\tilde{r}_w^h$ and $\tilde{r}_g^h$ are denoted the corresponding piecewise linear time dependent functions defined as in (5.56).

The following estimates follows:

Proposition 5.3. *Under the assumptions of Proposition 5.1 the following bounds, uniform with respect to h are valid:*

$$(r_\alpha^h)_h \text{ is uniformly bounded in } L^2(0, T; H^1(\Omega)),\ \alpha \in \{w, g\}, \tag{5.81}$$

$$(\tilde{r}_\alpha^h)_h \text{ is uniformly bounded in } L^2(0, T; H^1(\Omega)),\ \alpha \in \{w, g\}, \tag{5.82}$$

$$(\Phi\partial_t\tilde{r}_\alpha^h)_h \text{ is uniformly bounded in } L^2(0, T; V'),\ \alpha \in \{w, g\}. \tag{5.83}$$

Proof. First note that the functions r_α^h and $\tilde{r}_\alpha^h$ are uniformly bounded in $L^\infty(Q_T)$. For gradients it follows

$$\begin{aligned}\nabla r_w^h &= \sum_{k=1}^N \nabla(\rho_w(P_w^\eta(S^k,P^k))(1-S^k))\chi_{(t_{k-1},t_k]}(t)\\ &= \sum_{k=1}^N \rho_w'(P_w^\eta(S^k,P^k))(1-S^k)\nabla P_w^\eta(S^k,P^k)\chi_{(t_{k-1},t_k]}(t)\\ &- \sum_{k=1}^N \rho_w(P_w^\eta(S^k,P^k))\nabla S^k\chi_{(t_{k-1},t_k]}(t)\end{aligned}$$

and therefore

$$|\nabla r_w^h| \le C\sum_{k=1}^N |\nabla P_w^\eta(S^k,P^k)|\chi_{(t_{k-1},t_k]}(t) + C\sum_{k=1}^N |\nabla S^k|\chi_{(t_{k-1},t_k]}(t)$$

Using (5.27) one gets

$$|\nabla P_\alpha^\eta(S,P)| \le C|\nabla P| + C_\eta|\nabla S|$$

which gives

$$|\nabla r_w^h| \le C_\eta\sum_{k=1}^N(|\nabla P^k| + |\nabla S^k|)\chi_{(t_{n-1},t_n]}(t) = C_\eta(|\nabla P^h| + |\nabla S^h|),$$

and the same estimate holds for $|\nabla r_g^h|$. This proves (5.81). For (5.82), the proof is similar. From (5.57), for all $\varphi \in l_h(V)$ is valid

$$\begin{aligned}\int_0^T \langle\Phi\partial_t\tilde{r}_w^h,\varphi\rangle dt = &-\int_{Q_T}[\Lambda_w^\eta(S^h,P^h)\mathbb{K}\nabla P^h\cdot\nabla\varphi - A^\eta(S^h,P^h)\mathbb{K}\nabla S^h\cdot\nabla\varphi]dxdt\\ &+\int_{Q_T}[\lambda_w(S^h)\rho_w^\eta(S^h,P^h)^2\mathbb{K}\mathbf{g}\cdot\nabla\varphi - \rho_w^\eta(S^h,P^h)f_w(S^h,P^h)F_P\varphi]dxdt\\ &+\int_{Q_T}\rho_w^\eta(S^h,P^h)(1-S^{*,h})F_I\varphi dxdt.\end{aligned}$$

Using Proposition 5.2, the boundedness of the coefficients and the density of $l_h(V)$ in $L^2(0,T;V)$, one gets (5.83) for $\alpha = w$. For $\alpha = g$, the estimate is obtained using (5.58). □

5.3.3 Step 3. Passage to the Limit as $h \to 0$

Proposition 5.4. *Under the assumptions of Proposition 5.1 the following convergences for a subsequence, when h goes to zero are valid:*

$$\|r_\alpha^h - \tilde{r}_\alpha^h\|_{L^2(Q_T)} \to 0, \ \alpha \in \{w, g\}, \tag{5.84}$$

$$S^h \rightharpoonup S \text{ weakly in } L^2(0,T;V) \text{ and a.e. in } Q_T, \tag{5.85}$$

$$\beta^\eta(S^h) \rightharpoonup \beta^\eta(S) \text{ weakly in } L^2(0,T;V) \text{ and a.e. in } Q_T, \tag{5.86}$$

$$P^h \rightharpoonup P \text{ weakly in } L^2(0,T;V) \text{ and a.e. in } Q_T, \tag{5.87}$$

$$r_\alpha^h \to r_\alpha \text{ strongly in } L^2(Q_T), \ \alpha \in \{w, g\}, \tag{5.88}$$

Furthermore, $0 \le S \le 1$ *a.e. in* Q_T, $r_\alpha = \rho_\alpha(P_\alpha^\eta(S,P))S_\alpha$ *and*

$$\Phi\partial_t \tilde{r}_\alpha^h \rightharpoonup \Phi\partial_t(\rho_\alpha(P_\alpha^\eta(S,P))S_\alpha) \quad \text{weakly in } L^2(0,T;V'), \ \alpha \in \{w, g\}. \tag{5.89}$$

Proof. In order to prove (5.84), first note that by an easy calculation for any bounded function $\zeta = \zeta(x)$ id obtained

$$\|(r_\alpha^h - \tilde{r}_\alpha^h)\zeta\|_{L^2(Q_T)}^2 = \frac{h}{3}\sum_{k=1}^N \|(r_\alpha^k - r_\alpha^{k-1})\zeta\|_{L^2(\Omega)}^2.$$

The following test functions will be used: $\varphi = (r_w^k - r_w^{k-1})\zeta$ in (5.59) and $\psi = r_g^k - r_g^{k-1}$ in (5.60), where ζ is $C_0^1(\overline{\Omega})$ function, strictly positive in Ω, used to impose the boundary condition. From (5.59) one gets

$$\begin{aligned}
&\frac{1}{h}\int_\Omega \Phi(r_w^k - r_w^{k-1})^2\zeta dx \\
&\quad = -\int_\Omega [\Lambda_w^\eta(S^k,P^k)\mathbb{K}\nabla P^k - A^\eta(S^k,P^k)\mathbb{K}\nabla S^k]\cdot\nabla((r_w^k - r_w^{k-1})\zeta)dx \\
&\quad + \int_\Omega \big[\lambda_w(S^k)\rho_w^\eta(S^k,P^k)^2\mathbb{K}\mathbf{g}\cdot\nabla((r_w^k - r_w^{k-1})\zeta) \\
&\qquad\qquad - \rho_w^\eta(S^k,P^k)f_w(S^k,P^k)F_P^k(r_w^k - r_w^{k-1})\zeta\big]dx \\
&\quad + \int_\Omega \rho_w^\eta(S^k,P^k)(1 - S^{*,k})F_I^k(r_w^k - r_w^{k-1})\zeta dx.
\end{aligned}$$

The boundedness of the coefficients gives the following estimate,

$$\begin{aligned}\frac{\phi_m}{h}\int_\Omega (r_w^k - r_w^{k-1})^2\zeta dx &\leq C(1 + \|\nabla P^k\|_{L^2(\Omega)} + \|\nabla S^k\|_{L^2(\Omega)})\|\nabla((r_w^k - r_w^{k-1})\zeta)\|_{L^2(\Omega)} \\ &\quad + C(\|F_P^k\|_{L^2(\Omega)} + \|F_I^k\|_{L^2(\Omega)})\,\|(r_w^k - r_w^{k-1})\sqrt{\zeta}\|_{L^2(\Omega)}.\end{aligned}$$

This can further be estimated as

$$\begin{aligned}&\frac{\phi_m}{2h}\|(r_w^k - r_w^{k-1})\sqrt{\zeta}\|^2_{L^2(\Omega)} \\ &\leq C(1 + \|\nabla P^k\|_{L^2(\Omega)} + \|\nabla S^k\|_{L^2(\Omega)})(\|\nabla r_w^k\|_{L^2(\Omega)} + \|\nabla r_w^{k-1}\|_{L^2(\Omega)} + \|r_w^k - r_w^{k-1}\|_{L^2(\Omega)}) \\ &+ C(\|F_P^k\|^2_{L^2(\Omega)} + \|F_I^k\|^2_{L^2(\Omega)}).\end{aligned}$$

Multiplying by h and summing from 1 to N to obtain

$$\begin{aligned}\frac{\phi_m}{2}\sum_{k=1}^N \|(r_w^k - r_w^{k-1})\sqrt{\zeta}\|^2_{L^2(\Omega)} &\leq C\big(1 + \|\nabla P^h\|^2_{L^2(Q_T)} + \|\nabla S^h\|^2_{L^2(Q_T)} + 2\|\nabla r_w^h\|^2_{L^2(Q_T)} \\ &+ \|\nabla r_w^0\|^2_{L^2(\Omega)} + 2\|r_w^h\|^2_{L^2(Q_T)} + \|r_w^0\|^2_{L^2(\Omega)} + \|F_P^h\|^2_{L^2(Q_T)} + \|F_I^h\|^2_{L^2(Q_T)}\big).\end{aligned}$$

Using Proposition 5.2 and Proposition 5.3 one finds that

$$\sum_{k=1}^N \|(r_w^k - r_w^{k-1})\sqrt{\zeta}\|^2_{L^2(\Omega)} \leq C$$

with C independent of h, and therefore

$$\|(r_w^h - \tilde{r}_w^h)\sqrt{\zeta}\|_{L^2(Q_T)} \to 0 \text{ as } h \to 0.$$

Taking a subsequence, if necessary, one gets $(r_w^h - \tilde{r}_w^h)\sqrt{\zeta} \to 0$ a.e. in Q_T as $h \to 0$. Since ζ is strictly positive in Ω if follows $r_w^h - \tilde{r}_w^h \to 0$ a.e. in Q_T, and by Lebesgue's theorem $\|r_w^h - \tilde{r}_w^h\|_{L^2(Q_T)} \to 0$ as $h \to 0$. Now the wetting phase is treated similarly with $\zeta = 1$. This proves (5.84). From Proposition 5.2 the weak convergence of subsequences $(S^h)_h$ and $(P^h)_h$ is obtained.

Family $(\tilde{r}_\alpha^h)$ is bounded in $L^2(0,T;H^1(\Omega))$, while $\partial_t(\Phi\tilde{r}_\alpha^h)$ being bounded in $L^2(0,T;V')$. A small modification of a classical compactness result in [60] (see Lemma 5.4) gives that

$(\tilde{r}^h_\alpha)$ is relatively compact in $L^2(Q_T)$. Therefore, up to a subsequence, for $\alpha \in \{w, g\}$,

$$\tilde{r}^h_\alpha \to r_\alpha \text{ strongly in } L^2(Q_T) \text{ and a.e. in } Q_T.$$

Using (5.84) it follows

$$r^h_\alpha \to r_\alpha \text{ strongly in } L^2(Q_T) \text{ and a.e. in } Q_T.$$

By Lemma 5.2 and Remark 5.8 the mapping $(u, v) = G^\eta(S, P)$, defined by (5.41) has a continuous inverse $H^\eta \colon \mathcal{R} \to [0, 1] \times \mathbb{R}$. Therefore, from a.e. convergence in Q_T of $r^h_w = u^h = \rho_w(P^\eta_w(S^h, P^h))(1 - S^h)$ and $r^h_g = v^h = \rho_g(P^\eta_g(S^h, P^h))S^h$ one can conclude a.e. convergence in Q_T of S^h and P^h if shows that the measure of the set

$$E = \{(x, t) \in Q_T \colon (u^h(x, t), v^h(x, t)) \to (u, v) \in \overline{AB} \cup \overline{CD} = \overline{\mathcal{R}} \setminus \mathcal{R}\},$$

is zero ($\overline{AB}$ and $\overline{CD}$ are segments on $\partial\mathcal{R}$ denoted in Figure 5.2). But this follows from the fact that for $(x, t) \in E$ one has $|P^h(x, t)| \to +\infty$ and therefore

$$\int_{Q_T} |P^h(x, t)|^2 dxdt \geq \int_E |P^h(x, t)|^2 dxdt \to \infty$$

if $|E| > 0$. This is in contradiction with Proposition 5.2 and, as a consequence $|E| = 0$. The (5.85), (5.87) are proven, and (5.86) now follows. From pointwise convergence of S^h and P^h the limits r_α can be now identified as $r_w = \rho_w(P^\eta_w(P, S))(1 - S)$, and $r_g = \rho_g(P^\eta_g(P, S))S$. Finally, the weak limit in (5.89) exists because of the bound (5.83). □

Using the convergence results in Proposition 5.4 and the boundedness of all nonlinear coefficients, one can now pass to the limit as $h \to 0$ in the variational equations (5.57), (5.58) and find, for all $\varphi, \psi \in L^2(0, T; V)$

$$\begin{aligned}
&\int_0^T \langle \Phi \partial_t(\rho^\eta_w(S, P)(1 - S)), \varphi \rangle dt + \int_{Q_T} [\Lambda^\eta_w(S, P)\mathbb{K}\nabla P \cdot \nabla\varphi - A^\eta(S, P)\mathbb{K}\nabla S \cdot \nabla\varphi] dxdt \\
&\quad - \int_{Q_T} [\lambda_w(S)\rho^\eta_w(S, P)^2 \mathbb{K}\mathbf{g} \cdot \nabla\varphi - \rho^\eta_w(S, P) f_w(S, P) F_P \varphi] dxdt \\
&\quad = \int_{Q_T} \rho^\eta_w(S, P)(1 - S^*) F_I \varphi dxdt,
\end{aligned}$$

$$\begin{aligned}
&\int_0^T \langle \Phi\partial_t(\rho_g^\eta(S,P)S),\psi\rangle dt + \int_{Q_T}[\Lambda_g^\eta(S,P)\mathbb{K}\nabla P\cdot\nabla\psi + A^\eta(S,P)\mathbb{K}\nabla S\cdot\nabla\psi]dxdt\\
&\qquad - \int_{Q_T}[\lambda_g(S)\rho_g^\eta(S,P)^2\mathbb{K}\mathbf{g}\cdot\nabla\psi - \rho_g^\eta(S,P)f_g(S,P)F_P\psi]dxdt\\
&\qquad = \int_{Q_T}\rho_g^\eta(S,P)S^*F_I\psi dxdt.
\end{aligned}$$

From (A.1), $\rho_g(P_g^\eta(S,P))S, \rho_w(P_w^\eta(S,P))(1-S) \in L^2(0,T;H^1(\Omega))$ and $\partial_t(\Phi\rho_g(P_g^\eta(S,P))S)$, $\partial_t(\Phi\rho_w(P_w^\eta(S,P))(1-S)) \in L^2(0,T;V')$, it follows in a standard way that $\rho_g(P_g^\eta(S,P))S$, $\rho_w(P_w^\eta(S,P))(1-S) \in C([0,T];L^2(\Omega))$.

Using an integration by parts in the discrete and limit problems, with a test function of the form $\psi(x)\varphi(t)$, $\psi \in V$, $\varphi(0)=1$, $\varphi(T)=0$, w find

$$\int_0^T \langle \Phi\partial_t(\tilde{r}_\alpha^h),\psi\rangle\varphi(t)dt = -\int_{Q_T}\Phi\tilde{r}_\alpha^h\psi\varphi'(t)dxdt + \int_\Omega \Phi r_\alpha(s_0,p_0)\psi dx, \tag{5.90}$$

$$\int_0^T \langle \Phi\partial_t r_\alpha,\psi\rangle\varphi(t)dt = -\int_{Q_T}\Phi r_\alpha\psi\varphi'(t)dxdt + \int_\Omega \Phi r_\alpha(S,P)(0)\psi dx. \tag{5.91}$$

Passing to the limit as $h \to 0$ in (5.90) and subtracting from (5.91) one get for all $\psi \in V$,

$$\int_\Omega \Phi r_\alpha(S,P)(0)\psi dx = \int_\Omega \Phi r_\alpha(s_0,p_0)\psi dx.$$

Therefore, $r_\alpha(S,P)(0) = r_\alpha(s_0,p_0)$ for $\alpha \in \{w,g\}$ a.e. in Ω at $t=0$. This concludes the proof of Theorem 5.2.

5.4 Compactness Lemma

In this section a modification of a compactness result from [60] that is already used in subsection 5.3.3 and will be used in section 5.5 is going to be proved.

Lemma 5.4. *Let Ω be a bounded open set and $Q_T = \Omega\times]0,T[$. Let $(r^h)_{h>0}$ be a family of functions in $L^2(Q_T)$ and let $\Phi \in L^\infty(\Omega)$ be such that $0 < \phi_m \le \Phi(x) \le \phi_M < \infty$. Let $V \subset H^1(\Omega)$, dense in $L^2(\Omega)$ and $0 < \sigma \le 1$, $p \ge 2$. Assume that $(r^h)_{h>0}$ satisfy:*

- $(r^h)_{h>0}$ *is uniformly bounded in* $L^2(0,T;W^{\sigma,p}(\Omega))$*;*
- $(\partial_t(\Phi r^h))_{h>0}$ *is uniformly bounded in* $L^2(0,T;V')$*.*

Then $(r^h)_{h>0}$ *is relatively compact in* $L^2(Q_T)$*.*

The proof is based on the following simple modification of Lemma 8 in [60].

Lemma 5.5. *Let* Ω *be a bounded open set,* $\Phi \in L^\infty(\Omega)$ *be such that* $0 < \phi_m \leq \Phi(x) \leq \phi_M < \infty$*,* $V \subset H^1(\Omega)$*, dense in* $L^2(\Omega)$ *and* $0 < \sigma \leq 1$*,* $p \geq 2$*. Then*

$$\forall \eta > 0,\ \exists N,\ \forall v \in W^{\sigma,p}(\Omega), \quad \|v\|_{L^2(\Omega)} \leq \eta \|v\|_{W^{\sigma,p}(\Omega)} + N\|\Phi v\|_{V'}.$$

Proof. Note that $L^2(\Omega)$ is continuously embedded in V' and that $\|v\|_{L^2(\Omega)} \neq 0$ implies $\|\Phi v\|_{V'} \neq 0$. Set $V_n = \{v \in L^2(\Omega) \colon \|v\|_{L^2(\Omega)} < \eta + n\|\Phi v\|_{V'}\}$ is open in $L^2(\Omega)$ and grows when $n \to \infty$, such that $L^2(\Omega) = \cup_n V_n$. Due to the boundedness of Ω, the unit ball $S \subset W^{\sigma,p}(\Omega)$ is relatively compact in $L^2(\Omega)$ and therefore there exists N such that $S \subset V_N$. This yields

$$\|v\|_{L^2(\Omega)} \leq \eta \|v\|_{W^{\sigma,p}(\Omega)} + N\|\Phi v\|_{V'},$$

for $v \in S$, and by homogeneity for all $v \in W^{\sigma,p}(\Omega)$. $\square$

Proof. (Lemma 5.4) Note first that $(\Phi r^h)_{h>0}$ is compact in $L^2(0,T;V')$ by Theorem 3 (Corollary 1) in [60] since the embedding $L^2(\Omega) \subset V'$ is compact (as transpose of compact embedding $V \subset L^2(\Omega)$) and $(\Phi r^h)_{h>0}$ is bounded in $L^2(Q_T)$.

Then, given $\varepsilon > 0$ there exists a finite subset (r^{h_i}) such that for any r^h there exists h_i such that $\|\Phi r^h - \Phi r^{h_i}\|_{L^2(0,T;V')} < \varepsilon$. From Lemma 5.5 it follows

$$\begin{aligned} \|r^h - r^{h_i}\|_{L^2(0,T;L^2(\Omega))} &\leq \eta \|r^h - r^{h_i}\|_{L^2(0,T;W^{\sigma,p}(\Omega))} + N\|\Phi r^h - \Phi r^{h_i}\|_{L^2(0,T;V')} \\ &\leq \eta c + N\varepsilon, \end{aligned}$$

where c is the diameter of $(r^h)_{h>0}$ in $L^2(0,T;W^{\sigma,p}(\Omega))$. For given $\varepsilon' > 0$ take $\eta = \varepsilon'/2c$ and $\varepsilon = \varepsilon'/2N$, which gives $\|r^h - r^{h_i}\|_{L^2(0,T;L^2(\Omega))} \leq \varepsilon'$ and proves that $(r^h)_{h>0}$ is relatively compact in $L^2(Q_T)$. $\square$

5.5 Proof of Theorem 5.1

In this section the passage to the limit as $\eta \to 0$ in the regularized problem (5.54), (5.55) will be performed. The dependence of the regularized solution on the parameter η from now on will be denoted explicitly. In order to apply Theorem 5.2, the initial conditions s_0 and p_0 will be regularized with the regularization parameter η and by s_0^η and p_0^η regularized initial conditions are denoted. One may obviously assume that $s_0^\eta \to s_0$ and $p_0^\eta \to p_0$ in $L^2(\Omega)$ and a.e. in Ω when η tends to zero.

Lemma 5.6. *Let the sequence $(S^\eta, P^\eta)_\eta$ be defined by Theorem 5.2 for sufficiently small η, is set $P_\alpha^\eta = P_\alpha^\eta(S^\eta, P^\eta)$ and it is assumed $S^* = 1$. Then the following bounds uniform with respect to η hold true:*

$$(P^\eta)_\eta \ \text{ is uniformly bounded in } L^2(0,T;V), \tag{5.92}$$

$$(\beta^\eta(S^\eta))_\eta \ \text{ is uniformly bounded in } L^2(0,T;V), \tag{5.93}$$

$$(\sqrt{\eta}\nabla S^\eta)_\eta \ \text{ is uniformly bounded in } L^2(Q_T)^d, \tag{5.94}$$

$$(\Phi\partial_t(\rho_w(P_w^\eta)(1-S^\eta)))_\eta \text{ is uniformly bounded in } L^2(0,T;V'), \tag{5.95}$$

$$(\Phi\partial_t(\rho_g(P_g^\eta)S^\eta))_\eta \text{ is uniformly bounded in } L^2(0,T;V'). \tag{5.96}$$

Proof. Note that $S^* = 1$ implies that the estimate (5.77) is uniform with respect to η. Estimates (5.92), (5.93) and (5.94) then follow from (5.77) since weak lower semicontinuity of seminorms involved in (5.77) gives, after passage to limit as $h \to 0$,

$$\int_{Q_T} (|\nabla P^\eta|^2 + |\nabla \beta^\eta(S^\eta)|^2)\, dxdt + \eta \int_{Q_T} |\nabla S^\eta|^2 dxdt$$
$$\leq C \int_{Q_T} (|F_I|^2 + |F_P|^2 + 1) dxdt + \int_\Omega \Phi \mathcal{H}^\eta(s_0^\eta, p_0^\eta) dx.$$

As is already mentioned at the end of the proof of Proposition 5.2, the last integral in this estimate can be bounded, independently of η. For the last two estimates the equations

(5.54), (5.55) are used. For $\varphi \in L^2(0,T;V)$ is valid

$$|\int_0^T \langle \Phi\partial_t(\rho_w^\eta(S^\eta,P^\eta)(1-S^\eta)),\varphi\rangle dt| \leq |\int_{Q_T}[\lambda_w(S_w)\rho_w(S_w,p)\mathbb{K}\nabla P_w^\eta + \eta\mathbb{K}\nabla S]\cdot\nabla\varphi dxdt|$$
$$+|\int_{Q_T}[\lambda_w(S^\eta)\rho_w^\eta(S^\eta,P^\eta)^2\mathbb{K}\mathbf{g}\cdot\nabla\varphi - \rho_w^\eta(S^\eta,P^\eta)f_w(S^\eta,P^\eta)F_P\varphi]dxdt|.$$

Since (5.92) and (5.93) imply that $\sqrt{\lambda_\alpha(S^\eta)}\nabla P_\alpha^\eta$ is uniformly bounded in $L^2(Q_T)^d$ for $\alpha \in \{w,g\}$ it follows

$$|\int_0^T \langle \Phi\partial_t(\rho_w^\eta(S^\eta,P^\eta)(1-S^\eta)),\varphi\rangle dt| \leq C\|\varphi\|_{L^2(0,T;V)}.$$

This proves (5.95) and (5.96) is proved in the same way. □

Lemma 5.7. *(Compactness result in the degenerate case) For every $c > 0$ and for sufficiently small $\eta_0 > 0$ the following set*

$$\begin{aligned} E_c^{\eta_0} = \{&(\rho_w(P_w^\eta(S,P))(1-S), \rho_g(P_g^\eta(S,P))S) \colon 0 < \eta \leq \eta_0, \\ &\|P\|_{L^2(0,T;V)} \leq c, \quad \|\beta^\eta(S)\|_{L^2(0,T;V)} \leq c, \\ &\|\Phi\partial_t(\rho_w(P_w^\eta(S,P))(1-S))\|_{L^2(0,T;V')} + \|\Phi\partial_t(\rho_g(P_g^\eta(S,P))S)\|_{L^2(0,T;V')} \leq c\} \end{aligned}$$

is relatively compact in $L^2(Q_T) \times L^2(Q_T)$.

Proof. Recall that the inverse map of β is called $\mathcal{S}$ and also $\mathcal{S}^\eta = (\beta^\eta)^{-1}$. Let us introduce the map $G^\eta \colon [0,\beta^\eta(1)] \times \mathbb{R} \to \mathbb{R}^+ \times \mathbb{R}^+$, $(u^\eta, v^\eta) = G^\eta(\theta,P)$ by

$$u^\eta = \rho_w(P_w^\eta(S,P))(1-S), \quad v^\eta = \rho_g(P_g^\eta(S,P))S, \quad S = \mathcal{S}^\eta(\theta).$$

For $i = 1,2$ choose $\theta_i \in [0,\beta^\eta(1)]$, $P_i \in \mathbb{R}$ and set $S_i = \mathcal{S}^\eta(\theta_i)$. Assume $\theta_2 > \theta_1$ since the opposite case is treated in the same way. Now, it is valid that

$$\begin{aligned}
|v^\eta(\theta_1, P_1) - v^\eta(\theta_2, P_2)| &\leq |\rho_g(P_g^\eta(S_1, P_1))S_1 - \rho_g(P_g^\eta(S_1, P_2))S_1| \\
&+ |\rho_g(P_g^\eta(S_1, P_2))S_1 - \rho_g(P_g^\eta(S_2, P_2))S_1| \\
&+ |\rho_g(P_g^\eta(S_2, P_2))(S_1 - S_2)| \\
&\leq [\max_P \rho_g'(P) \max_P \omega^\eta(S_1, P) + 2 \max_P \rho_g(P)] \min(|P_1 - P_2|, 1) \\
&+ \max_P \rho_g'(P) \left| \int_{S_1}^{S_2} f_w(s, P_2) R_\eta(P_c'(s))\, ds \right| S_1 + \max_P \rho_g(P) |S_2 - S_1|.
\end{aligned}$$

For the term $X_1 = \left| \int_{S_1}^{S_2} f_w(s, P_2) R_\eta(P_c'(s)) ds \right| S_1$, in the case $S_1 < S_2$, it holds

$$X_1 \leq \frac{\rho_M}{\lambda_m \rho_m} S_1 \int_{S_1}^{S_2} \lambda_w(s) R_\eta(P_c'(s))\, ds.$$

Since $R_\eta(P_c'(S)) \leq P_c'(S)$ for $S > \eta$, for $S_2 > S_1 > S^\# > \eta$ it follows that

$$X_1 \leq \frac{\rho_M}{\lambda_m \rho_m} \int_{S_1}^{S_2} s \lambda_w(s) P_c'(s)\, ds \leq M_1 |S_1 - S_2|,$$

where the last inequality follows from boundedness of $\lambda_w(S) P_c'(S)$ on $\left[S^\#, 1\right[$ (see (A.4)). For $S_1 < S_2 \leq \eta$ can be obtained

$$\begin{aligned}
X_1 &\leq \frac{\rho_M \lambda_M}{\lambda_m \rho_m} S_1 \int_{S_1}^{S_2} R_\eta(P_c'(s)) ds \\
&\leq \frac{\rho_M \lambda_M}{\lambda_m \rho_m} 2S_1 \frac{P_c(\eta) - P_c(0)}{\eta} \int_{S_1}^{S_2} \left(1 - \frac{s}{\eta}\right) ds + \frac{\lambda_M \rho_M}{\rho_m \lambda_m} S_1 P_c'(\eta) \left| \int_{S_1}^{S_2} \left(2\frac{s}{\eta} - 1\right) ds \right| \\
&= 2 \frac{\lambda_M \rho_M}{\rho_m \lambda_m} S_1 \frac{P_c(\eta) - P_c(0)}{\eta} \left(S - \frac{S^2}{2\eta}\right) \Big|_{S_1}^{S_2} + \frac{\lambda_M \rho_M}{\rho_m \lambda_m} S_1 P_c'(\eta) \left| \left(\frac{S^2}{\eta} - S\right) \Big|_{S_1}^{S_2} \right| \\
&= \frac{\lambda_M \rho_M}{\lambda_m \rho_m} \left(2 \frac{P_c(\eta) - P_c(0)}{\eta} S_1 (S_2 - S_1) \left(1 - \frac{S_1 + S_2}{2\eta}\right) + S_1 (S_2 - S_1) P_c'(\eta) \left| \frac{S_2 + S_1}{\eta} - 1 \right| \right) \\
&\leq \frac{\rho_M \lambda_M}{\lambda_m \rho_m} S_1 (S_2 - S_1) [P_c'(\eta) + 2 \frac{P_c(\eta) - P_c(0)}{\eta}] \\
&\leq |S_2 - S_1|^\gamma [\eta^{2-\gamma} P_c'(\eta) + 2(P_c(\eta) - P_c(0))] \leq C |S_2 - S_1|^\gamma
\end{aligned}$$

where (A.5) is used. Finally, for $S \in]\eta, S^{\#}[$, using (5.15) in Remark 5.2 one obtains

$$X_1 \leq \frac{\rho_M \lambda_M}{\lambda_m \rho_m} S_1 \int_{S_1}^{S_2} P_c'(s) ds = \frac{\rho_M \lambda_M}{\lambda_m \rho_m} S_1 (P_c(S_2) - P_c(S_1)) \leq C|S_2 - S_1|^{\gamma}.$$

The estimates obtained so far give for any $0 < \tau < 1$

$$|v^\eta(\theta_1, P_1) - v^\eta(\theta_2, P_2)| \leq C(|P_2 - P_1|^{\tau\gamma} + |\mathcal{S}^\eta(\theta_2) - \mathcal{S}^\eta(\theta_1)|^{\gamma}),$$

where C is independent of η, and from Remark 5.7 it follows

$$|v^\eta(\theta_1, P_1) - v^\eta(\theta_2, P_2)| \leq C(|P_2 - P_1|^{\tau_1} + |\theta_2 - \theta_1|^{\tau_1}), \tag{5.97}$$

where $\tau_1 = \tau\gamma$ and the exponent τ is given in (A.8). For the function u^η assume $\theta_2 > \theta_1$. The opposite case is treated in the same way.

$$\begin{aligned} |u^\eta(\theta_2, P_2) - u^\eta(\theta_1, P_1)| \leq & |(\rho_w(P_w^\eta(S_2, P_2)) - \rho_w(P_w^\eta(S_2, P_1)))(1 - S_2)| \\ & + |(\rho_w(P_w^\eta(S_2, P_1)) - \rho_w(P_w^\eta(S_1, P_1)))(1 - S_2)| \\ & + |\rho_w(P_w^\eta(S_1, P_1))(S_2 - S_1)| \end{aligned}$$

This gives

$$\begin{aligned} |u^\eta(\theta_2, P_2) - u^\eta(\theta_1, P_1)| \leq & [\max_P \rho_w'(P) \max_P \omega^\eta(S_2, P) + 2 \max_P \rho_w(P)] \min(|P_2 - P_1|, 1) \\ & + \max_P \rho_w'(P) | \int_{S_1}^{S_2} f_g(s, P_1) R_\eta(P_c'(s))\, ds | (1 - S_2) \\ & + \max_P \rho_w(P) |S_2 - S_1|. \end{aligned}$$

In order to estimate the middle term, (5.16) is used. Since $R_\eta(P_c'(S)) \leq P_c'(S)$ for $S \geq S^{\#} > \eta$, for $S_2 > S_1 \geq S^{\#}$ is obtained

$$| \int_{S_1}^{S_2} f_g(s, P_1) R_\eta(P_c'(s))\, ds | (1 - S_2) \leq \frac{\rho_M \lambda_M}{\lambda_m \rho_m} (P_c(S_2) - P_c(S_1))(1 - S_2) \leq C_1 |S_2 - S_1|^{\gamma},$$

by (5.16). For all $S_1, S_2 \in [\eta, S^{\#}[$ it follows that

$$\left|\int_{S_1}^{S_2} \lambda_g(s) R_\eta(P_c'(s))\, ds\right| \le C|S_2 - S_1|,$$

for some constant C, since $\lambda_g(S)P_c'(S)$ is bounded in $]0, S^{\#}[$. For $S_1 < S_2 \le \eta$, where $R_\eta(P_c'(S))$ and $P_c'(S)$ are not the same, one has to consider only the case where $P_c'(S)$ has a singularity at $S = 0$. Then, in sufficiently small neighborhood of $S = 0$, $P_c''(S)$ must be negative and therefore $P_c'(\eta) \le (P_c(\eta) - P_c(0))/\eta$. Then it follows that

$$\begin{aligned}
|\int_{S_1}^{S_2} f_g(s, P_1) R_\eta(P_c'(s))\, ds| &\le \frac{\rho_M}{\lambda_m \rho_m}\lambda_g(\eta)\left|\int_{S_1}^{S_2} R_\eta(P_c'(s)) ds\right| \\
&\le \frac{\rho_M}{\lambda_m\rho_m}\lambda_g(\eta)\left(2\frac{P_c(\eta)-P_c(0)}{\eta}\int_{S_1}^{S_2}\left(1-\frac{s}{\eta}\right) ds + P_c'(\eta)\left|\int_{S_1}^{S_2}\left(2\frac{s}{\eta}-1\right) ds\right|\right) \\
&= \frac{\rho_M}{\lambda_m\rho_m}\lambda_g(\eta)\left(2\frac{P_c(\eta)-P_c(0)}{\eta}\left(s-\frac{s^2}{2\eta}\right)\Big|_{S_1}^{S_2} + \frac{P_c(\eta)-P_c(0)}{\eta}\left|\left(\frac{s^2}{\eta}-s\right)\Big|_{S_1}^{S_2}\right|\right) \\
&= \frac{\rho_M}{\rho_m\lambda_m}\lambda_g(\eta)\frac{P_c(\eta)-P_c(0)}{\eta}(S_2-S_1)\left(2\left(1-\frac{S_1+S_2}{2\eta}\right)+\left|\frac{S_1+S_2}{\eta}-1\right|\right) \\
&\le \frac{3\rho_M}{\lambda_m\rho_m}(S_2-S_1)\lambda_g(\eta)(P_c(\eta)-P_c(0))/\eta \\
&= \frac{3\rho_M}{\lambda_m\rho_m}\lambda_g(\eta)(S_2-S_1)^\gamma(S_2-S_1)^{1-\gamma}\eta^{-1}(P_c(\eta)-P_c(0)) \\
&\le C\lambda_g(\eta)(S_2-S_1)^\gamma\eta^{1-\gamma}\eta^{-1}(P_c(\eta)-P_c(0)) \\
&= C|S_2-S_1|^\gamma\eta^{-\gamma}\lambda_g(\eta)(P_c(\eta)-P_c(0)) \le C|S_2-S_1|^\gamma.
\end{aligned}$$

where in the last inequality (A.5) is used.Therefore, a constant C, independent of η can be found, such that for any $0 < \tau < 1$

$$|u^\eta(\theta_1, P_1) - u^\eta(\theta_2, P_2)| \le C(|P_2 - P_1|^\tau + |\mathcal{S}^\eta(\theta_2) - \mathcal{S}^\eta(\theta_1)|^\gamma),$$

and ((A.8)) and Remark 5.7 give for $\tau_1 = \gamma\tau$

$$|u^\eta(\theta_1, P_1) - u^\eta(\theta_2, P_2)| \le C(|P_2 - P_1|^{\tau_1} + |\theta_2 - \theta_1|^{\tau_1}). \tag{5.98}$$

Now, taking $0 < r < 1$ and using the Hölder continuity (5.97) and (5.98), one obtains for

$\sigma = r\tau_1$ and $p = 2/\tau_1$ (see [43] for details)

$$\begin{aligned}\|u^\eta\|_{L^p(0,T;W^{\sigma,p}(\Omega))} + \|v^\eta\|_{L^p(0,T;W^{\sigma,p}(\Omega))} \\ \leq C(\|P\|^{\tau_1}_{L^2(0,T;H^1(\Omega))} + \|\theta\|^{\tau_1}_{L^2(0,T;H^1(\Omega))} + 1).\end{aligned}$$

From the definition of the set E_c it follows that

$$\|u^\eta\|_{L^p(0,T;W^{\sigma,p}(\Omega))} + \|v^\eta\|_{L^p(0,T;W^{\sigma,p}(\Omega))} \leq C,$$

for some constant C. Applying Lemma 5.4 to (u^η) and (v^η) one gets that E_c is relatively compact in $L^2(Q_T) \times L^2(Q_T)$. □

Remark 5.9. *The compactness result in Lemma 5.7 can also be obtained in a "smaller" space, namely in* $L^2(0,T;W^{\tau',p}(\Omega))$, *for* $\tau' < r\tau_1$, $p = 2/\tau_1$.

Lemma 5.8. *(Strong and weak convergences) Up to subsequences the following convergence results hold for* $(\theta^\eta)_\eta$, $\theta^\eta = \beta^\eta(S^\eta)$ *and* $(P^\eta)_\eta$*:*

$$P^\eta \rightharpoonup P \quad \text{weakly in } L^2(0,T;V) \text{ and a.e. in } Q_T, \tag{5.99}$$

$$\theta^\eta \rightharpoonup \theta \quad \text{weakly in } L^2(0,T;V) \text{ and a.e. in } Q_T, \tag{5.100}$$

$$S^\eta \to \mathcal{S}(\theta) \quad \text{a.e. in } Q_T, \tag{5.101}$$

$$\begin{aligned}&\Phi\partial_t(\rho_w(P^\eta_w(S^\eta,P^\eta))(1-S^\eta)) \rightharpoonup \Phi\partial_t(\rho_w(P_w(\mathcal{S}(\theta),P))(1-\mathcal{S}(\theta))) \\ &\quad \text{weakly in } L^2(0,T;V')\end{aligned} \tag{5.102}$$

$$\Phi\partial_t(\rho_g(P^\eta_g(S^\eta,P^\eta))S^\eta) \rightharpoonup \Phi\partial_t(\rho_g(P_g(\mathcal{S}(\theta),P))\mathcal{S}(\theta)) \quad \text{weakly in } L^2(0,T;V'). \tag{5.103}$$

Moreover, $0 \leq \theta \leq \beta(1)$ *a.e. in* Q_T.

Proof. The uniform estimates (5.92) and (5.93) give the weak convergence results (5.99) and (5.100). Lemma 5.7 ensures, up to a subsequence, the following strong convergence results,

$$\begin{aligned}\rho_w(P^\eta_w(S^\eta,P^\eta))(1-S^\eta) \to r_w \quad &\text{in } L^2(Q_T) \text{ and a.e. in } Q_T \\ \rho_g(P^\eta_g(S^\eta,P^\eta))S^\eta \to r_g \quad &\text{in } L^2(Q_T) \text{ and a.e. in } Q_T.\end{aligned}$$

The following decomposition is used:

$$\begin{aligned}\rho_w(P_w^\eta(S^\eta, P^\eta))(1-S^\eta) &= (\rho_w(P_w^\eta(S^\eta, P^\eta)) - \rho_w(P_w(S^\eta, P^\eta)))(1-S^\eta)\\ &\quad + \rho_w(P_w(S^\eta, P^\eta))(1-S^\eta),\end{aligned}$$

and a similar one for $\rho_g(P_g^\eta(S^\eta, P^\eta))S^\eta$. From the uniform convergence in Lemma 5.3 it follows that

$$\begin{aligned}\rho_w(P_w(S^\eta, P^\eta))(1-S^\eta) &\to r_w \;\text{ in } L^2(Q_T) \text{ and a.e. in } Q_T\\ \rho_g(P_g(S^\eta, P^\eta))S^\eta &\to r_g \;\text{ in } L^2(Q_T) \text{ and a.e. in } Q_T.\end{aligned}$$

One can now prove, as in Proposition 5.4, that $P^\eta \to P$ and $S^\eta \to S$ a.e. in Q_T, where P is the weak limit in (5.99). Note also that $\theta^\eta = \beta^\eta(S^\eta) \to \beta(S)$ a.e. in Q_T due to the uniform convergence of $\beta^\eta \to \beta$ in Lemma 5.3. Now, from the weak convergence (5.100) this limit $\beta(S)$ is the same as the limit θ in (5.100).

Now the limits r_w and r_g can be identified and the convergence in (5.102) and (5.103) is a consequence of the bounds given in Lemma 5.6. □

Let us take a test function $\varphi \in C^1([0,T]; V)$ such that $\varphi(T) = 0$ and make integration by parts in (5.54). From (5.31), (5.5) and (5.36) if follows that

$$A^\eta(S^\eta, P^\eta)\nabla S^\eta = A(S^\eta, P^\eta)\nabla\beta^\eta(S^\eta) + \eta\nabla S^\eta,$$

and therefore

$$\begin{aligned}&-\int_{Q_T} \Phi\rho_w^\eta(S^\eta, P^\eta)(1-S^\eta)\partial_t\varphi dxdt\\ &\quad + \int_{Q_T} [\Lambda_w^\eta(S^\eta, P^\eta)\mathbb{K}\nabla P^\eta \cdot \nabla\varphi - A(S^\eta, P^\eta)\mathbb{K}\nabla\theta^\eta \cdot \nabla\varphi]dxdt\\ &\quad - \int_{Q_T} [\lambda_w(S^\eta)\rho_w^\eta(S^\eta, P^\eta)^2\mathbb{K}\mathbf{g} \cdot \nabla\varphi - \rho_w^\eta(S^\eta, P^\eta)f_w(S^\eta, P^\eta)F_P\varphi]dxdt\\ &\quad - \eta\int_{Q_T} \mathbb{K}\nabla S^\eta \cdot \nabla\varphi dxdt = \int_\Omega \Phi\rho_w^\eta(s_0^\eta, p_0^\eta)(1-s_0^\eta)\varphi(0)dx\end{aligned}$$

Pointwise convergence and boundedness of the coefficients allow to pass to the limit as $\eta \to 0$ in all nonlinear terms. The penalization term goes to zero because of (5.94) and all other coefficients converge due to pointwise convergence in Lemma 5.8 and uniform convergence in Lemma 5.3. Thus, it is valid that

$$
\begin{aligned}
-\int_{Q_T} \Phi\rho_w(S,P)(1-S)\partial_t\varphi dxdt + \int_{Q_T} [\Lambda_w(S,P)\mathbb{K}\nabla P\cdot\nabla\varphi - A(S,P)\mathbb{K}\nabla\theta\cdot\nabla\varphi]dxdt \\
-\int_{Q_T} [\lambda_w(S)\rho_w(S,P)^2\mathbb{K}\mathbf{g}\cdot\nabla\varphi - \rho_w(S,P)f_w(S,P)F_P\varphi]dxdt \\
= \int_\Omega \Phi\rho_w(s_0,p_0)(1-s_0)\varphi(0)dx
\end{aligned}
$$

where $S = \mathcal{S}(\theta)$. In the same way one gets for all $\psi \in C^1([0,T];V)$ such that $\psi(T) = 0$

$$
\begin{aligned}
-\int_{Q_T} \Phi\rho_g(S,P)S\partial_t\psi dt + \int_{Q_T} [\Lambda_g(S,P)\mathbb{K}\nabla P\cdot\nabla\psi + A(S,P)\mathbb{K}\nabla\theta\cdot\nabla\psi]dxdt \\
-\int_{Q_T} [\lambda_g(S)\rho_g(S,P)^2\mathbb{K}\mathbf{g}\cdot\nabla\psi - \rho_g(S,P)f_g(S,P)F_P\psi]dxdt \\
= \int_{Q_T} \rho_g(S,P)F_I\psi dxdt + \int_\Omega \Phi\rho_g(s_0,p_0)s_0\psi(0)dx
\end{aligned}
$$

Using the fact that the functions $\Phi\rho_g(S,P)S$ and $\Phi\rho_w(S,P)(1-S)$ belong to $C([0,T];V')$ and by an integration by parts, one easily concludes that the initial condition is satisfied in V'. This completes the proof of Theorem 5.1.

5.6 Conclusion

An existence result for the weak solutions of the coupled system under realistic assumptions on the data was established. The hypotheses required for some earlier results on immiscible compressible systems are weakened so that only physically relevant assumptions are made. In particular, the results cover the cases of a singular capillary pressure function, and discontinuous porosity and absolute permeability tensors.

Chapter 6

Conclusion

With the motivation of making the coupling of the derived equations (2.39)-(2.41) less strong, and giving the system a well defined mathematical structure, a new immiscible compressible two-phase flow model based on the concept of global pressure is introduced in this thesis. The system is written in a fractional flow formulation, which consists of a nonlinear parabolic equation (the global pressure equation) and a nonlinear diffusion-convection one (the wetting phase saturation equation). In order to make the problem solving more tractable, another model is discussed as well: a simplified fractional flow model. In this model, further simplifications are performed, so that the phase pressures are replaced by the global pressure in the calculation of the mass densities, where applicable. This model was introduced in [25], and, in this thesis, additional slight modifications are introduced into this model in order to make it more applicable.

A comparison between the fully equivalent model and the simplified model is made. The comparison reveals that the simplified model can be safely used in applications where mean field pressure is high, capillary pressure is low and the wetting phase is not highly compressible. This is the case in oil-gas systems, so the simplified model may be used for such systems. On the other hand, the analysis reveals that the simplification may not be appropriate for hydro-geological applications where capillary pressures are very high, like the numerical test case 2 presented in chapter 4.

The above conclusions are verified by means of numerical simulation performed for a simple heterogeneous one-dimensional test case where the wetting phase is an incompressible fluid. The simulation reveals that the difference in the phase pressures, in particular, in the new and the simplified model may be significant.

In order to validate the new model, it is tested on the numerical test cases [52], and the obtained results in the test case 2 are similar to those obtained by other authors [5,14]. This confirms that the model is applicable in the situations with high capillary pressures, and in highly heterogeneous porous media. Test case 3 shows its applicability in the simulations with initially fully saturated porous media by the wetting phase.

Furthermore, the existence result for the weak solutions of the coupled system under realistic assumptions on the data is established. While results on immiscible compressible systems already exist, the major difference of this work to the earlier results is that the required hypotheses are significantly weakened, so that only physically relevant assumptions are made. In particular, the presented results cover the cases of the singular capillary pressure function, and the discontinuous porosity and absolute permeability.

A suggestion for further work is to extend the existence results presented here towards porous media with several rock types. In these cases the capillary pressures and relative permeabilities curves are different in each type of porous media, which introduces nonlinear transmission conditions resulting from the continuity of the physical quantities at the interfaces separating different media. Another direction of suggested future research is extending the numerical simulation cases to higher dimensional problems.

Appendix A

Implementation of the Coefficients in the Two-phase Flow Model

In this appendix, the basic manipulations of the coefficient formulae in two different models are presented. Subsequently, an overview of the practical implementation of these coefficients is explained.

A.1 Coefficients in Fractional Flow Formulations

Before explaining the fractional flow coefficients implementation, one should be aware that they are obtained by algebraic manipulations of the following functions:

- Two-phase flow functions: capillary pressure ($P_c(S_w)$) and relative permeabilities ($kr_w(S_w)$, $kr_g(S_w)$).
- Fluid properties: μ_w, μ_g and $\rho_w(P_w), \rho_g(P_g)$, where the density of the phase α depends on its own pressure.

For the sake of simplicity, in this appendix coefficients are assumed to depend on wetting phase saturation. The coefficients entering the equations (2.39)-(2.41) can be written in the following general form:

$$\lambda_\alpha(S_w) = \frac{kr_\alpha(S_w)}{\mu_\alpha}, \quad \alpha = w, g \tag{A.1}$$

$$\lambda(S_w, P_g, P_w) = \rho_w(P_w)\lambda_w(S_w) + \rho_g(P_g)\lambda_g(S_w) \tag{A.2}$$

$$f_\alpha(S_w, P_g, P_w) = \frac{\rho_\alpha(P_\alpha)\lambda_\alpha(S_w)}{\lambda(S_w, P_g, P_w)}, \quad \alpha = w, g, \tag{A.3}$$

$$\rho(S_w, P_g, P_w) = \frac{(\lambda_w(S_w)\rho_w(P_w)^2 + \lambda_g(S_w)\rho_g(P_g)^2)}{\lambda(S_w, P_g, P_w)}, \tag{A.4}$$

$$\alpha(S_w, P_g, P_w) = \frac{\rho_w(P_w)\rho_g(P_g)\lambda_w(S_w)\lambda_g(S_w)}{\lambda(S_w, P_g, P_w)}, \tag{A.5}$$

$$b_g(S_w, P_g, P_w) = (\rho_w(P_w) - \rho_g(P_g))\alpha(S_w, P_g, P_w), \tag{A.6}$$

$$a(S_w, P_g, P_w) = -\alpha(S_w, P_g, P_w)P_c'(S_w) \tag{A.7}$$

Therefore, the coefficients in the (S_w, P_g) formulation given by the equations (2.39)-(2.41) are obtained by setting $P_w = P_g - P_c(S_w)$ in (A.1)-(A.7), and in that case they are assumed as functions dependent upon the variables S_w and P_g.

When the **fully equivalent fractional flow formulation**, introduced in the chapter 3, is used, the coefficients are calculated from (A.1)-(A.7) by setting $P_g = P_g(S_w, P)$ $P_w = P_w(S_w, P) = P_g(S_w, P) - P_c(S_w)$, where P is the global pressure. Naturally, here the formula for $P_g(S_w, P)$ needs to be provided, which can be obtained as a solution of the initial problem (3.14). Also, to complete the list of the coefficients entering the equations (3.23)–(3.25) one needs to know how to calculate the function $\omega(S_w, P)$, which is given by the equation (3.22).

When the **simplified fractional flow formulation** is used, it is assumed that the density of each phase depends on the global pressure, instead of its own phase pressure so when the calculation of the coefficients is done in the simplified model one needs to set $P_w = P_g = P$ in the coefficients (A.1)-(A.7). The function $\omega(S, P)$ is given by (3.45). After the equations are solved numerically, the calculation of the phase pressures is required. This can be performed by applying the numerical integration and using (3.30).

A.2 On the Implementation of the Coefficients

The coefficients are implemented as C++ classes, defined for each of the fractional flow formulations. Figure A.1 shows the classes UML diagram.

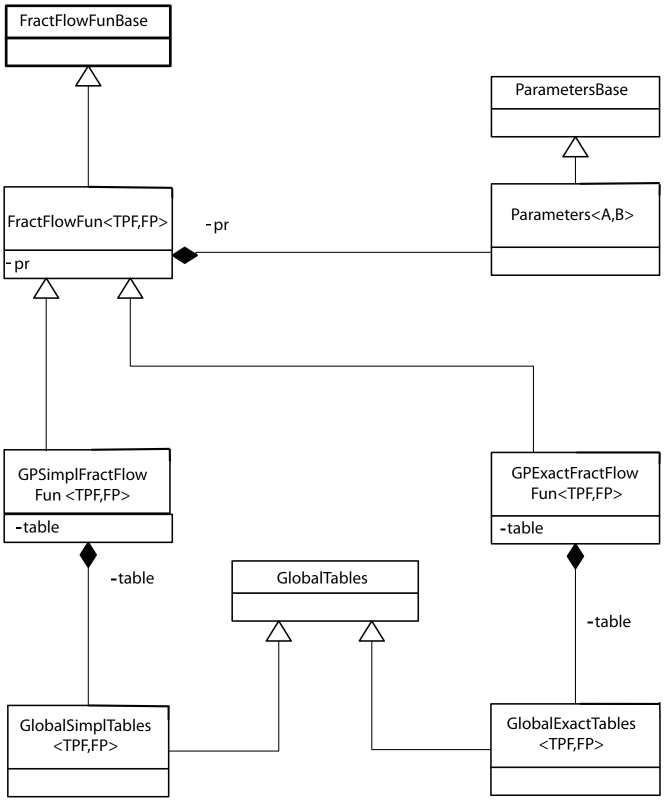


Figure A.1: UML diagram for the coefficients

The implementation is centered on the `FractFlowFunBase` class. This is the base class providing an interface for the two-phase flow (`TPF`) and fluid properties (`FP`) functions.

All the coefficients implementations take two arguments:

- Wetting phase saturation (that can be switched to capillary pressure)
- Pressure.

In this class, all the coefficients are defined as pure virtual functions.

The class `StaticFractFlowFun` is an auxiliary class used to implement formulae for the coefficients (A.1)-(A.7) and their partial derivatives as static functions. It is written as a template parametrized by the classes implementing `TPF` and `FP`. It contains all the coefficients, as the `FractFlowFunBase` class. For this class, note that the relevant functions had to be implemented as static, because of the requirements of GSL library [45] used in `GlobalExactTables` class.

The class `FractFlowFun` inherits the abstract class `FractFlowFunBase`. This class is implemented as a template parametrized by the `TPF` and `FP` classes. The pure virtual functions from the abstract `FractFlowFunBase` class are implemented here as virtual functions, depending on the wetting phase saturation and the nonwetting phase pressure as is presented in the formulae (2.33)-(2.37). These functions subsequently rely on the functions implemented in the classes `TPF`, `FP` and `StaticFractFlowFun`. So, the coefficient functions in the `FractFlowFun<TPF,FP>` class are implemented by calling the functions from `StaticFractFlowFun` class taking as arguments wetting phase saturation and the values of the virtual functions $\mathsf{P}_{\mathsf{n\_}}(\mathsf{S},\mathsf{P})$ and $\mathsf{P}_{\mathsf{w\_}}(\mathsf{S},\mathsf{P})$, which will be defined separately for each class inheriting the `FractFlowFun<TPF,FP>` class. In the class `FractFlowFun<TPF, FP>` is set to be

$$\mathsf{P}_{\mathsf{n\_}}(\mathsf{S},\mathsf{P}) = \mathsf{P} \tag{A.8}$$

$$\mathsf{P}_{\mathsf{w\_}}(\mathsf{S},\mathsf{P}) = \mathsf{P} - \mathsf{P}_{\mathsf{c}}(\mathsf{S}), \tag{A.9}$$

so, here the unknown P is assumed to be the gas pressure.

The class `FractFlowFun<TPF,FP>` also contains an object `pr` of the type `Parameters`. This object provides the parameters for the `TPF` and `FP` classes. As an example of the required parameters, van Genuchten's functions require parameters: `Pr`, `n`, residual saturation of wetting and nonwetting phase and the parameters for linearization of the capillary pressure. The task of the `Parameters` object is to store all the required parameters.

The `GPExactFractFlowFun<TPF,FP>` clas inherits the `FractFlowFun<TPF,FP>` class. This class implements the coefficients for the fully equivalent global pressure formulation. The following is set:

$$\mathsf{P}_{\mathsf{n\_}}(\mathsf{S},\mathsf{P}) = \mathsf{P}_{\mathsf{g}}(\mathsf{S},\mathsf{P}) \tag{A.10}$$

$$\mathsf{P}_{\mathsf{w\_}}(\mathsf{S},\mathsf{P}) = \mathsf{P}_{\mathsf{g}}(\mathsf{S},\mathsf{P}) - \mathsf{P}_{\mathsf{c}}(\mathsf{S}). \tag{A.11}$$

The nonwetting phase pressure $P_g(S,P)$ and the function $\omega(S,P)$ are calculated from the object `table` of the type `GlobalExactTables<TPF,FP>`.

The `GPSimplFractFlowFun<TPF,FP>` inherits the class `FractFlowFun<TPF,FP>` by setting:

$$\mathsf{P}_{\mathsf{n\_}}(\mathsf{S},\mathsf{P}) = \mathsf{P} \tag{A.12}$$

$$\mathsf{P}_{\mathsf{w\_}}(\mathsf{S},\mathsf{P}) = \mathsf{P}. \tag{A.13}$$

This class implements the coefficients for the simplified global pressure fractional flow formulation. The nonwetting phase pressure $P_g(S, P)$ and the function $\omega(S, P)$ are calculated from the object `table` of the type `GlobalSimplTables<TPF,FP>`.

The class `GlobalExactTables<TPF,FP>` implements a look-up table for the values of $P_g(S, P)$. For each value of the global pressure vector in a certain range (values ranging from P_{min} to P_{max}), $P_g(u, P)$ is calculated as a solution of the initial problem (3.15). The calculation is performed by using a GSL ODE solver. This class also provides a table of values for the function$\omega(S, P)$. The function $P_g(S, P)$ and $\omega(S, P)$ are calculated from the corresponding tables by linear interpolation.

The class `GlobalSimplTables<TPF,FP>` performs the equivalent task for the simplified coefficients case - it provides the calculation of $P_g(S, P)$. The difference is that, in this case, the tables are obtained by numerical integration.

The function of these two classes storing the tables is to calculate the required values only once at the beginning of each numerical simulation. When required in the later phase, the values are only looked up in the tables. For a large pressure range, this is obviously a very memory-intensive task.

The `TPF` classes contain relative permeabilities functions, capillary pressure and their derivatives. Currently, the implemented classes are `VanGenuchtenFun`, `BrooksCoreyFun`, `SimpleFun` $(kr_w(S_w) = S_w^2, kr_g(S_w) = (1 - S_w)^2, P_c(S_w) = Pr(1 - S_w))$. The variable in `TPF` class can be switched to the capillary pressure or the wetting phase saturation, so consequently all the coefficients can depend either on the wetting phase saturation or on the capillary pressure.

The examples of the `FP` classes are class `FluidCompress` which models densities as exponential functions, and `FluidCompInc` which models flow of water and gas (the density is given by the gas ideal law).

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Summary

In petroleum engineering and environmental engineering, many processes can be mathematically modelled as multiphase fluid flow in porous media. Carbon dioxide sequestration and long-term nuclear waste storage are examples of such processes.

This thesis studies immiscible compressible two-phase fluid flow in porous media. Such flows can be modelled by a set of partial differential equations. Multiple formulations and main variable selections are possible, and the choice of the formulation and the main variables strongly influences the PDEs system mathematical analysis and its solving by means of numerical methods.

In this thesis, a new formulation for modelling immiscible compressible two-phase flow in heterogeneous porous media is developed and studied. For each phase, the governing equations describing this type of flow are given by the mass balance law and Darcy-Muscat law. This original system of nonlinear evolutionary partial differential equations is transformed, using the concept of global pressure, to a system of PDEs which is more suitable for mathematical and numerical studies. The new model is fully equivalent to the starting one.

In order to make the problem solving more tractable, another model is discussed as well: a simplified model. In this model, further simplifications are performed where applicable: in the fractional flow formulations, phase pressures are replaced by the global pressure in the calculation of the mass densities. This model was introduced in [25], and an updated version is used in the scope of this thesis.

A numerical code based on the vertex centered finite volume method is developed. A comparison of the new model with the simplified fractional flow formulation is performed in two ways: by means of numerical simulations and by comparing the coefficients. The comparisons reveal that the simplified model can be used safely in applications where mean field pressure is high, capillary pressure is low and the wetting phase is not highly compressible.

In the presentation of the numerical simulations, a special attention is paid to the numerical treatment of highly heterogeneous media (multiple rock types) by the vertex centred finite volume method. The model is validated by numerical simulations on the benchmarks proposed by the French research group MoMaS. The benchmarks are related to the flow of water (incompressible) and gas such as hydrogen (compressible), concerning the gas migration through engineered and geological barriers for the deep repository of radioactive waste.

In the thesis, the existence result for the new formulation for two-phase compressible flow under realistic assumptions on the data is established. While earlier existence results on the existence of immiscible compressible systems are known, as in [44, 48], the major difference of the work presented to the earlier results is that the required hypotheses are significantly weakened, so that only physically relevant assumptions are made. In particular, the results presented cover the cases of a singular capillary pressure function, and the discontinuous porosity and absolute permeability tensors.

Sažetak

U naftnom inženjerstvu i ekoinženjerstvu česti su procesi koji se mogu matematički modelirati višefaznim protokom fluida kroz poroznu sredinu. Primjeri mogu biti procesi kod odlaganja nuklearnog otpada, podzemno spremanje ugljičnog dioksida i slično.

Doktorska disertacija razmatra dvofazni tok nemješivih kompresibilnih fluida u poroznoj sredini. Ovakav se tok modelira sustavom parcijalnih diferencijalnih jednadžbi, pri čemu je moguće više formulacija i odabira glavnih nepoznanica sustava. Odabir glavnih varijabli i formulacija sustava jednadžbi snažno utječe na matematičku analizu dobivenog problema i odabir numeričkih metoda za njegovo rješavanje.

U disertaciji se razmatra nova formulacija modela dvofaznog toka nemješivih kompresibilnih fluida u heterogenoj poroznoj sredini. Osnovne jednadžbe koje opisuju nemješivi višefazni tok proizlaze iz zakona očuvanja mase za svaku od faza te Darcy-Muscatovog zakona. Početni sustav nelinearnih evolucijskih jednadžbi transformira se pomoću koncepta globalnog tlaka. Cilj transformacija je postizanje bolje matematičke strukture sustava, pri čemu je nova formulacija potpuno ekvivalentna početnoj.

Nadalje, razmatra se pojednostavljena formulacija navedenog modela. U ovoj se formulaciji koristi aproksimacijska hipoteza da gustoće pojedinih fluida (faza) ovise o globalnom, a ne o faznom tlaku. Pojednostavljeni model zasnovan na konceptu globalnog tlaka uveden je u [25]. U ovoj disertaciji razmatra se izmijenjena inačica tog modela. Kako pojednostavljeni model predstavlja aproksimaciju originalne zadaće, primjena tako izvedenog modela je ograničena. U sklopu disertacije razmatra se primjenjivost pojednostavljenog modela.

U okviru izrade disertacije implementiran je i numerički kod baziran na metodi konačnih volumena s centrima u vrhovima mreže, te je u referentnom testu provedena usporedba nove i pojednostavljene formulacije. Usporedba pojednostavljene i nove formulacije provedena je na temelju koefcijenata jednadžbe i na temelju numeričke simulacije. Rezultati usporedbe otkrivaju kako se pojednostavljeni model može koristiti u primjenama gdje je srednji tlak visok, kapilarni tlak malen te vlažeća faza nije jako kompresibilna.

Prilikom numeričkih simulacija, poseban je naglasak stavljen na tretiranje heterogene porozne sredine s jakim kontrastima (porozna sredina sastavljena od više materijala) primjenom metode konačnih volumena s centrima u vrhovima mreže. Novi model provjeren je na referentnim testovima koje je predložila francuska istraživačka grupa MoMas. Referentni testovi razmatraju tok vode i plina, uglavnom vodika, vezano za migraciju plina kroz umjetne i geološke barijere i usmjereno na dugoročno skladištenje nuklearnog otpada.

U radu je prikazana i egzistencija slabog rješenja za model dvofaznog nemješivog toka u formulaciji globalnog tlaka, s realističnim pretpostavkama na ulazne podatke. Ranija istraživanja vezana za egzistenciju slabog rješenja nemješivog dvofaznog kompresibilnog toka u poroznoj sredini su razmatrana i u radovima drugih autora (npr. [44, 48]). No, u tim radovima primijenjene su izuzetno jake pretpostavke na oblik kapilarnog tlaka, ili je pokazana egzistencija aproksimacijskih modela. U sklopu ove disertacije, egzistencija je prikazana uz značajno oslabljene i fizikalno opravdane ulazne pretpostavke, Prikazani rezultati pokrivaju slučaj neograničenog kapilarnog tlaka te dopuštaju diskontinuitete u poroznosti i permeabilnosti.

Curriculum Vitae

Ana Žgaljić Keko was born in Rijeka, Croatia, on 8 June, 1980. After obtaining secondary education in Krk, she started the undergraduate studies of Applied Mathematics at the Faculty of Science, University of Zagreb in 1998, where she graduated in 2004. In the same year, she started the postgraduate studies at the same faculty. Starting with 2005, she works as a teaching and research assistant at the Faculty of Electrical Engineering and Computing at the University of Zagreb.

Životopis

Ana Žgaljić Keko rodena je u Rijeci 8. lipnja 1980. godine. Osnovnu i srednju školu završila je u Krku. Prirodoslovno-matematički fakultet Sveučilišta u Zagrebu upisuje 1998. godine i 2004. godine završava studij matematike, smjer primijenjena matematika. Iste godine upisuje poslijediplomski znanstveni studij matematike na istom fakultetu. Od 2005. godine zaposlena je kao asistent na Zavodu za primijenjenu matematiku Fakulteta elektrotehnike i računarstva Sveučilišta u Zagrebu.