Dynamic effect in two-phase flow in porous media:
a pore-scale network approach
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a pore-scale network approach

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Chapter 1

Introduction

Two-phase flow processes in porous media are very important in many natural and industrial systems. Examples of two-phase flow in natural porous media are groundwater contamination problems like oil spills, unsaturated flow (for example in the plant root zone), but also the flow of oil and gas or oil and water in an oil reservoir. An industrial example is flow of two fluid phases through a fluidized bed.

Groundwater contamination by oil spills is a complex problem. The current physical and mathematical description of the behaviour of an oil spill in the subsurface is based on various extensions of the simple relationship between pressure head and flow rate as proposed by Darcy in 1856 [20]. In the case of two-phase flow, this simple relationship is written for each of the two fluid phases, and coupling occurs through empirical parameters as relative permeability and capillary pressure. In general, these parameters are assumed to be a function of wetting fluid saturation only. For complex systems, this is too simple.

A deeper understanding of multiphase flow and transport phenomena in porous media, such as interfacial effects, capillary pressure, saturation effects and immiscible displacement, will enable a formulation for optimal strategies for remediation of NAPL contaminations. A higher accuracy in oil spill removal can be achieved if knowledge is gained on multiphase flow and transport phenomena.

This dissertation is concerned with an investigation at the pore scale of two-phase flow in porous media under transient conditions. Starting from the microscale, an extended description of macroscale fluid flow is studied by means of pore-scale network models. Insight is gained into transport mechanisms of two immiscible fluids in porous media. Thus, a contribution is given to the derivation of more reasonable macroscale equations for the description of complex multiphase flow than are generally used at this moment. With this, the extension of Darcy’s law for multiphase fluid flow receives a physical fundament.
1.1 Governing equations in two-phase flow in porous media

In the absence of sources and sinks, the continuum-scale formulation of two-phase flow in porous media is given by the following mass balance equations:

\[
\frac{\partial}{\partial t} (\phi S^\alpha \rho^\alpha) + \nabla \cdot (\rho^\alpha q^\alpha) = 0 \quad (\alpha = w, n)
\]  

(1.1)

where \(t\) is time, \(\phi\) porosity, \(S\) saturation, \(\rho\) fluid density and \(q\) is volumetric flux.

The equations of motion for the two fluids are given by:

\[
q^\alpha = -\frac{k k^{\alpha \alpha}}{\mu^\alpha} (\nabla P^\alpha - \rho^\alpha g \hat{e}_z) \quad (\alpha = w, n)
\]  

(1.2)

where \(k\) is intrinsic permeability tensor, \(k^{\alpha \alpha}\) \(\alpha\)-phase relative permeability, \(\mu\) dynamic viscosity, \(g\) gravitational attraction and \(\hat{e}_z\) a unit vector in vertical direction.

Substituting equations (1.2) in (1.1) yields

\[
\frac{\partial}{\partial t} (\phi S^\alpha \rho^\alpha) - \nabla \cdot \left( \rho^\alpha \frac{k k^{\alpha \alpha}}{\mu^\alpha} (\nabla P^\alpha - \rho^\alpha g \hat{e}_z) \right) = 0.
\]  

(1.3)

In the case of isothermal two-phase flow and assuming the intrinsic permeability of the porous medium, as well as the fluids’ dynamic viscosities \(\mu^\alpha\), to be known, equations (1.3) constitute two equations with eight unknowns: \(S^n, S^w, \rho^n, \rho^w, P^n, P^w, k^{rn}\) and \(k^{rw}\). Therefore, six additional equations are required to close the set of equations. These are:

\[
1 = S^w + S^n  \quad (1.4)
\]
\[
\rho^w = \rho^w (P^w)  \quad (1.5)
\]
\[
\rho^n = \rho^n (P^n)  \quad (1.6)
\]
\[
P^n - P^w = P^\alpha (S^w)  \quad (1.7)
\]
\[
k^{rw} = k^{rw} (S^w)  \quad (1.8)
\]
\[
k^{rn} = k^{rn} (S^n)  \quad (1.9)
\]

Relationships (1.5) and (1.6) are equations of state, relating fluid density to pressure and temperature. Relationship (1.7) describes the equilibrium relationship between wetting fluid saturation and capillary pressure, defined as the difference between nonwetting and wetting fluid pressure. Relationships (1.8) and (1.9) describe relative fluid permeabilities as a function of wetting fluid saturation.

Special attention should be paid to relationships (1.7), (1.8) and (1.9). Relationship (1.7) is an equilibrium relationship, i.e., it is determined under no-flow conditions. Relationships (1.8) and (1.9) have a dynamic nature. They are determined under flow conditions (see [4, page 465]). Measurements and interpretation of capillary pressure is further treated in next section.
1.2 Capillary pressure at core scale

1.2.1 Laboratory experiments

Traditionally, capillary pressure for multiphase flow in porous media is studied using pressure cells, in which quasi-static displacement experiments are performed. A schematic illustration of such a cell is given in figure 1.1.

![Cross section of a pressure cell.](image)

Figure 1.1: Cross section of a pressure cell.

In these experiments, also referred to as multistep outflow experiments, fluid flow is controlled by capillary forces. The difference between the pressures of the fluids across the inflow and outflow boundaries is increased in small steps each time when equilibrium between fluid phases has been achieved.

The pressure steps of a traditional multistep outflow experiment are shown as the dashed-dotted line in figure 1.2. The equilibrium points are shown as the grey dots. From these equilibrium points, the capillary pressure-saturation relationship is then determined. In figure 1.2, this is the dashed line. However, following this procedure, the dynamics of the flow inbetween the equilibria are not captured. The capillary pressure-saturation relationship one retrieves when including the flow dynamics is schematically shown as the solid line in figure 1.2. The solid line matches the results of Dahle et al.’s bundle-of-tube model [17] very well. This indicates, that a capillary pressure definition that is a function of wetting fluid saturation does not give a full explanation for the fluids’ behaviour.
Chapter 1. Introduction

Wetting fluid saturation ($-\$w$)
Capillary pressure (Pa)
Reservoir pressure difference
Quasi-static $P_c-S_w$ curve
Quasi-static $P_c-S_w$ curve including dynamics

An argument not less important for the indication of capillary pressure being a function of more than saturation alone is the time-scale at which measurements are taken. The duration of quasi-static experiments can be days, weeks or even longer. The time-scale of many two-phase flow processes is much smaller, for example in industrial processes. This again raises the question whether the traditional equilibrium $P_c-S_w$ relationship is accurate to describe the involved (nonequilibrium) two-phase processes. In systems where two fluid phases are not in equilibrium, a more general dynamic $(P^n - P^w) - S_w$ relationship should be used. Thus, an extended definition of capillary pressure is required.

As early as 1921, one has realised that the behaviour of capillary flow under (quasi-)static and transient conditions is different [69]. In the last four decades, several researchers found different capillary pressure-saturation relationships for static, steady-state and transient laboratory experiments [60, 64, 66, 68]. As an example, results of quasi-static and unsteady state drainage experiments by Topp et al. [60] are shown in figure 1.3.

A comprehensive overview of the literature on experimental work under transient conditions is given by Hassanizadeh et al. [36]. In this paper, also more recent experiments are discussed. Most of the discussed experiments involve unsaturated systems, where air is the nonwetting fluid and water is the wetting fluid. Only Kalaydjian [41] and O’Carroll [9] investigate dynamic displacement with oil as non-

Figure 1.2: Determination of a capillary pressure-saturation relationship curve. The dashed-dotted line shows the boundary pressure differences. The grey dots denote the equilibrium points, from which the quasi-static $P_c-S_w$ curve is determined (the dotted line). The solid line shows the $P_c-S_w$ relationship one retrieves when flow dynamics are not discarded [17].
1.2 Capillary pressure at core scale

wetting fluid phase and water as wetting fluid phase. Kalaydjian studies imbibition (water displacing oil), where O’Carrol studies drainage (oil displacing water).

Figure 1.3: Water content-pressure head data from drainage experiments of Topp et al. [60]

In the late 1970s, Stauffer investigated drainage in air-water systems [65, 66] through laboratory column experiments. In his work, he relates dynamic and quasi-static capillary pressure through a dependency on saturation rate of change, according to the following relationship:

\[ P_{\text{dyn}} = P_{\text{stat}} - \tau \frac{\partial S^w}{\partial t} \]  

(1.10)

where coefficient \( \tau \) may depend on various parameters. From intuitive arguments, supported by his observations, Stauffer suggests the following dependency for coefficient \( \tau \):

\[ \tau = \frac{\alpha \epsilon \mu}{\lambda \kappa} \left( \frac{P_e}{\rho w g} \right)^2 \]  

(1.11)

where \( \alpha \) is a dimensionless constant, \( \epsilon \) is porosity, \( \mu \) is water dynamic viscosity, \( \lambda \) is Brooks-Corey parameter, \( \kappa \) is intrinsic permeability, \( P_e \) is entry capillary pressure, \( \rho_w \) is water density and \( g \) is gravitational acceleration. This relationship is further discussed and investigated in Chapter 7.
1.2.2 Theoretical considerations

Upscaling

From the late 1970s through the early 1990s, Hassanizadeh and Gray published several papers on upscaling thermodynamic pore-scale equations to core scale [32, 33, 31, 29, 34, 35]. In the upscaled equations for capillary pressure in two-phase flow, a viscous term appeared that could be accounted for in a new definition of capillary pressure. As first approximation, the dependency between capillary pressure and saturation rate of change was assumed to be linear.

This linear relationship can be expressed through a dynamic or damping coefficient $\tau$. With this, the traditional (quasi-)static relationship is replaced by:

$$P^n - P^w = P^c_{stat} - \tau \frac{dS^w}{dt} = P^c_{dyn} \quad (1.12)$$

where $P^c_{stat}$ is traditional (quasi-static) capillary pressure, $P^c_{dyn}$ is dynamic capillary pressure, $S^w$ is wetting fluid saturation, $P^n$ and $P^w$ are nonwetting and wetting fluid pressures, respectively, and $\tau$ is a dynamic or damping coefficient. This relationship is similar to that proposed by Stauffer [65, 66].

Relaxation time

The difference between quasi-static and dynamic capillary pressure can also be explained by taking a relaxation time into account, that governs fluid redistribution under transient conditions [1, 2, 3, 49]. Based on the units of the parameters, this seems to be a completely different mechanism, but if one normalizes damping coefficient $\tau$ with pressure, e.g., entry capillary pressure, one retrieves a parameter with time as unit.

1.3 Investigation of two-phase flow with pore-scale models

The proposed relationship (1.12) needs to be tested, and the properties of $\tau$ investigated. However, a major problem encountered in research on multiphase flow in porous media is the difficulty to measure all variables of interest. Even under well-controlled laboratory conditions, not all properties can be measured. Examples are fluid-fluid interfacial area, local fluid pressures and capillary pressure throughout the porous medium.

As an alternative for laboratory experiments and theoretical studies, numerical pore-scale network models have therefore been developed. Network models consist of an assembly of tubes (as pore throats) and pore bodies connecting them. These models can represent virtual experiments where every step and every parameter in multiphase flow can be controlled and/or determined. Main advantage of pore-scale network models is the possibility to monitor every variable one is interested in. Also, the duration time of experiments is reduced dramatically. Disadvantage is
the required amount of computing power. Also, it is very difficult to compute fluid displacement in a real porous medium at the pore scale.

### 1.3 investigation of two-phase flow with pore-scale models

1.3.1 Early models

A historical overview of the development of network models starts with the concept of ‘bundle of tubes’. In this concept, a porous medium is represented by a set of parallel tubes. As early as 1921, Washburn studied dynamic invasion of fluid in a tube [69]. In 1941, Carman extended the bundle of tubes idea, using capillary tubes of varying diameters [8]. He also made comparisons to sand beds.

Bundle-of-tube models are in general not too complex. They offer the opportunity to gain more insight in two-phase systems. For this reason, bundle-of-tubes models are still used. Recent research examples are works by Celia, Dahle and Hassanizadeh [11, 17].

A second way of representing a porous medium was used by Haines in 1930. He used a so-called ‘sphere pack model’ to show hysteresis in two-phase flow. An important conclusion of his work is that changes in moisture distribution are generally not reversible, but depend on the direction of moisture change [30]. In other words, the relationship between capillary pressure and saturation depends on whether the capillary pressure increases (drainage) or decreases (imbibition).

1.3.2 Pore-scale network models

In 1956, Fatt published a series of three papers, in which he introduced pore-scale network models [23, 24, 25]. Fatt’s networks were two-dimensional. He made use of the simplest methods: he calculated capillary pressure characteristics with pencil and paper, and dynamic properties of the networks with the electrical analog method. The use of network models became more and more abundant with increasing computational power.

Numerous pore-scale network models have been developed in recent years and have been used as numerical surrogate for laboratory experiments (for an overview, see Dullien [22] or Celia et al. [12]). Topics that are studied are amongst others the effect of multiple phases on relative permeability, comparison of numerical and real porous media, the origin of hysteresis and the influence of interfacial area on multiphase flow development.

From the viewpoint of this research, pore-scale network models can be subdivided in two major categories: (quasi-)static and dynamic models. In (quasi-)static models, the assumption is made that fluid displacement is only affected by the local capillary pressure. Therefore, they can only be used for cases of low flow velocity.

Examples of (quasi-)static pore-scale network models are amongst others that of Lenormand et al. [45], who used etched glass micromodels as porous media. Jerault and Salter [40] studied the effect of pore structure on hysteresis in relative permeability and capillary pressure in a numerical network. Blunt et al. [7] made their network model physically more realistic by introducing an approximation of
viscous effects in a static model. Reeves and Celia [59, 58] mainly focussed on the relationship between capillary pressure, saturation and interfacial area.

Another type of pore-scale network models is the so-called dynamic network models. In these models, fluid-fluid interfaces are tracked in time and fluids flows are simulated. Clearly, the interfaces do not have to be at equilibrium positions. Instead of increasing inflow boundary fluid pressure in small steps to a maximum value, the simulations are carried out with the boundary pressure set equal to a (large) constant value from the start. See, e.g., Mogensen & Stenby [48], Dahle & Celia [16] and Celia et al. [10]. Alternatively, one can impose a constant nonwetting flux at the boundary (e.g., Blunt & King [6]). The difference between quasi-static and dynamic drainage experiments as used in this research is sketched in figure 1.4. In this study, a dynamic pore-scale network model is used to investigate transient effects in the capillary pressure-saturation relationship.

![Figure 1.4: Fluid reservoir pressure difference in time for a quasi-static and a dynamic experiment](image)

Dynamic pore-scale network models are mostly used to study relative permeabilities. The research performed in this dissertation is the first that employs a dynamic pore-scale network model to study the definition of dynamic capillary pressure.

### 1.4 Research objectives and structure of dissertation

Main objective of this research is to investigate the dynamic capillary pressure effect in two-phase flow in porous media. For this purpose, quasi-static and dynamic pore-scale network models are developed.

In Chapters 2, 3 and 4, the pore-scale network models that are developed and employed in the framework of this research are presented. In Chapter 2, the angular dynamic pore-scale network model is introduced. This model can simulate transient as well as quasi-static primary drainage. Results of numerical primary drainage experiments are shown. Despite its elegant formulation, the angular model had to
be abandoned because of problems that were too difficult to solve in the remaining time of the research project.

The research continues with a pore-scale network model with simplified geometry, namely the ball-and-stick formulation. In Chapter 3, the quasi-static network model is described. Typical results as capillary pressure and fluid distribution are shown. Chapter 4 introduces the dynamic pore-scale network model with the same geometrical properties. This model can actually also perform quasi-static drainage simulations.

In Chapter 5, test cases are shown with which possible drawbacks and limitations of the dynamic pore-scale model from Chapter 4 are investigated. Three different displacement regimes are treated. Also, the influence of placing a hydrophilic filter on the resulting capillary pressure-saturation curves is discussed.

In Chapter 6, a Representative Elementary Volume (REV) is determined, with which damping coefficient $\tau$ is calculated. Damping coefficient $\tau$ shown to be a function of wetting fluid saturation.

In Chapter 7, further dependencies of damping coefficient $\tau$ are investigated. The focus is on the influence of fluid viscosities and length scale or averaging domain size on $\tau$.

Finally, in Chapter 8 results of this research are summarized and conclusions are drawn. Recommendations for further research are given as well.
Chapter 1. Introduction
Chapter 2

The angular pore-scale network model

This chapter describes the pore-scale network model with elements (pore bodies and throats) of rectangular cross section. The shape of the elements allows two fluids to reside in the same network element at the same time. This has certain implications for handling the fluid conductances in the network elements.

In principle, this pore-scale network model is developed to handle both dynamic and quasi-static drainage. However, when simulating quasi-static and dynamic drainage, numerical problems occurred which made it technically impossible to simulate the performed laboratory experiments. Therefore, this network model could not be deployed to investigate dynamic effects in multiphase flow. Nevertheless, it is important to give a description of the model and to report on the kind of difficulties that were encountered in running the model.

The background physics and model description is given in Sections 2.1 through 2.4. Some numerical drainage experiments are described in Section 2.5. In this section, some typical results are presented. Also, a first computation of damping coefficient $\tau$ is given. Descriptions and explanations of encountered problems are given in Section 2.6.

2.1 Geometry and assumptions

The pore network is built as a regular lattice of pore bodies and pore throats. A pore body is cubic in shape, whereas a pore throat has the shape of a straight parallelepiped (see figures 2.1 and 2.2). The network consists of $N$ nodes. Pore body and throat sizes are assumed to follow a truncated log-normal distribution which is given in Section 3.1. The network is not necessarily regular, but in the current version a regular grid is used. The coordination number is therefore six for a 3D network and four for a 2D network. An example of a two-dimensional lattice is shown in figure 2.2.
Chapter 2. The angular pore-scale network model

Figure 2.1: Schematic representation of a pore body and adjacent pore throats in a 3D network with coordination number 6

The model is simplified using the following assumptions:

- Both fluids are considered to be incompressible; the solid matrix is rigid.
- The pore throats have negligible volume, but they offer hydraulic resistance to flow.
- The passage of a fluid-fluid interface through a pore throat occurs instantaneously (i.e. the residence time is negligible compared to the characteristic flow time).
- Flow in the pore throats is laminar and given by Hagen-Poiseuille formulae.
- Capillary pressure is constant in a pore body during a time step.
- Gravity is neglected, hence fluid flow is driven by pressure gradients only.

The angular pore-scale network model has the following important features:

- An interface can be tracked in time within a pore throat or a pore body.
- Two fluids can be simultaneously present and flowing within pore throats and/or pore bodies.
- Wetting phase is present and continuous along edges of pore throats and pore bodies.
- Residual saturation within a single pore body or pore throat is possible.
2.2 Governing pore-scale equations

In this section, pore-scale equations that are used in the network model under the assumptions mentioned in Section 2.1 are described. Pore bodies are denoted by a single subscript (e.g. \(i\)), pore throats by the double subscript \(ij\). Superscript \(w\) and \(n\) denote wetting and nonwetting fluid phases, respectively.

Continuity equations

In the absence of external sources and sinks, the principle of volume conservation for fluid phase \(\alpha\) in pore body \(i\) connected to neighbouring pore bodies \(j\) \((j \in N_i)\) can be written as:

\[
V_i \frac{\Delta S_i^\alpha}{\Delta t} + \sum_{j \in N_i} Q_{ij}^\alpha = 0, \quad (\alpha = w, n)
\]  

(2.1)

where \(V_i\) is volume, \(t\) is time, \(S_i^\alpha\) is the local \(\alpha\)-phase saturation (fraction of volume \(V_i\) filled by fluid \(\alpha\)), \(Q_{ij}^\alpha\) is the \(\alpha\)-phase flux from pore body \(i\) to \(j\), and \(N_i\) is the set of node numbers connected to node \(i\).

Since, by definition,

\[
S_i^w + S_i^n = 1,
\]  

(2.2)
summation of equations (2.1) for the two fluid phases results in the following system of equations:

\[ \sum_{j \in \mathcal{N}_i} (Q_{ij}^w + Q_{ij}^n) = 0, \quad (i = 1, N). \tag{2.3} \]

**Interfacial equilibrium equations**

It is possible for the two fluid phases to be present within a pore body at the same time. If this is the case, the two fluid pressures are related through the capillary pressure inside the pore body. This capillary pressure is chosen to be a function of the local saturation. This relationship is based on the curvature of the fluid-fluid interface and the pore body geometry. From the curvature of the interface, the prevailing capillary pressure can be calculated. Thus, local saturation and local capillary pressure are uniquely related for any given pore body:

\[ P_{ci} = P_i^n - P_i^w = f(S_i). \tag{2.4} \]

The derivation of this relationship is given in Section 2.4.3.

**Flux equations**

The flow of each phase within a pore throat \( ij \) is assumed to be given by modified Hagen-Poiseuille formulae. Wetting and nonwetting phase fluxes are expressed in terms of their corresponding phase pressures (neglecting gravitational terms):

\[ Q_{ij}^\alpha = K_{ij}^\alpha (P_i^\alpha - P_j^\alpha), \quad (\alpha = w, n) \tag{2.5} \]

where \( K_{ij}^\alpha \) is the \( \alpha \)-phase apparent conductivity of the pore throat connecting nodes \( i \) and \( j \) and \( P_i^\alpha \) and \( P_j^\alpha \) are \( \alpha \)-phase pressures. \( K_{ij}^\alpha \) depends on the fluid occupancy of pore throat \( ij \). Resistance to flow is expressed in terms of the effective cross-sectional area and the effective hydraulic radius for the considered fluid phase in a pore throat, and a dimensionless resistance that takes into account the angular shape of the pore throat \([21, 71, 48]\). Details are given in Section 2.4.6.

### 2.3 Model equations

Equations (2.1) through (2.5) suffice to describe two-phase flow in the angular pore-scale network model. However, using these equations only, one would have to solve for flow of both fluid phases simultaneously. This is not only CPU time consuming, but also inconvenient because of the general lack of knowledge of the exact location of the fluid-fluid interface. Therefore, the two-phase flow equations (2.1) - (2.5) are solved in a different manner. This procedure is described in this section.
Saturation-weighted total pressure

To make solving the flow equations in a drainage simulation more efficient, a change of variables has been employed. First, a total fluid pressure is defined, that is a weighted sum of the two phase pressures:

$$P_i = S_w^i P^w_i + S_n^i P^n_i.$$  \hspace{1cm} (2.6)

Using the definition of capillary pressure (equation (2.4)), phase pressures in each pore body can then be retrieved:

$$P^w_i = P_i - S_n^i P^c_i$$ \hspace{1cm} (2.7)

$$P^n_i = P_i + S_w^i P^c_i.$$ \hspace{1cm} (2.8)

Final system of linear equations

Equations (2.3), (2.5), (2.7) and (2.8) can be combined to obtain a set of linear equations in terms of $P$. For a given node $i$, the typical equation reads:

$$\sum_{j \in N_i} \left[ (K^w_{ij} + K^n_{ij}) (P_i - P_j) + F_i P^c_i + F_j P^c_j \right] = 0$$ \hspace{1cm} (2.9)

where $F_i$ and $F_j$ are coefficients given by:

$$F_i = K^n_{ij} S_w^i - K^w_{ij} (1 - S_w^i)$$

$$F_j = K^w_{ij} (1 - S_w^j) - K^n_{ij} S_w^j.$$  

Writing equation (2.9) for all nodes will yield a system of equations for $P_i$ that can be solved if $S_w^i$ is known. The algorithm for solving equations (2.9) and (2.4) is given in the following section.

2.4 Model description

In this section, the algorithms used for solving the pore-scale equations of the angular network model are described. Note that at this stage, the angular pore-scale network model is limited to drainage-type displacement, i.e., nonwetting fluid displacing wetting fluid.

The angular pore-scale network can simulate two types of laboratory experiments for the measurement of capillary pressure-saturation relationships: it is capable of performing both dynamic and quasi-static drainage experiments. In the dynamic drainage experiments, a large pressure is imposed on the nonwetting fluid reservoir at time $t = 0$. Fluid-fluid interfaces are then tracked in time until equilibrium between the two fluid phases has been achieved, or until all continuous wetting fluid has been drained from the network.

In the quasi-static drainage experiments, a small pressure is imposed on the nonwetting fluid reservoir at $t = 0$. Again, fluid-fluid interfaces are tracked until equilibrium between the two fluid phases has been achieved. Then, nonwetting fluid
Chapter 2. The angular pore-scale network model

Pressure is increased with an increment, and the fluid-fluid interfaces move to new equilibrium positions. This procedure is repeated until the boundary pressure equals the boundary pressure used in the dynamic experiment. As such, the quasi-static drainage experiments consists of a series of dynamic drainage experiments.

The flow chart of the pore-scale network model is given in figure 2.3. It illustrates the procedure that is followed during the numerical simulations. The governing equations presented in Section 2.2 are solved for $P$ and $S_w$ using an IMPES (IMplicit Pressure - Explicit Saturation) algorithm. Equation (2.9) is solved implicitly in terms of $P$, assuming that $S_w$ (and therefore, $P_c$) and $K_{ij}'$'s are known from the previous time step. Then, equations (2.7) and (2.8) are used to update phase pressures which are then used to calculate fluid fluxes (equation (2.5)). The fluxes are substituted in equation (2.1) and local phase saturations are calculated. Finally, equation (2.4) is used to update capillary pressure. The procedure is then repeated.

The flow chart gives a correct representation of the simulation procedure, but the stopping criteria are not mentioned. The steps in the flow chart are repeated as long as the number of time steps does not exceed the given maximum number of time steps, or until global (average) wetting fluid saturation doesn’t change anymore.

2.4.1 Initial and boundary conditions

Initially, the network is fully saturated with wetting fluid. The top layer of pore bodies acts as an infinite nonwetting fluid reservoir with $S_w = 0$. The bottom layer acts as an infinite wetting fluid reservoir with $S_w = 1$. Initially, total fluid pressure $P$ in all the pore bodies is zero. Since $S_w = 0$ in the network, this pressure represents wetting fluid pressure.

Pressure boundary conditions in the pore-scale network model are of Dirichlet type: constant pressure is prescribed at the top and the bottom of the network. The network does not have any pore throats pointing outward. Thus, flow is not possible through the sides of the network and, virtually, no-flow conditions are applied. The boundary conditions are sketched in figure 2.4.

To avoid breaktrough of nonwetting fluid into the wetting fluid reservoir, a hydrophilic filter can be applied. The pore throats adjacent to the wetting fluid reservoir can be reduced in size by a given factor. Thus, the entry capillary pressure is increased. If the increase is large enough, nonwetting fluid will not be able to enter the wetting fluid reservoir.

Saturation-weighted total pressure $P$ has a dual character at the top and bottom layer. From equations (2.7) and (2.8), it follows that pressure $P$ at the top of the network represents nonwetting fluid pressure, while $P$ at the bottom of the network represents wetting fluid pressure.

2.4.2 Time step size determination

The time step is chosen to be variable in the numerical model. It is determined as follows. First, a filling time is calculated for all internal (i.e. non-boundary) pore
bodies. This filling time is the time needed for a pore body to filled up or down to a target state. Target states are the following:

1. $S_i^w = 1$
2. $S_i^w = S_*^w$
3. $S_i^w = S_{w, min,i}$.

$S_*^w$ is the wetting fluid saturation of the pore body at the moment that the nonwetting phase has filled a sphere inscribed within the cubic pore body. On geometrical grounds, it is easy to see that this value corresponds to $1 - \frac{\pi}{6} \approx 0.48$ for all pore bodies.
Chapter 2. The angular pore-scale network model

$S_{w, min,i}$ is a pre-specified minimum saturation that depends on the maximum allowable capillary pressure in the network and the size of the pore body. The maximum capillary pressure is the difference between the fluid pressures in the boundary nodes. This is explained in Section 2.4.3.

The choice of target state is dependent on the current state, and on the sign of the net fluid flux, as described in the following two paragraphs, where it is also explained how the filling times are computed.

**Local drainage**

If the net nonwetting fluid flux in a node is positive, this node will be (partly) drained in next time step. The saturation in the node determines the allowed change in saturation for next time step, based on the target states defined above. In other words, it determines how much nonwetting fluid can enter in this time step. For local drainage, there are two possibilities:

- Wetting fluid saturation $S^w_i$ is larger than $S^w_{\ast}$. This is shown in figure 2.5, as situation I. Then, the target saturation is $S^w_{\ast}$. The filling time that belongs to the node is thus given by:

\[
\Delta t_i = \frac{V_i (S^w_i - S^w_{\ast})}{|q_{nw,i}|}.
\] (2.10)

- Wetting fluid saturation $S^w_i$ is between $S^w_{\ast}$ and $S^w_{w, min,i}$, see figure 2.5, situation II. Then, the target saturation is $S^w_{w, min,i}$. Filling time is given by:

\[
\Delta t_i = \frac{V_i (S^w_i - S^w_{w, min,i})}{|q_{nw,i}|}.
\] (2.11)
2.4.3 Capillary pressure in a pore body

In the network model, a relationship between wetting fluid saturation and capillary pressure in a pore body is required. Capillary pressure is related to the curvature of the fluid-fluid interface by the Young-Laplace equation [4]:

\[ P^c = \sigma \left( \frac{1}{r_1} + \frac{1}{r_2} \right) \]  

(2.13)
where $\sigma$ is interfacial tension and $r_1$ and $r_2$ are the principal radii of curvature of the fluid-fluid interface. When the two principal radii of curvature are equal, equation (2.13) can be written as:

$$P^c = \frac{2\sigma}{r_c}$$

(2.14)

where $r_c$ is the mean radius of curvature of the fluid-fluid interface.

Figure 2.6: In a corner of a cubic pore body, both principal radii of curvature of a fluid-fluid interface are equal (left). Along the edge, one of the principal radii of curvature is infinite (right).

In a cubic pore body, interfaces between the two fluids can have either one or two finite radii of curvature. In a corner of a pore body, the interface is one eighth of a sphere (see figure 2.6). Thus, both principal radii of curvature are equal and capillary pressure is given by equation (2.14). Along the edges of a pore body, the interface is one fourth of a cylinder. Thus, one of the principal radii of curvature is infinite, as illustrated in figure 2.6.

For assigning capillary pressure to a pore body, four domains in wetting fluid content of that pore body are distinguished. In fact, two domains and two states are distinguished, but for enhanced readability, the two states are referred to as domains as well. The domains are listed below. For each of these, capillary pressure is prescribed as in figure 2.7.

1. Domain I: $S^w = 1$
2. Domain II: $S^w < S^w < 1$
3. Domain III: $S^w_{\min} < S^w < S^w$
4. Domain IV: $S^w = S^w_{\min}$

where $S^w$ is the wetting fluid saturation when nonwetting fluid occupies the inscribed sphere of the pore body, as defined previously. This value can be easily seen to be $S^w = 1 - \frac{\pi}{6} S^w_{\min}$. $S^w_{\min}$ is the minimum possible wetting fluid saturation based on the maximum capillary pressure and the pore body size.
Figure 2.7: Illustration of the four domains that are used to determine capillary pressure from saturation in a pore body. For each of these domains, a different prescription for capillary pressure is used. The values on the y-axis are based on results given in figures 2.9 and 2.10.

If local saturation is in domain I, capillary pressure is zero. That is, capillary pressure is zero if there is only wetting fluid phase present. If local saturation is in domain II, capillary pressure is set to the capillary pressure that belongs to $S_w$. Then, the fluid-fluid interface is the inscribed sphere of the pore body. The curvature of the interface is such, that the capillary pressure is equal to the entry capillary pressure of a cylindrical tube with the same radius as the pore body. Equation (2.13) then reduces to (see Section 2.4.4):

$$P_i^c = \frac{2\sigma \cos \theta}{R_i}$$

where $R_i$ is the radius, or half-width of the pore body. If saturation is in domain III, an approximation of an analytical expression based on the mean radius of curvature of the fluid-fluid interface inside the pore body is used. Both the analytical expression and the approximation are given in the text below. If local saturation is in domain IV, capillary pressure is set to the maximum capillary pressure in the system, the difference between the nonwetting and the wetting fluid pressure in the end reservoirs.
Analytical expression

To derive the analytical expression for the relationship between capillary pressure and wetting fluid saturation for $S_w > S > S_{w,min}$ (domain III), the pore body is subdivided into 8 corners and 12 edges, as illustrated in figure 2.8. Let $r_{c1}$ be the mean radius of curvature of the fluid-fluid interface in a corner of a cubic pore body, and $r_{c2}$ the mean radius of curvature along an edge of that cubic pore body. The fluid-fluid interface in each of the corners has the shape of $\frac{1}{8}$ of a sphere with radius $r_{c1}$. The interface in the 12 edges can be merged into three cylinders with length $L_{edge}$ and radius $r_{c2}$.

Figure 2.8: Schematic representation of the assumed fluid-fluid interfaces in a pore body, as used to determine capillary pressure from saturation. The radii of curvature of the fluid-fluid interfaces in the corners are twice as large as the radii of curvature of the quarter cylinders along the sides of the cube.

The total volume of wetting fluid in the eight corners is equal to the volume of wetting fluid in a pore body of half-width $r_{c1}$, minus the volume of the inscribed sphere of the cube. This volume equals:

$$V_{corners}^w = \left(8 - \frac{4}{3}\pi\right)r_{c1}^3. \quad (2.16)$$

The length of an edge in the pore-scale network model is defined as the width of the cube minus the length of the corners (twice the mean radius of curvature):

$$L_{edge} = 2(R_i - r_{c1}). \quad (2.17)$$

The volume of wetting fluid in all twelve edges is given by:

$$V_{edges}^w = 12L_{edge}r_{c2}^2 \left(1 - \frac{\pi}{4}\right). \quad (2.18)$$
Therefore, the total volume of wetting fluid in a pore body equals:

\[ V_{w} = \left(8 - \frac{4}{3}\pi\right)r_{c1}^3 + 24(R_i - r_{c1})r_{c2}^2 \left(1 - \frac{\pi}{4}\right). \tag{2.19} \]

Under the assumption that capillary pressure is constant in a pore body during a time step, and using equation (2.13), it can be seen, that \( r_{c1} \) and \( r_{c2} \) are then related as \( r_{c1} = 2r_{c2} \). The total volume of wetting fluid is a pore body can thus be written in terms of \( r_{c1} \) only:

\[ V_{w} = (8 - \frac{4}{3}\pi)r_{c1}^3 + (6 - \frac{3}{2}\pi)(R_i - r_{c1})r_{c1}^2. \tag{2.20} \]

Using equation (2.14) to replace \( r_{c1} \) with \( P_c \), the relationship between wetting phase saturation in a pore body of square cross section and capillary pressure can be found to be:

\[ S_{w} = \frac{(2 + \frac{1}{6}\pi)(\frac{2\pi}{P_c})^3 + (6 - \frac{3}{2}\pi)R_i(\frac{2\pi}{P_c})^2}{8R_i^3} \] for \( S_{w_{min,i}} < S_{w} \leq S_{w} \tag{2.21} \]

where \( S_{w} \) is the wetting phase saturation if the pore body is filled with an inscribed sphere of nonwetting fluid.

**Approximation**

To determine capillary pressure as a function of saturation, the analytical expression (2.21) has to be inverted. However, no explicit inversion of this expression is possible. Therefore, a curve-fitting is made to write \( P_c \) as function of \( S_{w} \). The found relationship is given by:

\[ P_{c} = \frac{2\sigma \cos \theta}{r_{c}^{mod}} \tag{2.22} \]

where the denominator is the modified radius of curvature, related to saturation by:

\[ r_{c}^{mod} = 1.3404 R_i (S_{w})^{0.3991}. \tag{2.23} \]

These equations relate geometry and saturation to capillary pressure.

Note that equations (2.22) and (2.23) are only valid for wetting fluid saturation between \( S_{w_{min}} \) and \( S_{w} \) in a pore node. If the wetting fluid saturation is larger than \( S_{w} \), capillary pressure is given by:

\[ P_{c} = \frac{2\sigma \cos \theta}{R_i}. \tag{2.24} \]

If wetting fluid saturation equals 1, capillary pressure is zero, and if wetting saturation equals the minimum saturation, capillary pressure is maximum.

In figure 2.9, the difference between the analytical expression as given in equation (2.21) and the approximation (2.22) is shown. The compared expressions are only valid for \( S_{w_{min}} < S_{w} < S_{w} \).
Table 2.1: Local mean radius of curvature and capillary pressure

<table>
<thead>
<tr>
<th>Domain</th>
<th>$r_c$</th>
<th>$P_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>-</td>
<td>0</td>
</tr>
<tr>
<td>II</td>
<td>$R \left( \frac{\sigma}{\gamma} (1 - S_w) \right)^{\frac{1}{3}}$</td>
<td>$\frac{2\sigma \cos \theta}{R}$</td>
</tr>
<tr>
<td>III</td>
<td>$1.3404R \left( S_w \right)^{0.3991}$</td>
<td>$\frac{2\sigma \cos \theta}{r_c}$</td>
</tr>
<tr>
<td>IV</td>
<td>$1.3404R \left( S_{w_{\min}} \right)^{0.3991}$</td>
<td>$P^c_{\max}$</td>
</tr>
</tbody>
</table>

$R$ is pore body radius (half-width), $r_c$ is local mean radius of curvature inside the pore body.

Figure 2.9: Comparison of the semi-analytical and the approximated relationship for capillary pressure as a function of wetting fluid content in a pore body. Radius (half-width) of the pore body is 0.09 mm.

Note that local capillary pressure is assumed to be constant in a pore body for $S_w > S_{w_{\max}}$, although local mean radius of curvature changes.

In figure 2.10, it can clearly be seen that the capillary pressure inside a pore body not only depends on the maximum allowed capillary pressure, but also on the radius (half-width) of the pore body. In the figure, local capillary pressure-saturation relationships are given for different pore body sizes and constant maximum capillary pressure. For a large pore body, the inscribed sphere has a higher radius of curvature, and therefore a lower capillary pressure in the domain where $S_w < S_{w_{\max}}$.

This also has an effect on the minimum saturation $S_{w_{\min}}$, which depends on the maximum value of capillary pressure and pore size as well. The maximum
2.4 Model description

Figure 2.10: Graph of local capillary pressure-saturation curves for three different pore sizes and a constant maximum capillary pressure.

value of capillary pressure gives a minimum curvature. In a small pore body, this minimum curvature will lead to a relatively large amount of remaining nonwetting fluid, whereas in a large pore body, only a small amount of nonwetting fluid will remain. This is also evident in figure 2.10.

2.4.4 Entry capillary pressure of a pore throat

Entry capillary pressure of a pore throat is found following Young-Laplace equation [4]:

\[ P^c = \sigma \left( \frac{1}{r_1} + \frac{1}{r_2} \right) \] (2.25)

where \( \sigma \) is interfacial tension and \( r_1 \) and \( r_2 \) are principal radii of curvature of the fluid-fluid interface. In a cylinder, the meniscus is part of a sphere. Thus, both principal radii of curvature are equal, and Young-Laplace equation reduces to \( P^c = \frac{2\sigma}{r_c} \), where \( r_c \) is mean radius of curvature. Mean radius of curvature of the meniscus can in turn be related to the radius of the cylinder by \( r_c = r \cos \theta \), yielding

\[ P^c = \frac{2\sigma \cos \theta}{r} \] (2.26)

where \( r \) is the radius of the circular pore throat and \( \theta \) is the contact angle.
For an angular pore throat, the expression is a more complex function of contact angle $\theta$ [44, 57, 21, 71]. Entry capillary pressure is then given by:

$$P_c = \frac{\sigma}{r} \left( \frac{\theta + \cos^2 \theta - \frac{\pi}{4} - \sin \theta \cos \theta}{\cos \theta - \sqrt{\frac{\pi}{4} - \theta + \sin \theta \cos \theta}} \right).$$ \hspace{1cm} (2.27)

For a perfectly wetting solid, $\theta$ equals 0 and capillary pressure takes the form:

$$P_c = \frac{\sigma}{r} \left( 1 - \frac{\pi}{4} \right) = \frac{\sigma}{r} \left( 1 + \sqrt{\frac{\pi}{4}} \right).$$ \hspace{1cm} (2.28)

Capillary pressure in a pore throat must be exceeded before an interface moves into the pore throat. Comparing equations (2.26) and (2.28), it is clear that the entry capillary pressure of an angular tube is less than that of a circular tube.

When a pore throat has been drained, both fluids are present in the throat with the wetting fluid filling the edges of the pore throat. The fluid phase conductivities are a function of cross-sectional interfacial area, which in turn is a function of the radius of curvature.

### 2.4.5 Interfacial area in a pore body

Following a similar procedure as in Section 2.4.3, local interfacial area can easily be computed. For each of the four domains stated in Section 2.4.3, a mean radius of curvature of the fluid-fluid interface can be determined, based on the dimensions of the pore body and the volume of nonwetting fluid inside that pore body. Local interfacial area can then be expressed in terms of local mean radius of curvature and pore body dimensions. This is given in table 2.2.

The dependency of local interfacial area on local saturation is shown in figure 2.11. In this figure, pore body radius $R$ is 0.09 mm. Knowing the local mean radius of curvature the interfacial area over the whole saturation range of a pore body can be computed.

<table>
<thead>
<tr>
<th>Domain</th>
<th>$r_c$</th>
<th>$a_{\text{wn}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>$-$</td>
<td>0</td>
</tr>
<tr>
<td>II</td>
<td>$R \left( \frac{S_w}{2} \right)^\frac{1}{3}$</td>
<td>$4\pi r_c^2$</td>
</tr>
<tr>
<td>III</td>
<td>$1.3404R (S_w)^{0.3991}$</td>
<td>$4\pi r_c^2 + 6\pi r_c (R - r_c)$</td>
</tr>
<tr>
<td>IV</td>
<td>$1.3404R (S_{\text{min}})^{0.3991}$</td>
<td>$4\pi r_c^2 + 6\pi r_c (R - r_c)$</td>
</tr>
</tbody>
</table>

$R$ is pore body radius, $r_c$ is local mean radius of curvature inside the pore body.
2.4 Model description

Figure 2.11: Interfacial area in a pore body as a function of local saturation. Radius of the pore body is 0.09 mm.

![Graph showing interfacial area vs. wetting fluid saturation for a single pore body.]

Figure 2.12: Interfacial area in three pore bodies as a function of local saturation. Radii of the pore bodies are 0.06 mm, 0.12 mm, and 0.18 mm. Irreducible wetting fluid saturation depends on boundary pressure and pore body size (see also figure 2.10).

![Graph showing interfacial area vs. local wetting fluid saturation for three pore bodies with different radii.]
2.4.6 Fluid occupancy in a pore throat

The fluid occupancies in a pore throat are the key to the computations of the flow through the pores of the network. Based on the fluid occupancies, phase conductivities are determined, which are not only used to calculate the fluid phase fluxes in the pore throats, but also to set up the right hand side of the set of linear equations in terms of $\overline{F}$, see equation (2.9).

Interface stability

In the pore-scale network model, a set of displacement rules determines the fluid occupancy in the pore throats. An illustration of these rules is given in figure 2.13. In this figure, nonwetting fluid is shown in dark grey, wetting fluid in white. A solid X through a pore throat indicates that flow of the shown fluid phase is prohibited. Note that a dark grey pore throat means that both wetting and nonwetting fluid reside in that throat, as nonwetting fluid cannot reside inside the corners. Wetting fluid is always considered to be mobile. The displacement rules are the following:

- An interface between the nonwetting and wetting fluid may migrate from a pore body into its adjacent throats when the volume of nonwetting fluid has the dimension of the inscribed sphere of the pore body, thus when $S^w \leq S^w_w$. It is allowed to do so if the capillary pressure at the interface exceeds the entry capillary pressure of the adjacent pore throat. This is shown as Ia in figure 2.13.

  If the capillary pressure at the interface does not exceed the entry capillary pressure of the pore throat, the pore throat will remain filled with wetting fluid only. This is illustrated as Ib in figure 2.13.

- When at a previous time step, nonwetting fluid was trapped in a throat, and one of the adjacent pore bodies is drained beyond $S^w_w$, the nonwetting fluid is allowed to move again. This is illustrated as situation II.

- When a throat has been drained at a previous time, and in both adjacent pore bodies the saturation has increased again to a higher value than $S^w_w$, the nonwetting fluid in the throat is considered to be trapped. The wetting fluid is still allowed to move. This is shown as situation III.

Phase conductivities

Phase conductivities for flow in a pore throat are based on the fluid occupancy of that throat. Three possible combinations of phase conductivity are distinguished [48]. These are listed below. Subscript $ij$ denotes pore throat $ij$, superscript $n$ and $w$ denote nonwetting and wetting fluid phases, respectively.
2.4 Model description

Figure 2.13: Check for mobility of interfaces, and consequent change in fluid occupancy. These fluid occupancies determine the fluid phase conductivities, and are also used in the calculation of $\mathbf{F}$. Nonwetting fluid is shown in dark grey, wetting fluid in white. A dark grey pore throat is filled by both fluid phases, as the nonwetting fluid cannot reside in the corners of the throat. A solid X through a pore throat indicates that flow of the shown fluid phase is prohibited. Wetting fluid is always allowed to move, except in case Ib.

1. wetting fluid flows in corners, nonwetting fluid is trapped

\[ K_{ij}^w = \frac{4 - \pi}{\beta \muw l_{ij}} \left( r_{ij}^c \right)^4 \]  \hspace{1cm} (2.29)

\[ K_{ij}^n = 0 \]  \hspace{1cm} (2.30)

where

\[ r_{ij}^c = \frac{\sigma}{P_{ij}^c} \]  \hspace{1cm} (2.31)
where $r_{ij}^c$ is mean radius of curvature of the cross-sectional fluid-fluid interface, $\mu$ is dynamic fluid viscosity, $l$ is pore throat length, and $\beta$ is a resistance factor that takes the angular shape of a pore throat into account [57], $P_{ij}^c$ is capillary pressure (see below) and $\sigma$ is interfacial tension.

2. wetting fluid flows, no nonwetting fluid present in pore throat

\[
\begin{align*}
K_{ij}^w &= \frac{\pi}{8\mu^w l_{ij}} \left( r_{ij}^{\text{eff}} \right)^4 \\
K_{ij}^n &= 0
\end{align*}
\] (2.32)

where

\[
r_{ij}^{\text{eff}} = \sqrt{\left( \frac{4}{\pi} \right) r_{ij}}
\] (2.34)

where $r_{ij}^{\text{eff}}$ is effective hydraulic radius of pore throat $ij$ and $r_{ij}$ is half-width of pore throat $ij$.

3. both wetting and nonwetting fluids flow

\[
\begin{align*}
K_{ij}^w &= \frac{4 - \pi}{\beta \mu^w l_{ij}} \left( r_{ij}^c \right)^4 \\
K_{ij}^n &= \frac{4}{8\mu^n l_{ij}} \left( r_{ij}^{\text{eff}} \right)^4 \\
K_{ij}^c &= \frac{\sigma}{P_{ij}^c}
\end{align*}
\] (2.35)

\[
\begin{align*}
r_{ij}^c &= \frac{\sigma}{P_{ij}^c} \\
r_{ij}^{\text{eff}} &= \frac{1}{2} \left( \sqrt{\frac{a_{ij}^{nw}}{\pi}} + r_{ij} \right) \\
a_{ij}^{nw} &= (r_{ij})^2 - (4 - \pi) \left( r_{ij}^c \right)^2
\end{align*}
\] (2.37)

(2.38)

(2.39)

where $a_{ij}^{nw}$ is cross-sectional area of nonwetting fluid in a pore throat.

As is evident in equations (2.29), (2.35) and (2.36), the fluid conductivities for funicular flow (when two fluid phases reside in one pore throat) depend not only on the dimensions of the pore throat, but also on the capillary pressure in the pore throat. However, fluid pressures, and thus capillary pressure, are only evaluated in the pore bodies and not in the pore throats. Therefore, capillary pressure in a pore throat is defined as the average of the capillary pressures in its neighboring pore bodies:

\[
P_{ij}^c = \frac{1}{2} \left[ P_{i}^c + P_{j}^c \right].
\] (2.40)
This equation has an important drawback which has been observed in simulations. When $P_{ij}^c$ is too low, effective radius $r_{ij}^{eff}$ can become larger than throat radius $r_{ij}$. This may lead to negative cross-sectional area of the nonwetting fluid, which is impossible. From equations (2.37) and (2.39), it can be derived that for a physical solution, $P_{ij}^c$ should match the following condition:

$$P_{ij}^c \geq \sqrt{4 - \pi} \frac{\sigma}{r_{ij}}.$$  \hspace{1cm} (2.41)

When this condition is not fulfilled, fluid conductivities depend on the dimensions of the pore throat only. The conductivities are then computed based on the fluid configuration where the pore throat is filled with an inscribed cylinder of nonwetting fluid. The remaining space is filled with wetting fluid. In that case, equations (2.35) and (2.36) change to:

$$K_{ij}^w = \frac{4 - \pi}{\beta \mu_w l_{ij}} (r_{ij})^4 \hspace{1cm} (2.42)$$  

$$K_{ij}^n = \frac{\pi}{8 \mu_n l_{ij}} (r_{ij})^4 \hspace{1cm} (2.43)$$

### 2.4.7 Equilibrium conditions

In dynamic and quasi-static drainage simulations, for a given set of boundary conditions (which correspond to a global capillary pressure) eventually the flow of fluids stop and an equilibrium distribution is obtained. In a dynamic displacement process, this is the end state. In a quasi-static drainage process, the boundary capillary pressure will be increased by a given pressure step until a predefined end boundary pressure has been achieved. The equilibrium state in a quasi-static simulation is considered to be the situation in which $\frac{dS_w}{dt}$ equals zero.

In drainage simulations, the length of a time step is determined by local changes in saturation, as described in Section 2.4.2. If there are no local saturation changes possible anymore under the prevailing boundary conditions, equilibrium between the two fluid phases must have been achieved. However, if local saturation cannot change anywhere in the network, next time step size will be undetermined. As a result of that, the saturation rate of change cannot be computed.

The chosen solution is that when no time step size can be determined, a predefined time step size is selected. As no local saturation changes are possible at equilibrium, $\frac{dS_w}{dt}$ will be zero. The condition $\frac{dS_w}{dt} = 0$ can then be replaced by a condition that requires that $S_w$ doesn’t change in a predescribed limited number of subsequent time steps.

### 2.4.8 Drainage procedure

The drainage procedure, the displacement of wetting fluid by nonwetting fluid is sketched in figures 2.14(a) to (d). Let’s assume that the pore body with coordination number 4 in a two-dimensional grid is going to be drained from the left throat (a). The drainage of the pore throat happens instantaneously, since the pore throat is
assumed to have no volume. Once a pore throat has been drained, nonwetting fluid is allowed to flow into the adjacent pore body.

Figure 2.14: Illustration of four saturation states in a pore body during drainage. The pore body is first drained until the inscribed sphere has been replaced by nonwetting fluid, as shown in (a) and (b). Wetting fluid saturation is then $S_w^w$. From the situation in (b) onward, the nonwetting fluid may migrate into adjacent pore throats, whenever the entry capillary pressure has been exceeded. With continuing drainage in the pore body, the fluid-fluid interface retreats into the corners (c) until a minimum wetting fluid saturation $S^w_{\text{min}}$ has been achieved (d).

The pore body is first drained (in one or more time steps) until the inscribed sphere is displaced by nonwetting fluid (b). Wetting fluid saturation is then $S^w_w$. During this drainage, capillary in the pore body is assumed to be constant. This capillary pressure has the value $P^c = \frac{2\sigma \cos \theta}{R}$, where $R$ is the radius of the inscribed sphere. Only after the nonwetting fluid has displaced the inscribed sphere, it may
move into the adjacent pore throats. This is of course allowed only if the entry capillary pressure of the pore throat has been exceeded (such a possible invasion is not shown in figure 2.14).

If the nonwetting fluid saturation increases further, capillary pressure increases. The wetting fluid retracts in the edges and corners, where the mean radius of curvature of the fluid-fluid interface decreases. This is illustrated in figure (c). This drainage can continue until a minimum wetting fluid saturation, $S_{\text{w, min}}$, has been achieved. This minimum wetting fluid saturation is defined by the maximum allowable capillary pressure in the porous medium. This is illustrated in (d).

Note that in figures 2.14(c) and 2.14(d), it appears as if the nonwetting fluid has displaced the water in the edges of the cubical pore body. This of course does not occur unless capillary pressure becomes infinite, which is not allowed in the angular pore-scale network model.

### 2.4.9 Averaging procedure

Macroscale variables are obtained by averaging their corresponding pore-scale variables. Averaging is performed over fluid phases and over fluid-fluid interfacial area. The macroscale pressures are obtained by volume averaging of the pore body pressures:

$$
\langle P^\alpha \rangle_{\text{vol}} = \frac{1}{\delta V^\alpha} \int_{\delta V^\alpha} P^\alpha \, dV = \frac{\sum_i^N P^\alpha_i S^\alpha_i V_i}{\sum_i^N S^\alpha_i V_i} \tag{2.44}
$$

where $N$ is number of pore bodies, $P^\alpha$ is $\alpha$-phase fluid pressure, $S^\alpha$ is $\alpha$-phase saturation and $V$ is volume. Subscript $i$ denotes pore body $i$.

Then, one may define volume-average capillary pressure:

$$
\langle P_c \rangle_{\text{vol}} = \langle P_n \rangle_{\text{vol}} - \langle P_w \rangle_{\text{vol}}. \tag{2.45}
$$

Alternatively, one may define an area-averaged macroscale capillary pressure given by:

$$
\langle P_c \rangle_{\text{area}} = \frac{1}{\delta a_{wn}} \int_{\delta a_{wn}} P_c \, da = \frac{\sum_i^N P^c_{i} a^{wn}_{i}}{\sum_i^N a^{wn}_{i}} \tag{2.46}
$$

where the averaging is only carried out over interfaces that reside in pore bodies. Here, $P^c$ is local capillary pressure and $a^{wn}$ is local fluid-fluid interfacial area.

Macroscale wetting and nonwetting fluid saturations are defined as:

$$
\langle S^w \rangle = \frac{V^w}{V^n + V^w} = \frac{\sum_i^N S^w_i V_i}{\sum_i^N V_i} \tag{2.47a}
$$

$$
\langle S^n \rangle = 1 - \langle S^w \rangle. \tag{2.47b}
$$
2.5 Description of numerical drainage experiments

In this section, numerical drainage experiments that are performed with the angular pore-scale network model are described and results are shown. The pore-scale network model is used to simulate typical laboratory experiments for the measurement of capillary pressure-saturation relationships. Simulations are performed on 2D- and 3D-networks. First, the drainage of a 3×3 node network is treated. This network is so small that the dimensions of the 9 pore bodies and 8 pore throats are manually selected. Next, larger networks are constructed that consist of 10×20 and 5×5×5 nodes, respectively. The geometrical properties of these networks are given in table 2.3. The porosity of the 3D pore-scale network was calculated to be 0.21.

<table>
<thead>
<tr>
<th>Table 2.3: Lattice network parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice dimensions</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>Coordination number</td>
</tr>
<tr>
<td>Lattice spacing (10⁻³ m)</td>
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<tr>
<td>Min pore body radius (10⁻³ m)</td>
</tr>
<tr>
<td>Max pore body radius (10⁻³ m)</td>
</tr>
<tr>
<td>Mean pore body radius (10⁻³ m)</td>
</tr>
<tr>
<td>Min pore throat radius (10⁻³ m)</td>
</tr>
<tr>
<td>Max pore throat radius (10⁻³ m)</td>
</tr>
<tr>
<td>Mean pore throat radius (10⁻³ m)</td>
</tr>
<tr>
<td>Standard deviation of distribution</td>
</tr>
</tbody>
</table>

2.5.1 Fluid properties

The fluid properties that are used in the numerical experiments are given in table 2.4. They are not chosen randomly, but don’t reflect any specific fluid either. The interfacial tension is that of TCE (trichloroethylene) and water. TCE has a dynamic viscosity of 5.7·10⁻⁴ kg m⁻¹ s⁻². However, viscosity ratio is set to 1. This makes it easier to investigate the pressure field inside the network.

2.5.2 Initial and boundary conditions

The numerical experiments performed are dynamic and quasi-static primary drainage experiments. For 2D networks, only results of dynamic simulations are shown in this chapter. As mentioned in Section 2.4.1, the network is fully saturated with wetting fluid, initially. The top layer of pore bodies acts as an infinite nonwetting fluid.
2.5 Description of numerical drainage experiments

Table 2.4: Fluids’ parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contact angle (°)</td>
<td>0.0</td>
</tr>
<tr>
<td>Interfacial tension (kg s(^{-2}))</td>
<td>0.03</td>
</tr>
<tr>
<td>Wetting fluid viscosity (kg m(^{-1})s(^{-1}))</td>
<td>0.001</td>
</tr>
<tr>
<td>Nonwetting fluid viscosity (kg m(^{-1})s(^{-1}))</td>
<td>0.001</td>
</tr>
</tbody>
</table>

reservoir with \(S^w = 0\). The bottom layer acts as an infinite wetting fluid reservoir with \(S^w = 1\). Initially, fluid pressure \(P\) in all the pore bodies is zero.

Table 2.5: Boundary conditions

<table>
<thead>
<tr>
<th>Condition</th>
<th>Quasi-static</th>
<th>Dynamic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure wetting fluid reservoir (Pa)</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Starting pressure nonwetting fluid reservoir (Pa)</td>
<td>1150</td>
<td>11000</td>
</tr>
<tr>
<td>Pressure step (Pa)</td>
<td>1150</td>
<td>-</td>
</tr>
<tr>
<td>End pressure nonwetting fluid reservoir (Pa)</td>
<td>11000</td>
<td>11000</td>
</tr>
</tbody>
</table>

At the boundaries, Dirichlet pressure conditions are applied. Throughout all simulations, pressure at the wetting fluid reservoir is kept constant at 0 kPa. For dynamic drainage simulations, pressure at the nonwetting fluid reservoir is kept constant at 10.5 kPa for the 2D networks and 11 kPa for the 3D networks. For quasi-static drainage simulations, pressure at the nonwetting fluid reservoir is initially set to 1.15 kPa, which is well below entry capillary pressure. Pressure in the nonwetting fluid reservoir is increased in steps of 500 Pa when equilibrium between the two fluid phases has been achieved. The end value of the nonwetting fluid reservoir pressure in the quasi-static drainage simulations is 11 kPa.

In the 3×3 node case, a hydrophilic filter is applied between the internal (non-boundary) nodes and the wetting fluid reservoir. The size of the pore throats in that layer is reduced to increase entry capillary pressure, as can be seen in figure 2.16.

2.5.3 Local resaturation

A physical realistic property of the angular pore-scale network model is the occurrence of local resaturation during drainage. A pore body that has been drained in a previous time step can get (partly) resaturated in a next time step.

An example of resaturation of pore bodies during drainage is given in figure 2.15. In this graph, local wetting fluid saturations are shown for the center three nodes in a 3×3 node network. It is clearly visible that node 4 gets resaturated after it has been drained to \(S^w\). Also in node 5, wetting fluid displaces some of the nonwetting fluid during the drainage experiment.

The actual fluid distributions for the initial and first 11 time steps are shown in
Figure 2.15: Local resaturation during drainage in a 3×3 node network

In figure 2.17, the drainage procedure in part of a 10×20 nodes network is visualised. Shown are rows 10 through 18 of 20. Figures 2.17(a) through 2.17(c) show the fluid distribution in three subsequent time steps, figure 2.17(d) shows the situation few time steps later. Special attention should be paid to the drainage behaviour of the pore body fourth from the bottom, fourth from the left. This pore body is further referred to as node A. In figure 2.17(a) the pressure in node A is such, that the pore body below it (node B) can be (partly) drained. In figure 2.17(b), one can clearly see that the nonwetting fluid has vanished completely from node A. The full nonwetting fluid content in node A has moved to node B. As drainage continues (figure 2.17(c)), node A gets partly filled again through the connection with its upper neighbour. As wetting fluid saturation in node B is larger than $S_w^\omega$, the nonwetting fluid conductivity in the pore throat connecting nodes A and B is set to zero. In figure 2.17(d), it is evident that nonwetting fluid has passed through node B into adjacent nodes, but that node A is fully filled with the wetting phase again.

2.5.4 Typical results from 3D networks

Standard output of the angular pore-scale network model is volume- and area-averaged capillary pressure, wetting fluid saturation change in time, and interfacial area as function of wetting fluid saturation. In figure 2.18, two dynamic capillary pressure-saturation curves are given. The geometrical properties are given in table
2.5 Description of numerical drainage experiments

Figure 2.16: Visualisation of drainage in a 3×3 network. Figure (a) shows the initial fluid distributions. Nonwetting fluid is light grey, wetting fluid is dark. Figures (b) through (k) show the fluid distribution in 9 subsequent time steps, figure (l) shows the final fluid distribution. A hydrophilic filter is applied at the bottom layer.

2.3, the fluid properties in table 2.4. Applied external capillary pressure is 11 kPa, as given in table 2.5. In this table, also the quasi-static boundary conditions are given. The averaging was performed as mentioned in Section 2.4.9. The area-averaged capillary pressures increases for decreasing wetting fluid saturation, whereas the volume-averaged capillary pressure is more or less constant until irreducible wetting fluid saturation has been reached. This is remarkable, as the definition of $\overline{P}$ does not allow nonwetting fluid pressure to be less than wetting fluid pressure at the pore scale. Equations 2.8 and 2.7 state, that

$$P_n^i = \overline{P_i} + S_i^w P_c^i$$
Local capillary pressure $P_{ci}$ is always either zero or positive and local wetting fluid saturation $S_{wi}$ is always between $S_{wmin}$ and 1. Thus, local nonwetting fluid pressure $P_{ni}$ is always larger than local wetting fluid pressure $P_{wi}$.

The irreducible wetting fluid saturation in the two capillary pressure curves in figure 2.18 is practically zero. This is a result of the angular shape of the network elements in combination with the high boundary capillary pressure. At the end of the drainage procedure, capillary pressure in all pore bodies equals the boundary capillary pressure. The curvature of the fluid-fluid interface in the pore bodies is then so high, that almost all wetting fluid is pushed out of the network.

In figure 2.19, interfacial area during primary drainage is given for quasi-static and dynamic experiments. The curves differ from the local interfacial area curves given in figures 2.11 and 2.12. Latter curves have their maximum at (local) wetting fluid saturation $S_{w}$, where the macroscale curves show an increasing amount of interfacial area for decreasing wetting fluid saturation, until the network is almost completely drained. Apparently, fluid-fluid interfacial area is created during drainage.
2.5 Description of numerical drainage experiments

Figure 2.18: Volume- and area-averaged capillary pressure curves from the 3D network given in table 2.3.

until very low wetting fluid saturation values. The shape of the curves are in good agreement with experimental [43, 62] and numerical results [42, 61, 53, 19].

The dynamic and quasi-static curves shown in figure 2.19 are different. At high wetting fluid saturation values, the dynamic curve is higher than the quasi-static curve. As drainage proceeds, quasi-static interfacial area becomes higher than dynamic interfacial area. This difference is due to the fact that in the dynamic drainage experiment, more pore throats, and therefore, more pore bodies, are accessible for the nonwetting fluid phase at the onset of drainage. At the start of drainage, more interfacial area is created. In the quasi-static experiment, less pore bodies are accessible at the onset of drainage. As drainage proceeds, more interfacial area is created in the quasi-static case. The nonwetting fluid front may behave less like a piston moving through the porous medium than in the dynamic case. Deviation from a stable piston-like fluid front creates additional interfacial area. At the end, all pore bodies go to $S_{\text{w}_{\text{min}}}$ saturation, giving minimum interfacial area. Then, the dynamic and quasi-static interfacial areas are equal.

2.5.5 Computation of damping coefficient $\tau$

In the first chapter of this thesis, dynamic capillary pressure is introduced [60, 1]. Dynamic capillary pressure is assumed to be related to static capillary pressure by
Figure 2.19: Interfacial area from the dynamic and quasi-static drainage of the 3D network given in table 2.3.

\[ P_{\text{dynamic}}^c - P_{\text{static}}^c = -\tau \frac{\partial S_w}{\partial t}. \]  
\[ (2.48) \]

This can be rewritten as:

\[ \tau = \frac{P_{\text{dynamic}}^c - P_{\text{static}}^c}{-\frac{\partial S_w}{\partial t}} = \frac{\Delta P^c}{-\frac{\partial S_w}{\partial t}}. \]  
\[ (2.49) \]

Using the angular pore-scale network model, damping coefficient \( \tau \) can be calculated. Preliminary results of this analysis are published in [26]. The procedure is as follows\(^1\): first, from typical results as given in figure 2.20, both \( P_{\text{dynamic}}^c - P_{\text{static}}^c \) and \(-\frac{\partial S_w}{\partial t}\) are obtained at a specific wetting fluid saturation. Then, using equation (2.49), damping coefficient \( \tau \) is computed for each of these saturations. These results are then plotted in a graph.

For the computation of damping coefficient \( \tau \) a 5x5x20 node network has been used. Geometrical properties of the network are given in table 2.3, fluid properties in table 2.4. Imposed boundary conditions for the dynamic and quasi-static drainage simulations are given in table 2.5.

Area-averaged capillary pressure curves are used for the computation of damping coefficient \( \tau \), since the explanation of the rather constant volume-averaged capillary

\(^1\)This procedure has been refined in a later stage. The modified method is used in Chapters 6 and 7.
2.5 Description of numerical drainage experiments

Figure 2.20: Dynamic and quasi-static capillary pressure curves (left) and wetting fluid saturation in time (right) for the computation of $\tau$.

pressure curve in Figure 2.18 is uncertain. In Figure 2.21, dynamic and quasi-static capillary pressure are shown as functions of wetting fluid saturation. The capillary pressure curves are not smooth. The irregularity in the capillary pressure curves is so large, that they touch at wetting fluid saturation $S^w = 0.6$. At the onset of drainage, the quasi-static curve has strong jumps, and is above the dynamic capillary pressure curve. The dynamic curve is above the static curve for wetting fluid saturations 0.9 and below. This is due to the fact that the nonwetting fluid distribution is different for the dynamic and the quasi-static experiments at the onset of drainage.

To process the data, a polynomial fit is applied to these data. The fitted curves are not shown in the graphs. In Figure 2.22, wetting fluid saturation is plotted versus time. The saturation rate of change is fairly constant at 0.61 s$^{-1}$.

Using equation (2.49), damping coefficient $\tau$ can now be computed. This has been done for wetting fluid saturations $S^w = 0.95, 0.90, \ldots, 0.05$. The found relationship between damping coefficient $\tau$ and wetting fluid saturation is plotted in Figure 2.23. From this graph, it follows that $\tau$ is a function of wetting fluid saturation. The value of $\tau$ is ranges from 498 Pa s at wetting fluid saturation $S^w = 0.95$ to 2426 Pa s at $S^w = 0.05$. These values are rather low in comparison to that found in literature (hassanzadeh, dahle, kalaydjian, stauffer). The shape of the curve in Figure 2.23 is similar to the results found by Dahle et al. [18, 17].

The value of damping coefficient $\tau$ increases as drainage proceeds. At first sight, this is contrary to expectations. One would expect damping coefficient $\tau$ to decrease for later stages of drainage, as the dynamic capillary pressure curve converges to the static curve. However, as can be seen in Figure 2.21, the dynamic and quasi-static curve do not converge before wetting fluid saturation becomes practically zero (except for the jump in the dynamic curve at $S^w = 0.6$).
Chapter 2. The angular pore-scale network model

Figure 2.21: Dynamic and quasi-static capillary pressure curves of the 3D network given in table 2.3.

Figure 2.22: Wetting fluid saturation in time of the 3D network given in table 2.3. Saturation rate of change is $0.61 \text{ s}^{-1}$. 
2.6 Difficulties encountered in the angular model

The development of the angular pore-scale network model was abandoned because of a number of problems that couldn’t be solved in the remaining time of the research project. Main problems are the determination of equilibrium between the fluids and the time step size. Although these problems are closely related, they will be treated in following two separate sections. To illustrate the difficulties, results from a 2D network have been used. Geometrical properties and fluid properties are given in tables 2.6 and 2.7. Pressure at the top fluid reservoir is 11 kPa, at the bottom reservoir 1 kPa.

2.6.1 Time step size

During simulations, it has been observed that the time step size can decrease to practically zero. An example is given in figure 2.24. In this figure, time step size is plotted against the first 1000 time steps. Clearly, time step size varies considerably between practically zero and 0.007 seconds.

As treated in Section 2.4.2, at every time step a filling time is determined for each pore body. The smallest filling time is used as the next overall time step size. The filling times $\Delta t_i$ can be seen to be $\Delta t_i \sim \frac{V_i \Delta S^{\text{w}}}{|\eta|}$ where $V_i$ is constant. There are two possible explanations for a very small time step size in the angular model: either the net fluid phase flux is very high, or the local change in saturation is very small in combination with regular net flux values.
Table 2.6: Lattice network parameters

<table>
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<th>Parameter</th>
<th>Value</th>
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<tr>
<td>Lattice dimensions</td>
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<td>Coordination number</td>
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</tr>
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<td>Lattice spacing (10^{-3} m)</td>
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<tr>
<td>Min pore body radius (10^{-3} m)</td>
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<tr>
<td>Max pore body radius (10^{-3} m)</td>
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<tr>
<td>Mean pore body radius (10^{-3} m)</td>
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<td>Mean pore throat radius (10^{-3} m)</td>
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<td>Standard deviation of distribution</td>
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Table 2.7: Fluids’ parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contact angle (°)</td>
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<tr>
<td>Interfacial tension (kg s^{-2})</td>
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</tr>
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</tr>
<tr>
<td>Wetting fluid viscosity (kg m^{-1}s^{-1})</td>
<td>0.001</td>
</tr>
</tbody>
</table>

Which mechanism causes the observed small time step size can be found through investigation of the (global) saturation change per time step. If the net fluid flux $q_i$ is very high, local and global saturation will change in each time step. If the local change in saturation is small, this is less likely. In that case, there might be a net change in global wetting fluid saturation, but this would be negligible.

To illustrate this, three parts of figure 2.24 have been enlarged and shown with the corresponding change in global wetting fluid saturation in the same figure. These are given in figures 2.25 through 2.27. From these figures it follows that global saturation does not change when time steps are small. Thus, the extremely small time step sizes are caused by small local saturation changes.

Three explanations for these very small time steps sizes can be given. The first explanation lies in the explicit computation of local saturation in the used IMPES-scheme. When saturation target states $S^w_i$ and $S^{w_{min}}_i$ are computed, round-off errors may occur. A minimum time step size is computed based on a target state, and net fluid phase flux is multiplied with that time step to arrive at the target state. Sometimes, the target state is not exactly reached. An example of this is given in figures 2.15 and 2.16. Between time step 9 and 10 (figures 2.16(j) and 2.16(k)), saturation doesn’t visibly change in any node. In time step 9, pore body 4 has target state 0.48 ($S^w_i$), but it was computed to be $0.48 + \epsilon$, where $\epsilon$ is $1.7 \cdot 10^{-10}$. Time step size determining node for time step 10 is then pore body 4 again, as filling time is
2.6 Difficulties encountered in the angular model

Figure 2.24: Time step size for the first 1000 time steps during drainage in a 20×62 node network

Figure 2.25: Plot of time step size and wetting fluid saturation for time steps 200 – 300 in figure 2.24.
Figure 2.26: Plot of time step size and wetting fluid saturation for time steps 300 – 500 in figure 2.24.

Figure 2.27: Plot of time step size and wetting fluid saturation for time steps 750 – 850 in figure 2.24.
2.6 Difficulties encountered in the angular model

It is to be expected for larger networks that this mechanism will give rise to at most few subsequent small time step sizes.

A second explanation for the small time step sizes can be found in the oscillatory behaviour of drainage at pore bodies. When the entry pressure of a pore throat is overcome, the throat will be drained instantaneously and the downstream adjacent pore body will be partially drained in the current time step, as shown in graph I in figure 2.28. Since the pore throats are rectangular in cross section, part of the wetting fluid may move back into the upstream pore body where the nonwetting fluid came from. This is shown in graph II in figure 2.28. This increases local wetting fluid saturation in the upward pore body. Saturation might even be increased beyond its value of either minimum saturation $S_{\text{min}}^w$ or $S_{\text{n}}^w$, as explained in Section 2.4.2. When the saturation increases just above one of the two states, it is very likely that the upstream pore body will determine next the (smallest) time step in the network. This is shown in graphic III in figure 2.28. This time step will then continue to become smaller and smaller every time step. This mechanism is expected to cause only few small time step sizes per pore body. Eventually, it is difficult to determine the distinction between this mechanism and the above-mentioned round-off error mechanism.

In addition to this single node oscillation, it can happen that few pore bodies exchange back and forth a small amount of fluid in subsequent time steps. This is observed frequently during simulations. An example is given in figure 2.29. In this figure, time step size determining node and global wetting fluid saturation are plotted for the same time steps as the ones in figure 2.24. It can be seen that in periods where wetting fluid saturation does not change, time step size is determined by two nodes only. These nodes do not have to be adjacent. In the last 200 times...
steps in figure 2.29, time step size determining nodes are 267 and 352, with only one exception. It is remarkable that these nodes are directly connected in the 20×62 node network. It is very well possible that these nodes are connected through a single cluster of nonwetting fluid.

![Figure 2.29: Time step size determining nodes and global wetting fluid saturation per time step in a 20×62 nodes network.](image)

To see whether this oscillatory behaviour is limited in time, a simulation was run for 20,000 time steps. The input of this simulation is -except for the maximum number of time steps- identical that of the simulation from which data figure 2.29 was constructed. The oscillatory movement of fluid between nodes 267 and 325 continued throughout the simulation (starting from around time step 800).

Most troublesome aspect of this behaviour is that the temporal description of fluid flow in a porous medium is not governed by the physics at the fluid displacement front itself. In other words, the nonwetting fluid might have drained 60% of the pore-scale network, while the time step size that is computed for that situation is governed by the local pressure field somewhere in the top 20% of the network.

Another problem with the occurrence of very small time step sizes is that it affects the determination of equilibrium between the two fluid phases in the quasi-static simulations. This is further addressed in next section.

### 2.6.2 Determination of equilibrium

The use of the total fluid pressure \( P \) helps to speed up the simulations. However, as a result, determination of equilibrium between the two fluid phases was made
problematic. When fluids in a pressure cell are at equilibrium, in the absence of gravity, as is the case in the angular network simulations, the two continuous fluid pressures should have the same pressures as their corresponding reservoirs.

Using the definition of $P$, one can see that $P$ represents nonwetting fluid pressure in the top reservoir and wetting fluid pressure in the bottom reservoir. A typical solution of the pressure field would therefore be a more or less linear gradient in $P$ over the height of the network. The definition of $P$ in equation (2.6) shows that this pressure is a combination of wetting and nonwetting fluid pressures. In order to arrive at a hydrostatic pressure distribution, the nonwetting fluid part and the wetting fluid part have to be separated. This is only possible when the continuous nonwetting fluid phase is disconnected from the continuous wetting fluid phase. This disconnection can only be established by setting both phase conductivities in the throat between the continuous fluids to zero. Thus, the (continuous) fluids will be completely separated, and saturation-weighted total pressure $P$ represents the individual fluid phase pressures, just like in the fluid reservoirs at the top and bottom of the pore-scale network.

However, because of the angular shape of the pore throats, wetting fluid will always reside in a throat, even when that throat is drained. This presence of wetting fluid implies a nonzero wetting fluid conductance throughout the porous medium. This leads to the above-mentioned gradient in $P$. Using capillary pressure, the local fluid phase pressures are then be found. This local capillary pressure depends not only on boundary capillary pressure, but also on the size of the pore body. The gradient in $P$ and the difference in size between two neighbouring pore bodies may result in phase pressure gradients, even when equilibrium between the two fluid phase pressures should have been achieved. Due to the angular shape of the pore throats, the nonwetting and wetting fluid pressures cannot be separated. Thus, establishing a hydrostatic pressure distribution in the continuous fluids uniquely implies disregarding the specific angular shape of the pore throats, such that only a single fluid is allowed to occupy a pore throat at each time.

In the angular pore-scale network model, equilibrium was assumed to be achieved when global wetting fluid saturation did not change in a certain number of subsequent time steps (see Section 2.4.7). In Section 2.6.1, it is shown that time step size can be practically zero for a large number of subsequent time steps. During such an event, global wetting fluid saturation has been shown not to change. As the two fluids in the network are considered to be incompressible, this can only hold when influx of nonwetting fluid is zero. Thus, the occurrence of small time step sizes during drainage make it very difficult to determine whether equilibrium between the two fluid phases has been achieved.

2.7 Summary

In this chapter, a pore-scale network model with elements (pore bodies and pore throats) of rectangular cross section is presented. The shape of the elements allows two immiscible fluids (wetting and nonwetting) to reside in the same network element.
Chapter 2. The angular pore-scale network model

at the same time. This model is referred to as the angular pore-scale network model.

In principle, the angular pore-scale network model is developed to handle both
dynamic and quasi-static drainage. However, when simulating quasi-static and dy-
namic drainage, numerical problems occurred which made it technically impossible
to simulate performed laboratory experiments at the same scale. For a smaller
porous medium sample, an indication of the behaviour of damping coefficient $\tau$
could be given.

Preliminary results show that $\tau$ is function of wetting fluid saturation. Results in
this chapter also indicate that averaging over the area of fluid-fluid interfaces gives a
better representation of capillary pressure than averaging over fluid phase volumes.

The strong advantage of this model is its weak point at the same time: because of
its angular geometry, it can simulate two-phase flow in a more realistic way than the
traditional (circular) ball-and-stick models. However, this angular geometry allows
countercurrent imbibition, with lead to uncontrolled oscillations.
Chapter 3

The quasi-static circular pore-scale network model

In this chapter, the quasi-static pore-scale network model is described. The geometrical properties, assumptions, boundary conditions and fluid properties are given in Sections 3.1 through 3.3. In Section 3.4, the modelling procedure is covered. Results of primary drainage simulations in 2D and 3D pore-scale networks are given in Section 3.5. Summarising conclusions are drawn in last section of this chapter.

3.1 Geometry and assumptions

The pore network is a regular lattice of pore bodies and pore throats. A pore body is spherical in shape, a pore throat is a cylinder (see figure 3.1). Pore body and throat sizes are assumed to follow a truncated log-normal distribution, defined by:

\[
f(r; \sigma_{nd}) = \frac{\sqrt{2} \exp \left[ -\frac{1}{2} \left( \frac{\ln r}{\sigma_{nd}} \right)^2 \right]}{\sqrt{\pi \sigma_{nd}^2} r} \left[ \text{erf} \left( \frac{\ln r_{ch}}{\sqrt{2} \sigma_{nd}} \right) - \text{erf} \left( \frac{\ln r_{min}}{\sqrt{2} \sigma_{nd}} \right) \right]
\]

(3.1)

where \( r \) is radius, \( r_{ch} \) is mean radius, \( r_{min} \) is minimum radius, \( r_{max} \) is maximum radius and \( \sigma_{nd} \) is standard deviation. For pore bodies and pore throats, the same standard deviation, but different mean, minimum and maximum radii are used.

The following simplifying assumptions are made in this model:

- Both fluids are considered to be incompressible; the solid matrix is rigid and perfectly wetting.
- The volumes of pore throats are negligible compared to those of pore bodies. Therefore, the pore throat volumes are not included in the computation of average saturation. However, the resistance to the flow offered by pore throats
is much larger than that of pore bodies. Therefore, resistance to flow by pore bodies is neglected.

- The passage of a fluid-fluid interface through a pore throat occurs instantaneously (i.e. the residence time is negligible compared to the characteristic flow time).
- Only one fluid resides in a pore throat at a time.
- Local capillary pressure is zero for all pore bodies. Thus, pressures of the two fluids are equal, i.e. there is only one pressure, at a pore body.
- Gravity is neglected, hence fluid flow is driven by pressure gradients only.

### 3.2 Boundary conditions

A typical property of quasi-static models is that fluids pressures and distribution are determined at equilibrium states. Therefore, time is not a primary variable. Fluid-fluid interfaces are not tracked explicitly in time. Instead, their equilibrium positions are determined based on the boundary conditions. As such, it is not necessary to set up and solve the full set of equations governing the change of fluid pressures and saturation. As gravity is not taken into account and only equilibrium points are considered, both fluid phases are assigned their corresponding reservoir pressure throughout the simulation.

The boundary conditions in the quasi-static model are Dirichlet type. The top and bottom layers of pore bodies represent infinite fluid reservoirs with fixed pressure and saturation. The upper and lower boundaries are connected to nonwetting and wetting fluid reservoirs, respectively. Their pressure difference is called "the imposed
capillary pressure” of the network. Initially, the network is filled with the wetting fluid and the imposed capillary pressure is such, that the nonwetting fluid cannot enter the network. Then, pressure at the nonwetting fluid boundary is increased with a predefined pressure step, until drainage starts. When no interface can move any further, equilibrium between the two fluid phases has been achieved. Nonwetting fluid pressure is everywhere equal to the upper boundary pressure and the wetting fluid pressure is everywhere equal to the lower boundary pressure. Now, pressure in the nonwetting fluid boundary is increased and the interfaces are interrogated again. This is repeatedly done until a preset maximum pressure difference between the fluid reservoirs has been reached.

As the model is constructed to simulate laboratory experiments, also hydrophobic and hydrophilic filters are modelled. For this, two conditions should be met: wetting fluid is not allowed to flow into the nonwetting fluid reservoir, and nonwetting fluid is not allowed to enter the wetting fluid reservoir. The first condition is always met in simulations of drainage from above under Dirichlet boundary conditions. The pressure in the top layer, representing the nonwetting fluid boundary is always higher than that of a layer below. The second condition is not automatically met, however. If no measures are taken, nonwetting fluid can enter the wetting fluid reservoir when entry pressure of the pore throats adjacent to the bottom boundary is overcome. To avoid this, the fluid conductivity of a drained pore throat adjacent to the wetting fluid reservoir is set to zero. The (nonwetting) fluid inside the throat becomes immobile. In terms of boundary conditions, this implies that at that pore throat, a no-flow condition for the nonwetting phase is employed.

### 3.3 Fluid properties

Interfacial tension is the only relevant parameter that describes the fluid-fluid interaction in this quasi-static model. As gravity is neglected, density effects do not occur. Also, values of fluid viscosity are redundant as flow is not modelled. Fluid viscosities can be used to find the pressure field in the two fluids during flow. However, in the quasi-static model, only points where the two fluids are at equilibrium points are relevant.

### 3.4 Procedure

The quasi-static pore-scale network model uses an invasion-percolation principle [13]. For a given imposed capillary pressure, all pore throats with the interface at the upper boundary are checked for entry pressure. If their entry pressures are less than the imposed capillary pressure, they will be invaded by the nonwetting fluid. Alternatively, Young-Laplace equation [4] can be used to find an entry radius $r_{\text{entry}}$:

$$P_{\text{entry}}^c = \frac{2\sigma \cos \theta}{r}$$  \hspace{1cm} (3.2)
Chapter 3. The quasi-static circular network model

$$r_{\text{entry}} = \frac{2\sigma \cos \theta}{P_{\text{entry}}}.$$  \hspace{1cm} (3.3)

The entry radius defines the accessible pore throat radii. If the radius of a pore throat is larger than the entry radius, wetting fluid in that throat is replaced by nonwetting fluid. Also, the adjacent (downstream) pore body is completely drained, an interface is placed at the entrance of all other pore throats that are connected to that pore body. Then, the check for entry pressure is repeated. This procedure is referred to as the interface stability test.

This procedure is repeated until no interfaces in the network can move any further. At this stage, all pore throats (and adjacent pore bodies) whose radius is larger than $r_{\text{entry}}$ and are connected to the nonwetting phase boundary are invaded by nonwetting fluid. The fluids are now at equilibrium. The average saturation is computed as well as the average capillary pressure, which is the pressure difference between the nonwetting and the wetting fluid boundary. These two values define a data point on the quasi-static $P_c - S^w$ curve.

Then, the imposed capillary pressure is increased by increasing the pressure at the nonwetting fluid boundary with a predefined pressure step, and the check for interface stability can be performed again. The whole procedure is repeated until the nonwetting fluid boundary pressure has reached a predefined end value or the wetting phase irreducible saturation is reached.

The fluid-fluid interfaces thus move from equilibrium position to equilibrium position, as schematically illustrated in figure 3.2. In this figure, a 1D column of pore bodies and pore throats is shown at 4 subsequent states a through d. The boundary nodes represent infinite fluid reservoirs. A boundary pressure and saturation are assigned to them. Saturation in boundary nodes is kept constant throughout the simulations, where pressure is increased stepwise.

Initially, only the top node is filled with nonwetting fluid, and the other nodes and throats are filled with wetting fluid (a). When the pressure in the top node is increased stepwise with with a small amount, eventually the entry capillary pressure of its adjacent throat will be overcome. At that moment, the pore throat and the adjacent pore body will be drained. The pore throat between the second and third pore body is smaller than the one between the first and the second. Therefore, its entry capillary pressure is such that the nonwetting fluid cannot move further under the present boundary conditions. Thus, equilibrium has been achieved. Average saturation and capillary pressure are computed to give second point on the capillary pressure-saturation curve (b).

Then, pressure in the top node increased again, until the entry capillary pressure of the pore throat between the second and third pore body is overcome. At that point, the pore throat and the third pore body is filled with nonwetting fluid. Since the radius of the pore throat between the third and the fourth pore body is larger than the ones already drained, this pore throat and its neighbouring pore body are drained as well. The interface stops at the entrance of the last pore throat due to the entry capillary pressure threshold. At this point, the two fluids are at equilibrium again. Average saturation and capillary pressure are computed to define next point
3.5 Results

on the capillary pressure-saturation curve (c). Similarly, last point on the capillary pressure-saturation curve is found (d).

![Diagram](image)

Figure 3.2: Schematic representation of three subsequent steps in a one-dimensional drainage procedure. Pressure in the top node is increased in small steps every time the fluid-fluid interface is blocked by entry capillary pressure of a pore throat. The corresponding capillary pressure curve is shown on the right.

Averaging is done only over the internal nodes. The nodes representing fluid reservoirs are ignored. This has no effect on the value of capillary pressure, and the full saturation range from 0 to 1 is covered.

3.5 Results

The quasi-static pore-scale network model is capable of simulating both two-dimensional and three-dimensional networks. For both types of networks, examples of results are given in this section. Boundary conditions and fluid properties are the same for two-dimensional and three-dimensional simulations. Boundary conditions are given in table 3.1. The initial imposed capillary pressure is too small for the onset of drainage.

<table>
<thead>
<tr>
<th>Boundary conditions</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure of wetting fluid reservoir (kg \cdot m^{-1} \cdot s^{-2})</td>
<td>0.0</td>
</tr>
<tr>
<td>Starting pressure of nonwetting fluid reservoir (kg \cdot m^{-1} \cdot s^{-2})</td>
<td>1000.0</td>
</tr>
<tr>
<td>Pressure steps size (kg \cdot m^{-1} \cdot s^{-2})</td>
<td>50.0</td>
</tr>
<tr>
<td>Final pressure of nonwetting fluid reservoir (kg \cdot m^{-1} \cdot s^{-2})</td>
<td>10000.0</td>
</tr>
</tbody>
</table>
Fluid properties are based on those of water and PCE. Interfacial tension between the two fluids is 0.0475 kg s$^{-2}$. Geometrical properties are given in table 3.2. The properties are chosen to match a model sand (called Zeijen) as explained in Chapter 6.

<table>
<thead>
<tr>
<th>Table 3.2: Lattice network parameters</th>
<th>40×40</th>
<th>10×10×20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice dimensions</td>
<td>40×40</td>
<td>10×10×20</td>
</tr>
<tr>
<td>Coordination number</td>
<td>4</td>
<td>6</td>
</tr>
<tr>
<td>Lattice spacing (10$^{-4}$ m)</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>Min pore body radius (10$^{-4}$ m)</td>
<td>0.8</td>
<td>0.8</td>
</tr>
<tr>
<td>Max pore body radius (10$^{-4}$ m)</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Mean pore body radius (10$^{-4}$ m)</td>
<td>0.9</td>
<td>0.9</td>
</tr>
<tr>
<td>Min pore throat radius (10$^{-4}$ m)</td>
<td>0.01</td>
<td>0.01</td>
</tr>
<tr>
<td>Max pore throat radius (10$^{-4}$ m)</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>Mean pore throat radius (10$^{-4}$ m)</td>
<td>0.125</td>
<td>0.125</td>
</tr>
<tr>
<td>Standard deviation of distribution</td>
<td>1.0</td>
<td>1.0</td>
</tr>
</tbody>
</table>

### 3.5.1 2D network: 40×40 nodes

For the visualisation of the fluid distributions in a 2D network, a network that consists of 40×40 nodes is used. A primary drainage curve is computed and shown in figure 3.3. At three points, indicated by A, B and C in the graph, fluid distributions are illustrated. This is done in figures 3.4 through 3.6. The capillary pressure-saturation curve is not smooth, as the equilibrium points are connected by straight lines. The pressure steps are very small, only 50 Pa. The homogeneous character of the porous medium is reflected by the size of the plateaus in figure 3.3.

In figures 3.4 through 3.6, nonwetting fluid is shown in light grey and wetting fluid in dark colour. It is obvious from figure 3.4 that the nonwetting fluid does not move through the porous medium as a stable horizontal front. Due to capillary restrictions, the nonwetting fluid drains the network on the left side first. The drainage pattern is sensitive to capillary thresholds because of the small size of the capillary pressure increment.

Also clearly visible are patches of wetting fluid that are disconnected from the wetting fluid reservoir. These patches can not be reconnected to their reservoir, and only contribute to the irreducible wetting fluid saturation. Once a volume of wetting fluid is disconnected (gets trapped), it will stay like that throughout the rest of the drainage procedure. These wetting fluids will not redistribute.
3.5 Results

Figure 3.3: Quasi-static capillary pressure-saturation curve from the 2D network described in table 3.2. A, B and C indicate points at which a visualisation of the fluid distribution was generated. These are shown in figures 3.4 (A), 3.5 (B) and 3.6 (C).

3.5.2 3D network: $10 \times 10 \times 20$ nodes

For the visualisation of the fluid distributions in a 3D network, a network that consists of $10 \times 10 \times 20$ nodes is used. A primary drainage curve is computed and shown in figure 3.7. At four points, indicated by A, B, C and D in the graph, fluid distributions are illustrated. This is done in figures 3.8 through 3.11.

The two-dimensional and three-dimensional networks have the same geometrical properties, except for the number of nodes and the coordination number. As a result of the increased size, the capillary pressure-saturation curve from the three-dimensional network is more smooth, as can be seen in figure 3.7.

Similar to the displacement pattern in the two-dimensional case, the nonwetting fluid enters the network in distinct fingers rather than as a stable front. The explanation for this is the same as in the previous section. As gravity is not taken into account and only equilibrium points are considered, both fluid phases are assigned their corresponding reservoir pressure throughout the simulation. Therefore, the spreading is controlled by the pore throat distribution. Or, to be more precise, by the combination of the radius and the location of each of the pore throats.

In figures 3.8 and 3.9, this is clearly visible. Although the nonwetting fluid should spread equally fast downward as sideways, it can be seen that first one or more fingers are formed that spread downward and laterally when the imposed capillary pressure is increased.

This is due to the combination of the structure of the porous medium and the small size of the pressure increments.
The small pressure increments increase the possibility of bypassing larger volumes of wetting fluid in the network. These volumes can become entrapped. One would expect that this would not happen much in the three-dimensional network, as connectivity is higher than in the two-dimensional network. The relatively high irreducible wetting fluid saturation of 0.2 at the end of the drainage procedure contradicts this idea. Connectivity in the 3D network is higher than in the 2D network, but the effect doesn’t show too clearly because of the relatively small lateral size of the network. It is to be expected that connectivity becomes more important when the network is larger, especially when the size of the pore throats can vary as much as they do in these simulations.

In figures 3.10 and 3.11, it can be seen that a small change in saturation leads to a very large change in capillary pressure. The high increase in capillary pressure occurs when the nonwetting fluid has reached the bottom layer that represents the wetting fluid reservoir. As a hydrophilic filter is modelled, nonwetting fluid cannot enter the bottom layer. As nonwetting fluid is always connected to its reservoir, wetting fluid that was bypassed can become definitely immobile when the nonwetting fluid reaches the wetting fluid reservoir. As the spreading of nonwetting fluid continues not only in the center of the porous medium, but also at the bottom, more and more wetting fluid becomes disconnected from its reservoir. Accordingly, it becomes more and more difficult to drain the wetting fluid from the network. This can happen in a short phase of the drainage, leading to a strong change in capillary pressure over
3.6 Summary

In this chapter, a quasi-static pore-scale network model is presented. In this model, pore bodies are spheres and pore throats are cylinders. Pore throats are considered to have no volume with respect to the pore bodies.

The displacement procedure is similar to that in percolation theory: based on boundary conditions (external capillary pressure) and accessibility and allowability.
Chapter 3. The quasi-static circular network model

Figure 3.6: Final fluid distribution in the 2D network at wetting fluid saturation 0.26, at point C in figure 3.3. Nonwetting fluid is light grey, wetting fluid is dark.

Figure 3.7: Quasi-static capillary pressure-saturation curve from the 3D network described in table 3.2.

(through entry capillary pressure of connected pore throats), nonwetting fluid drains
3.6 Summary

Figure 3.8: Fluid distribution in the 3D network at wetting fluid saturation 0.82, indicated by A in figure 3.7. Nonwetting fluid is light grey, wetting fluid is dark.

the porous medium. Since the fluid pressure field does not have to be solved, the required amount of computational time is very small.

Partially filled pore bodies do not exist in this model. The error created by ignoring partially filled pore bodies when comparing quasi-static capillary pressure with dynamic capillary pressure is marginal, as shown in Appendix B.
Figure 3.9: Fluid distribution in the 3D network at wetting fluid saturation 0.46, indicated by B in figure 3.7. Nonwetting fluid is light grey, wetting fluid is dark.
Figure 3.10: Fluid distribution in the 3D network at wetting fluid saturation 0.24, indicated by C in figure 3.7. Nonwetting fluid is light grey, wetting fluid is dark.
Figure 3.11: Fluid distribution in the 3D network at wetting fluid saturation 0.20, indicated by D in figure 3.7. Nonwetting fluid is light grey, wetting fluid is dark.
Chapter 4

The dynamic circular pore-scale network model

This chapter describes the dynamic pore-scale network model that has been developed in the framework of this research project. This model is basically similar to the model of Blunt & King [6]. The main difference is that Blunt & King imposed a constant flux of nonwetting fluid phase at the inflow boundary as they were interested in investigating relative permeability relationships. In the dynamic model presented here, however, a constant nonwetting fluid phase pressure at the inflow boundary is imposed. This makes it possible to simulate quasi-static drainage experiments as performed in laboratories. For this purpose, algorithms have been included for calculating average capillary pressure and saturation.

4.1 Geometry and assumptions

The pore network is a regular lattice of pore bodies and pore throats. A pore body is spherical in shape, a pore throat is a cylinder (see figure 4.1). Pore body and throat sizes are assumed to follow a truncated log-normal distribution given in Section 3.1.

The following simplifying assumptions are made in this model:

- Both fluids are considered to be incompressible, the solid matrix is rigid and perfectly wetting.

- The volumes of pore throats are negligible compared to those of pore bodies. Therefore, the pore throat volumes are not included in the computation of average saturation. However, the resistance to flow offered by pore throats is much larger than that of pore bodies. Therefore, resistance to flow by pore bodies is neglected.

- The passage of a fluid-fluid interface through a pore throat occurs instantaneously (i.e. the residence time is negligible compared to the characteristic
Chapter 4. The dynamic circular network model

Figure 4.1: Schematic representation of a pore body and adjacent pore throats in a 3D network with coordination number six (left) and a 2D network with coordination number four (right). Grid spacing is constant. Pore body and throat radii follow a truncated log-normal distribution.

flow time).

- Flow in the pore throats is laminar and its rate is given by Poiseuille’s formula.

- Local capillary pressure is zero for all pore bodies. Thus, pressures of the two fluids are equal, i.e. there is only one pressure, at a pore body.

- Only one fluid resides in a pore throat in a time (i.e. film flow and corner flow are neglected).

- Gravity is neglected, hence fluid flow is driven by pressure gradients only.

From these assumptions, it follows that only one fluid pressure field for the whole network has to be solved at any given time. Nevertheless, there is a local-scale capillary pressure originating from pore throats entry pressure. It is equal to the difference in pressures of nonwetting and wetting phases occupying pore bodies adjacent to the given pore throat.

4.2 Governing pore-scale equations

In this section, pore-scale equations that are used in the dynamic pore-scale network model under the assumptions mentioned in Section 4.1 are described. Subscript \( i \) denotes pore body \( i \), \( j \) denotes one of its neighbouring pore bodies, and \( ij \) the connecting pore throat. Superscripts \( w \) and \( n \) denote wetting and nonwetting fluid phases, respectively.
4.2 Governing pore-scale equations

Continuity equations
In the absence of external sources and sinks, the principle of volume conservation for a pore body $i$ connected to neighboring pore bodies $j$ ($j \in N_i$) can be written as:

$$V_i \frac{\Delta S_i^\alpha}{\Delta t} + \sum_{j \in N_i} Q_{ij}^\alpha = 0, \quad (\alpha = w, n) \quad (4.1)$$

where $V_i$ is volume, $t$ is time, $S_i^\alpha$ is the local $\alpha$-phase saturation (fraction of volume $V_i$ filled by fluid $\alpha$), $Q_{ij}^\alpha$ is the $\alpha$-phase flux from pore body $i$ to $j$, $N_i$ is the number of pore bodies connected to $i$.

Since, by definition,

$$S_i^w + S_i^n = 1 \quad (4.2)$$

summation of equation (4.1) for both phases results in the following system of equations:

$$\sum_{j \in N_i} (Q_{ij}^w + Q_{ij}^n) = 0. \quad (4.3)$$

Flux equations
The flow of each phase within a pore throat is assumed to be given by Hagen-Poiseuille formulae. Wetting and nonwetting phase fluxes are expressed in terms of the wetting and nonwetting phase pressures (neglecting gravitational terms):

$$Q_{ij}^\alpha = K_{ij}^\alpha \left( P_i^\alpha - P_j^\alpha \right), \quad (\alpha = w \text{ or } n) \quad (4.4)$$

where $K_{ij}^\alpha$ is the $\alpha$-phase conductivity of the pore throat between pore bodies $i$ and $j$, $P_i^\alpha$ and $P_j^\alpha$ are $\alpha$-phase pressures in pore body $i$ and $j$, respectively. $K_{ij}^\alpha$ depends on the fluid occupancy of the pore throat $ij$:

$$K_{ij}^\alpha = \frac{\pi R_{ij}^4}{8 \mu^\alpha L_{ij}} \quad (4.5)$$

where $R_{ij}$ is radius, $L_{ij}$ is length, and $\mu^\alpha$ is the $\alpha$-phase dynamic viscosity. For a given pore throat, equation (4.4) will be written either for $\alpha = w$ or $\alpha = n$ depending on the phase occupancy of that throat at that instance.

Final system of linear equations
Equations (4.3) and (4.4) can be combined to obtain a set of linear equations in terms of $P$. For a given pore body $i$, the typical equation reads:

$$\sum_{j \in N_i} \left[ (K_{ij}^w + K_{ij}^n) (P_i - P_j) \right] = 0. \quad (4.6)$$

Only one pressure field, rather than both fluid phase pressure fields has to be solved. The summation of conductivities is allowed since only one fluid can occupy a pore throat at a time. If wetting phase occupies the pore throat, $K_{ij}^n$ equals zero, and vice versa.
4.3 Model description

In this section, the initial and boundary conditions, and algorithms used in the dynamic pore-scale network model are described. At this stage, the model is limited to simulate primary drainage experiments only. The flow chart describing the steps taken in the pore-scale network model is given in figure 4.2.

![Flow chart of the pore-scale network model](image)

**Figure 4.2: Flow chart of the pore-scale network model**

4.3.1 Initial and boundary conditions

Initially, the network is fully saturated with wetting fluid. The top layer of pore bodies acts as an infinite nonwetting fluid reservoir with $S^w = 0$. The bottom layer acts as an infinite wetting fluid reservoir with $S^w = 1$. Initially, pressure in all the pore bodies is zero.

Boundary conditions in the dynamic network model are of Dirichlet type: constant pressure is prescribed at the top and the bottom of the network. The network does not have any pore throats pointing outward. Thus, flow is not possible through...
4.3 Model description

![Diagram of boundary conditions](image)

Figure 4.3: Boundary conditions as used in the pore-scale network model

the sides of the network and, virtually, no-flow conditions are applied. The boundary conditions are sketched in figure 4.3.

### 4.3.2 Time step determination

The time step size is a variable in the numerical model. It is determined as follows. For all internal nodes, net wetting and nonwetting fluid phase fluxes are determined based on the current node pressures. From these fluxes, also the wetting fluid saturation is calculated. When the nonwetting fluid flux in a pore body is positive, the pore body is drained. When it is negative, it is imbibed.

Next, for all internal nodes, the filling time is determined. This is done based on the current wetting fluid saturation. When the node is drained, its filling time is given by:

\[
t_{\text{fill},i} = \frac{V_i S_{\text{w},i}}{|q_{\text{nw},i}|},
\]

(4.7)

When a node is imbibed, its filling time is given by:

\[
t_{\text{fill},i} = \frac{V_i (1 - S_{\text{w}}^n)}{|q_{\text{w},i}|}.
\]

(4.8)

The length of next time step is then set to the smallest filling time found. This means that at least one pore body will be completely drained. Other pore bodies will be only partially drained. Since the model is limited to primary drainage simulations only, it is not to be expected that imbition of a pore body is the time step determining process.

### 4.3.3 Fluid occupation in a pore throat

The fluid occupation in a pore throat is of major importance to the fluid displacement in the network. The fluid phase conductivities are elements of the coefficient matrix
Chapter 4. The dynamic circular network model

in equation (4.6), from which the pressure field is determined. These conductivities are a function of the dimensions of the pore throat and of the viscosity of the fluid occupying the pore throat.

The fluid occupancy in a pore throat is determined by a set of displacement rules. An illustration of these rules is given in figure 4.4. The rules are the following:

- An interface between nonwetting and wetting fluid may migrate from a pore body into an adjacent pore throat when two conditions are fulfilled. First, the pore body from which the interface starts must be completely drained. Second, the entry pressure of the pore throat must be overcome. When these conditions are fulfilled, wetting fluid in the pore throat is replaced by nonwetting fluid. This is shown as case Ia.

- When the entry pressure is not overcome, the wetting fluid in the pore throat is considered to be temporarily immobile. The physical background of this rule is that when the interface cannot move, it will act as a no-flow boundary. This can only be expressed with nonmoving wetting phase. This is shown as case 1b. This condition allows pressure of the nonwetting fluid phase in node $i$ to build up so that, in a later stage, entry pressure eventually can be overcome.

- When wetting fluid in a pore throat is enclosed by completely drained pore bodies, it is considered to be trapped. This implies that no flow is possible through that pore throat. This is shown as case II.

- When nonwetting fluid occupies a pore throat and both adjacent pore bodies are reimbibed to a finite saturation level, the nonwetting fluid is considered to be disconnected from that in the pore bodies. It is then treated as trapped and immobile fluid. This is shown as case III.

- A special case occurs when a pore throat adjacent to the wetting fluid boundary reservoir gets filled with nonwetting fluid. Since nonwetting fluid is not allowed to enter the wetting fluid reservoir, the nonwetting fluid instantaneously becomes immobile. Thus, the exit throat is blocked. This affects the pressure field by contributing to pressure build-up in the nonwetting phase. Consequences of this special boundary condition are treated in section 4.4.

4.3.4 Numerical solution procedure

The governing equations presented in section 4.2 are solved for fluid pressure $P$ and wetting fluid saturation $S^w$ using an IMPES (IMplicit Pressure - Explicit Saturation) algorithm. Equation (4.6) is solved implicitly for $P$, assuming that $S^w$ and the throat conductances $K_{ij}$'s are known from the previous time step. Then, equation (4.4) is used to calculate fluid fluxes. The fluid fluxes are substituted in equations (4.1) and local phase saturations are calculated. The procedure is then repeated.

To solve the set of equations (4.6), a Preconditioned Conjugate Gradient Method (PCGM) algorithm is used. Alternatively, the system can be solved using a direct
Figure 4.4: Illustration of the interface stability test. Wetting fluid in a pore throat is replaced by nonwetting fluid when entry capillary pressure of that throat is overcome (Ia). Depending on the fluid occupancy in a pore throat and its adjacent pore bodies, throats might be temporarily closed for fluid flow (Ib, II and III). The dashed X indicates that the fluid in the pore throat is either open or closed to flow. When nonwetting fluid enters a throat adjacent to the wetting fluid reservoir, that throat is closed to flow for the rest of the simulation.

solver for the banded matrices. These solvers are basically the same as the one used in the model described in Chapter 2. However, a significant improvement to the PCGM solver has been made for simulations with the cylindrical pore-scale network model. During drainage simulations it has been observed, that many iterations were necessary before convergence was achieved. This is due to the following. When expressing throat radii of a network mimicking a fine sand, the conductivity has been observed to be of the order of magnitude $10^{-17}$ in SI-units, since conductivity scales with $r^4$. This value is placed in the conductivity matrix that is used to solve for pressure, see equation 4.6. Since pressure does not need to be solved for boundary nodes and trapped nodes, the matrix element that belongs to those has unit value.
Thus, there can be 17 orders of magnitude difference in the matrix that has to be solved. To avoid problems associated with stiffness of the matrix, the unit value matrix elements and their corresponding solution vector elements are rescaled by $r^4$.

4.3.5 Drainage procedure

The drainage procedure is illustrated by showing a portion of a small 2D network, as given in figure 4.5. Nonwetting fluid is shown in grey, wetting in white. Starting situation is given top left. Nonwetting fluid has fully drained the top layer of nodes, but the pressure difference over the adjacent throats is too low for them to be drained. The adjacent pore throats are therefore temporarily blocked. After solving the pressure field, entry capillary pressure is overcome in the two left vertical pore throats. From the figure, it can be seen that the left pore body in the second layer had the smallest filling time. Its neighbouring node gets partly filled. This is the node that has the next smallest time step.

In the illustration, the drainage procedure is then repeated several time steps. In a real simulation, this procedure is repeated until all nodes are drained, until a given maximum number of time steps is exceeded, or until a given maximum time is exceeded.

4.3.6 Averaging procedure

The pore-scale variables are averaged to arrive at the macro scale, where the results can be interpreted. The macro-scale pressures are defined as:

\[
\langle P^\alpha \rangle = \frac{1}{\delta V^\alpha} \int_{\delta V^\alpha} P^\alpha \, dV = \frac{\sum_i^N P^\alpha_i S^\alpha_i V_i}{\sum_i^N S^\alpha_i V_i} \quad (4.9a)
\]

\[
\langle P^c \rangle = \langle P^\alpha \rangle - \langle P^w \rangle \quad (4.9b)
\]

where $N$ is number of pore bodies, $P^\alpha$ is $\alpha$-phase fluid pressure, $S^\alpha$ is $\alpha$-phase saturation and $V_i$ is volume in pore body $i$. Average wetting and nonwetting fluid saturations are defined as:

\[
\langle S^w \rangle = \frac{V^w}{V^n + V^w} = \frac{\sum_i^N S^w_i V_i}{\sum_i^N V_i} \quad (4.10a)
\]

\[
\langle S^n \rangle = 1 - \langle S^w \rangle \quad (4.10b)
\]

For enhanced readability, the angular brackets are discarded in the remainder of this work. Averaging is only performed over pore bodies, pore throat volume is neglected. The error that is made as a result of this is estimated in Appendix A.

The fluid phase pressure averaging is only applied to fluid that is connected to its reservoir. Fluid that is disconnected from its reservoir contributes to the irreducible wetting fluid saturation. Local pressures of disconnected fluid are not taken.
4.3 Model description

Figure 4.5: Illustration of the drainage procedure in a 2D network. Nonwetting fluid is shown in grey. An X indicates that capillary entry pressure for the pore throat is not overcome. The fluid conductivity in that throat is then set to zero for that time step.

into account. Since the fluids are considered to be incompressible, pressure exerted on the interface between the continuous and disconnected fluid is incorporated in the pressure of that node. Thus, the pressure in that node passively takes on the pressure from its neighbouring node(s). If the pressure in the disconnected node would be taken into account in the (volume-) averaging of fluid pressures, it would progressively get a more important weight as drainage continues. Eventually, this would lead to a situation where all wetting fluid in the porous medium would be discontinuous, and average capillary pressure would be finite or even zero.

An algorithm is applied that checks pore bodies and adjacent pore throats on fluid phase content. Based on the outcome, it creates clusters of fluid phase. When a cluster is disconnected from its reservoir, all fluid that belongs to that cluster is considered to be trapped. In the flow equation for all nodes in that cluster, conductance is set to unity, so that pressure does not change anymore.

Volume averaging can be performed over different domains in the network. The averaging domains are always in the center of the network, as their size is determined
by the number of layers from the top and bottom of the network that is discarded in
the averaging procedure. Let the network size be \(NX \times NY \times NZ\), then the number of
pore bodies \(N_n\) in the averaging domain is \(NX \times NY \times (NZ-2 \times nskip)\). This is sketched
in figure 4.6.

Except for some results shown in Chapter 6, the top and bottom layers are
always discarded from the averaging domain. When they are not discarded, then
initial saturation is less then unity.

![Figure 4.6: Different averaging domains in the network model, controlled by the
number of layers to be skipped in the averaging procedure (nskip)](image)

### 4.4 Special boundary conditions

There is one important feature to the chosen setup that has to be noted here. The
pore-scale network is originally designed to mimic the laboratory experiment that is
performed to construct a capillary pressure-saturation curve. In these experiments,
hydrophobic and hydrophilic filters avoid wetting fluid to enter the nonwetting fluid
reservoir and vice versa.

In the pore-scale network model, no particular attention has been paid to the
hydrophobic filter, which is located between the nonwetting fluid reservoir and the
porous medium sample. This filter has a very low entry pressure. This can be
modelled by using large pore throats. In the dynamic simulations, entry pressure
is usually overcome for all pore throats adjacent to the nonwetting fluid reservoir.
Should a pore throat not be drained at the first time step, then the conductivity of
that pore throat is set to zero, as is indicated in figure 4.4, case Ib.

The hydrophilic filter, which is located between the wetting fluid reservoir and
the porous medium sample, has a very high entry pressure. This property can be
modelled by resizing the pore throat radii in the corresponding layer throats to a
small enough value. However, this has a major influence on the pressure field inside
the network. When pore throat radii in the bottom layer of vertical throats are much
smaller than the ones inside the network, then the imposed pressure gradient will
be mostly accounted for in the filter layer. The gradient in fluid pressure inside the network decreases. This reduced gradient leads to a smaller difference in average phase pressures during drainage. Capillary pressure will then be smaller than in absence of the bottom filter. Also, the time scale of the drainage process is increased, since the fluids move slower through the porous medium. The observed time scale is then characterised by the filter rather than by the porous medium under study.

As the retrieved macroscale capillary pressure is dominated by the properties of the hydrophilic filter rather than by the porous medium, the abovementioned method is discarded. Instead, the following procedure was chosen: whenever nonwetting fluid reaches the bottom layer of pore throats, this fluid becomes instantaneously immobile. The exit pore throats are then blocked. Although this affects the pressure distribution inside the porous medium, its impact on the pressure distribution is not as large as when all throat radii at the bottom are set to a very small value. Blocking exit pore throats actually alters the type of applied boundary condition: at the blocked pore throat, the Dirichlet boundary condition (for wetting fluid) is replaced by a no-flow condition (for nonwetting fluid).

The magnitude of the effect of the blocking of pore throats adjacent to the wetting fluid reservoir depends on the stability of the nonwetting fluid front during drainage. This in turn is determined by the chosen fluid viscosity ratio, as the pressure drop in each fluid phase is determined by its viscosity. This property is further investigated in Chapter 5.

4.5 Summary

In this chapter, the dynamic circular pore-scale network model is presented. The network generation is identical to that in the quasi-static model that is presented in Chapter 3. Pore bodies are spheres and pore throats are cylinders. Pore throats are considered to have no volume with respect to the pore bodies. The pore throats do govern hydraulic resistance to flow.

Dirichlet boundary conditions are applied to the top and bottom layer of pore bodies, which act as infinite nonwetting and wetting fluid phase reservoirs, respectively.

The displacement procedure in the dynamic pore-scale network model differs from the displacement procedure in the quasi-static model. Since transient displacement is computed here, the fluid pressure field has to be solved every time step in each node in the network. Based on the fluid content and pressure difference between two adjacent pore bodies, displacement of fluids is computed. To solve the fluid pressures numerically, an IMPES-schedule is applied. Fluid pressure is computed implicitly, while saturation is solved explicitly. Within a pore body, capillary pressure is assumed to be zero. Therefore, only a single fluid pressure has to be solved from the system of equations.
Chapter 5

Numerical pore-scale experiments: test cases

To test the cylindrical dynamic pore-scale network model, several scenarios have been investigated. This work must not be seen as a validation of the model against the reality, but as an investigation of possibilities and limitations of the pore-scale network model. In this chapter, two points are focussed on: the effect of fluid viscosity ratio on interface stability and fluid pressures and the effect of the hydrophilic filter at the wetting fluid reservoir on the fluid pressures inside the network.

This chapter has four sections. In the first section, the used pore-scale network model and its set up are given. In the second, the effects of fluid viscosity ratio on the average fluid phase pressures and the fluid distribution are investigated. For the simulations in this section 5.2, no hydrophilic filter is modelled at the bottom layer of pore throats (i.e. no extremely small radii). In Section 5.3, the effect of applying a hydrophilic filter on the average fluid phase pressures is studied. In the last section of this chapter, findings are summarized and conclusions are drawn.

5.1 Virtual experimental set up

In this section, the used pore-scale network model and its set up, including initial and boundary conditions and fluid properties, are given. The networks are identical for all simulations treated in this chapter, except for the simulations where a hydrophilic filter is applied.

5.1.1 Geometrical properties

The used pore-scale network consists of $10 \times 10 \times 20$ pore bodies. Coordination number of the network is 6. The geometrical properties of the network are given in table 5.1. The radii of the pore bodies and pore throats obey the truncated log-normal
distribution given in section 3.1. The used network is identical for all simulations treated in this chapter.

Table 5.1: Lattice network parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice dimensions</td>
<td>10×10×20</td>
</tr>
<tr>
<td>Coordination number</td>
<td>6</td>
</tr>
<tr>
<td>Lattice spacing (10^{-3} m)</td>
<td>0.2</td>
</tr>
<tr>
<td>Min pore body radius (10^{-3} m)</td>
<td>0.08</td>
</tr>
<tr>
<td>Max pore body radius (10^{-3} m)</td>
<td>0.10</td>
</tr>
<tr>
<td>Mean pore body radius (10^{-3} m)</td>
<td>0.09</td>
</tr>
<tr>
<td>Min pore throat radius (10^{-3} m)</td>
<td>0.01</td>
</tr>
<tr>
<td>Max pore throat radius (10^{-3} m)</td>
<td>0.05</td>
</tr>
<tr>
<td>Mean pore throat radius (10^{-3} m)</td>
<td>0.0125</td>
</tr>
<tr>
<td>Standard deviation of distribution</td>
<td>1.0</td>
</tr>
</tbody>
</table>

5.1.2 Fluid properties

The fluid properties are given in table 5.2. Interfacial tension is based on PCE (perchloroethylene) and water as fluid phases. As the effect of stable, neutral and unstable displacement regimes is investigated, nonwetting fluid viscosity is set to 10, 1 and 0.1 Pa s, respectively, in Section 5.2. For the simulations in section 5.3, the fluid viscosity ratio is set to 10.

Table 5.2: Fluids’ parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contact angle (°)</td>
<td>0.0</td>
</tr>
<tr>
<td>Interfacial tension (kg s^{-2})</td>
<td>0.0475</td>
</tr>
<tr>
<td>Wetting fluid viscosity (kg m^{-1}s^{-2})</td>
<td>0.001</td>
</tr>
<tr>
<td>Nonwetting fluid viscosity (kg m^{-1}s^{-1})</td>
<td></td>
</tr>
<tr>
<td>stable</td>
<td>0.010</td>
</tr>
<tr>
<td>neutral</td>
<td>0.001</td>
</tr>
<tr>
<td>unstable</td>
<td>0.0001</td>
</tr>
</tbody>
</table>

5.1.3 Initial and boundary conditions

The initial pressure in the network is 0 kPa. Throughout all simulations, pressure at the wetting fluid reservoir is kept constant at 0 kPa. Pressure at the nonwetting fluid reservoir is kept constant at 10 kPa.
5.2 Effect of fluid viscosity ratio

For the simulations in Section 5.2, no hydrophilic filter is modelled at the bottom layer of pore throats; that is, extremely small radii are not assigned to pore throats adjacent to the wetting fluid reservoir. However, when nonwetting fluid moves into a throat adjacent to the wetting fluid reservoir, it is instantaneously considered to be immobile. The exit throat then becomes blocked. This measure is taken to avoid the situation that nonwetting fluid would enter the wetting fluid reservoir.

5.2 Effect of fluid viscosity ratio

In this section, the effect of fluid viscosity ratio $M$ on the displacement is investigated. Viscosity ratio $M$ is defined as the ratio between the invading and the receding fluid inside the porous medium:

$$M = \frac{\mu_{\text{invading}}}{\mu_{\text{receding}}}$$  \hspace{1cm} (5.1)

where $\mu$ is dynamic viscosity. In the case of primary drainage, $M = \frac{\mu_n}{\mu_w}$, where superscripts $n, w$ indicate nonwetting and wetting fluid, respectively. Fluid-fluid interface stability is dictated by viscosity ratio. Three different flow regimes are investigated here:

- stable displacement
- neutral displacement
- unstable displacement

When displacement is stable, the fluid-fluid interface is a stable front and nonwetting fluid sweeps through the porous medium as a piston. When displacement is unstable, the fluid-fluid interface breaks up and fingering occurs.

Stable displacement is investigated with viscosity ratio $M = 10$, unstable displacement with $M = 0.1$. In the neutral case, both fluids have the same dynamic viscosity. Reference fluid is water, with dynamic viscosity $\mu_w = 0.001 \text{ kg m}^{-1} \text{ s}^{-1}$.

Dynamic displacement simulations have been performed, draining the network from $S^w = 1.0$ down to $S^w = 0.5$. Both wetting and nonwetting fluid then occupy 50% of the pore volume. At this point, the simulation was halted to compare the shape of the nonwetting fluid front for the different viscosity ratios.

5.2.1 Stable displacement: $M = 10$

The fluid distribution at wetting fluid saturation $S^w = 0.5$ is shown in figure 5.1. The two fluids are clearly separated by a more or less horizontal interface. Thus, the nonwetting fluid moves through the network as a piston. Under Dirichlet conditions, the pressure drop in nonwetting fluid pressure is 10 times smaller than the pressure drop in the wetting fluid.

In figure 5.2, the average wetting fluid saturation per layer is shown as a function of time. The saturation profile is plotted for every fifth time step. It shows the typical...
Figure 5.1: Visualisation of the fluid distribution at $S^w = 0.5$. Nonwetting fluid is shown in light grey, wetting fluid in dark grey. Viscosity ratio $M$ equals 10. The interface is a stable front with minor protrusions.

S-shaped curve. From this graph, it is clear that almost all wetting fluid is displaced by the passing front. The saturation profiles are practically parallel, which proves piston displacement by the nonwetting fluid.
Figure 5.2: Saturation profiles for viscosity ratio $M = 10$. The profiles are plotted every fifth time step, until $S_w^* = 0.5$. Almost all wetting fluid is displaced from a layer by the nonwetting front.

Figure 5.3: Average fluid pressures for the case where $M = 10$. Due to the difference in viscosity, the average wetting fluid pressure decreases more than the average nonwetting fluid pressure for ongoing drainage.
In figure 5.3, volume-averaged nonwetting and wetting fluid phase pressures are shown, as well as their difference, average capillary pressure. Both nonwetting and wetting fluid pressure show a sharp rise at the onset of drainage, near $S^w = 1$. The high value of average nonwetting fluid is due to the Dirichlet boundary condition at the nonwetting fluid reservoir. The average wetting fluid responds to that with a similar but smaller increase, as the pressure in the wetting fluid also increases, but the pressure is averaged over a larger volume. The drainage procedure is such, that per time step, a single pore body becomes completely filled. All other pore bodies accessible to nonwetting fluid will be partially drained. In these partially filled nodes, wetting fluid and nonwetting fluid are equal. Thus, the average wetting fluid pressure is high at the beginning, and decreases as drainage proceeds.

The decrease in the average wetting fluid pressure is higher than that in the average nonwetting fluid pressure, as a result of which, average capillary pressure increases. This is due to the difference in fluid viscosity. As the nonwetting fluid is more viscous, the largest pressure drop will be in that phase. For ongoing drainage, the average wetting fluid pressure will therefore decrease more than the average nonwetting fluid pressure.

The shape of the average nonwetting and wetting fluid pressure curves is very similar to those found in Appendix B, where average fluid phase pressures are shown as function of interface location in a single tube. The figure in the appendix corresponding to the results in this section are shown in figure C.7. Interface location in a single tube corresponds to nonwetting fluid saturation in a pore-scale network. However, in the single-tube case, capillary pressure is found to be independent of interface location.

### 5.2.2 Neutral displacement: $M = 1$

The fluid distribution at wetting fluid saturation $S^w = 0.5$ is shown in figure 5.4. The interface between the two fluids is not as horizontal as in figure 5.1. Some protrusions of nonwetting fluid exist, but these have not developed into fingers. Comparing figures 5.1 and 5.4, one can see that in the case where $M = 1$, more wetting fluid remains behind after the passing of the bulk nonwetting fluid. This is also visible in figure 5.5, where the average wetting fluid saturation per layer is shown as a function of time. The saturation profile is plotted for every fifth time step. The typical S-shape is recognisable, but less evident in comparison with the stable case in figure 5.2. Also, the saturation fronts are less parallel. At the beginning of drainage, the saturation front is less steep than in the stable case. When the nonwetting fluid front arrives at layer 10, there is a kink in the graph. At this point, there seems to be a capillary barrier, that causes the nonwetting fluid front to become more horizontal. This could be due to the small lateral size of the network (10×10 nodes). As the front moves onward, the slope of the saturation front is steeper, but still less steep than in figure 5.2.

In figure 5.6, volume-averaged nonwetting and wetting fluid phase pressures are shown, as well as their difference, average capillary pressure. As the fluids are isoviscous, the average phase pressures drop is more linear than in the stable case.
5.2 Effect of fluid viscosity ratio

Both nonwetting and wetting fluid pressures show a sharp rise at the onset of drainage, near $S^w = 1$. The high value of average nonwetting fluid is due to the Dirichlet boundary condition at the nonwetting fluid reservoir. The value of average nonwetting fluid pressure is higher than in the stable case, because there, pressure

Figure 5.4: Visualisation of the fluid distribution at $S^w = 0.5$. Nonwetting fluid is shown in light grey, wetting fluid in dark grey. Viscosity ratio $M$ equals 1. The interface is a relatively stable front with distinct protrusions. These protrusions have not developed into fingers.
Figure 5.5: Saturation profiles for viscosity ratio $M = 1$. The profiles are plotted every fifth time step, until $S^w = 0.5$. Some of the wetting fluid remains behind after the passing of the nonwetting fluid front.

drop over the nonwetting phase is much higher. In other words, the boundary pressure is transferred faster through the nonwetting fluid than in the stable case.

The average wetting fluid pressure follows this sharp rise, as is explained in the previous section. However, as the pressure drop in the wetting phase is larger than in the stable case, average phase pressure will decrease less than in the stable case. Also, the displacement is slightly less piston-like than in the stable case. When the nonwetting fluid front is smeared, this can give rise to more partially filled pore bodies than in the stable case. As argumented there, more wetting fluid pressure will have the same pressure as the nonwetting fluid. Capillary pressure is therefore less high than in stable case. From figure 5.6, it can be seen that capillary pressure decreases slightly for ongoing drainage.

An explanation for this shape of the $P^c-S^w$ curve is in the application of volume-averaging in combination with the set up of the pore-scale network. In figure 5.4, the nonwetting fluid front has reached to a point just below the center of the network. Since fluids are isoviscous in this case, pressure is transferred similarly in the two fluid phases. Pressure drop in the wetting fluid phase is equal to the pressure drop in the nonwetting fluid phase. Thus, as the fluid front moves below the center of the porous medium, the nonwetting fluid phase pressure is slightly lower than the wetting fluid pressure that is above the center of the porous medium. In combination with averaging over fluid volumes, capillary pressure does not increase as much (or even decreases slightly) as in the stable case. This analysis holds for any horizontal
5.2 Effect of fluid viscosity ratio

Figure 5.6: Average fluid pressures for the case where $M = 1$. Average wetting fluid decreases less than in the stable case, whereas average nonwetting fluid decreases more than in the stable case. This leads to lower capillary pressure.

layer in the porous medium when the two fluids are isoviscous.

Also, partially filled nodes can complicate matters. Since at a pore body, capillary pressure is assumed to be zero, nonwetting fluid pressure is equal to wetting fluid pressure in a partially filled pore body. In primary drainage, nonwetting fluid is always continuous and connected to the nonwetting fluid reservoir. When the wetting fluid in a partially filled node is continuous, the pressure is in that partially filled node is transferred into the wetting fluid phase. Thus, the wetting fluid phase is assigned a higher value than it should have. Thus, again, capillary pressure does not increase as much (or even decreases slightly) as in the stable case.

5.2.3 Unstable displacement: $M = 0.1$

In figure 5.7, the fluid distribution is shown at $S^w = 0.5$. It can easily be seen that the nonwetting fluid has penetrated fully through the network. The fluid-fluid interface has broken up into separate fingers. An important boundary effect is evident from this illustration: nonwetting fluid cannot enter the wetting fluid reservoir. At the moment that nonwetting fluid occupies a pore throat adjacent to the wetting fluid reservoir, the fluid conductivity of that throat is set to zero, as described in Section 4.4. As the pressure drop in the nonwetting fluid is small with respect to the pressure drop in the wetting fluid phase, the difference between nonwetting fluid pressure and wetting fluid in a neighbouring pore body will be
large. Overcoming capillary entry pressures of neighbouring throats, the nonwetting fluid will start to spread out sideways, as can be seen in the figure. This observation

Figure 5.7: Visualisation of the fluid distribution at $S^w = 0.5$. Nonwetting fluid is shown in light grey, wetting fluid in dark grey. Viscosity ratio $M$ equals 0.1. The interface has developed into fingers. As the nonwetting fluid reaches the wetting fluid reservoir, it is blocked, and can only move sideways. Thus, the nonwetting fluid gathers at the bottom of the network.

is also clearly visible in figure 5.8 where the saturation of wetting phase in the pore
5.2 Effect of fluid viscosity ratio

bodies near the bottom decreases fast. In figure 5.8, it can be seen that after the nonwetting fluid has reached the wetting fluid reservoir (layer 20), wetting fluid saturation in layer 19 decreases to zero in about 45 time steps. The average wetting fluid saturation per layer remains relatively high with respect to the average wetting fluid saturation in figures 5.2 and 5.5.

In figure 5.9, volume-averaged nonwetting, wetting and capillary pressures are given. For the unstable case, most of the pressure drop will be in the wetting fluid phase. The nonwetting fluid phase thus decreases less than in the cases where \( M = 10 \) and \( M = 1 \), which are shown in figures 5.3 and 5.6, respectively.

The effect of fluid viscosity ratio on wetting fluid pressure is extreme. Average wetting fluid increases with decreasing wetting fluid saturation. The mechanism behind this is the following. As viscosity is higher in the wetting fluid phase than in the nonwetting fluid phase, the larger pressure drop is in the wetting fluid phase. The pressure is transferred much more easily in the nonwetting fluid phase. Thus, the nonwetting fluid pressure at the fluid-fluid interface is still relatively high as the interface moves away from the top reservoir. The interface develops in fingers, as the interface is unstable. The fluid pressure in the wetting fluid is affected by this relatively high pressure through partially filled nodes. As the nonwetting fluid invades the network further, it will affect more and more wetting fluid. Thus, wetting fluid pressure is kept artificially high. As a result of this, average wetting fluid pressure is high as well.

In figures 5.9 and 5.10, a sudden decrease in average wetting fluid pressure and the corresponding increase in capillary pressure can be seen. This is a result of the used averaging technique. In figure 5.7, it can be seen that fingers of nonwetting fluid have reached the bottom layer in the network. From figure 5.8, it follows that this happens at high wetting fluid saturation.

As the nonwetting fluid cannot progress into the wetting fluid reservoir, it spreads sideways, causing snap-off of wetting fluid residing in the network. Thus, a large portion of wetting fluid which has an artificially high pressure becomes disconnected.

Now, the averaging only takes pressure of connected and mobile fluids into account. The pressure of the disconnected fluid is therefore ignored.

5.2.4 Summary

To summarize the findings in this section, all three volume-averaged capillary pressure curves for the \( 10\times10\times20 \) node network given in table 5.1 are shown in figure 5.10. As capillary pressure cannot decrease for decreasing wetting fluid saturation, it must be concluded that the pore-scale network model is limited to stable displacement only when investigating (dynamic) capillary pressure.

A fundamental issue that needs to be re-examined here is the traditional definition of average pressure, namely intrinsic phase volume average pressure. This issue has been recently investigated and alternatives have been proposed by Nordbotten et al. [50].
Figure 5.8: Saturation profiles for viscosity ratio $M = 0.1$. The profiles are plotted every fifth time step, until $S^w = 0.5$. Most of the wetting fluid remains behind after the passing of the nonwetting fluid front.

5.3 Effect of hydrophilic filter at bottom reservoir

In the pore-scale network model, a hydrophilic filter is applied between the internal nodes and the wetting fluid boundary nodes. This filter allows wetting fluid to pass, but immobilises nonwetting fluid as it enters the filter.

To study the effect of such a hydrophilic filter at the wetting fluid reservoir, the drainage simulations are now continued until irreducible wetting fluid saturation has been reached. This is done for two scenario’s. In the first case, the hydrophilic filter is applied so that nonwetting fluid cannot enter the wetting fluid reservoir. In the second scenario, no filter is applied. Nonwetting fluid can move into the wetting fluid reservoir. The phase pressures and saturations are averaged over the internal nodes only.

These two scenarios are computed for three different viscosity ratios. The results for these displacement experiments are shown in figures 5.11 through 5.13. For the case where viscosity ratio equals 10, there is practically no difference between the two scenarios. The nonwetting fluid moves like a piston through the network, so almost all nonwetting fluid arrives at the hydrophilic filter at the same time. The influence of the hydrophilic filter on capillary pressure is therefore negligible.

For the case with viscosity ratio 1, irreducible wetting fluid is the same for the two scenarios. The effect of the presence of a hydrophilic filter is marginally visible
5.3 Effect of hydrophilic filter at bottom reservoir

Figure 5.9: Average fluid pressures for the case where \( M = 0.1 \). Due to the difference in viscosity, the average wetting fluid pressure decreases more than the average nonwetting fluid pressure for ongoing drainage.

in the capillary pressure value, although the filter is activated much earlier (see figure 5.12). Once the filter becomes active (i.e., when a pore throat adjacent to the wetting fluid reservoir is drained by nonwetting fluid, and thus blocked), the pressure field changes. The reason for this is the change in boundary condition type. Before the nonwetting fluid becomes blocked, its pressure is influenced by the pressure at the wetting fluid boundary. When the nonwetting fluid becomes immobile, the influence of the wetting fluid reservoir is lost.

Thus, for both cases \( M = 10 \) and \( M = 1 \), applying a hydrophilic filter has only marginal impact on the computed capillary pressure-saturation curves.

A remarkable effect of the hydrophilic filter is shown in figure 5.13, where viscosity ratio \( M = 0.1 \). In this figure, irreducible wetting fluid saturation differs tremendously for the two boundary condition cases. This difference can be explained by lateral spreading of nonwetting fluid at the bottom layer. The nonwetting fluid thus breaks the connection of a large part of the wetting fluid inside the network with the wetting fluid reservoir.

The absence of corners and crevices gives rise to the existence of partially filled nodes. Since locally, capillary pressure is zero, nonwetting fluid pressure equals wetting fluid pressure in these nodes. As the displacement continues, there are more and more partially filled nodes, which lead to much bigger differences. In the unstable case (viscosity ratio equals 0.1), the difference between the cases with and without hydrophilic filter is therefore much more pronounced than in the more stable
Figure 5.10: Average capillary pressure for various viscosity ratios $M$ from the network given in table 5.1.

Figure 5.11: Effect of blocking exit throats on average capillary pressure for a 10x10x20 nodes network when viscosity ratio is 10.
5.3 Effect of hydrophilic filter at bottom reservoir

Figure 5.12: Effect of blocking exit throats on average capillary pressure for a 10x10x20 nodes network when viscosity ratio is 1.

Figure 5.13: Effect of blocking exit throats on average capillary pressure for a 10x10x20 nodes network when viscosity ratio is 0.1.
5.4 Summary and conclusions

In this chapter, the dynamic pore-scale network model from Chapter 4 is tested on its possibilities and limitations. Attention is paid to the effect of viscosity ratio $M = \frac{\mu_o}{\mu_w}$ on the displacement of the two fluids. This ratio affects the pressure field in the nodes of the network, and therefore plays a role in the displacement of the fluids.

From the tests performed with the dynamic pore-scale network model, it must be concluded that the model is limited to simulating stable drainage only. This means, that viscosity ratio must be larger than unity. The applied method of volume averaging does not give reliable results when the nonwetting fluid front becomes unstable.

When nonwetting fluid reaches the bottom layer of pore bodies, which represents the reservoir with wetting fluid, the imposed Dirichlet boundary condition (constant pressure) is changed to a no-flow Neumann condition (no-flow boundary). This change does not affect the results for stable displacement. For unstable displacement, the change in boundary condition type has a significant effect on both irreducible wetting fluid saturation and (average) capillary pressure.
Chapter 6

Numerical pore-scale experiments: Determination of damping coefficient $\tau$

In this chapter, numerical experiments that are performed with the circular pore-scale network models (described in Chapters 3 and 4) are described. First, the virtual experimental set up is discussed. The network models are built such that they mimic Zeijen sand. Next, the Representative Elementary Volume (REV) for the selected pore body and pore throat size distribution is determined. Performing numerical drainage experiments with this REV, damping coefficient $\tau$ is computed.

6.1 Virtual experimental set up

6.1.1 Pore space properties

To perform the drainage experiments, the geometry of the pore space needs to be characterised. The properties of Zeijen sand are used to define the porous medium under study. The Zeijen sand’s grain size distribution is given in figure 6.1. From this figure, it can be seen that the Zeijen sand is very homogeneous, and that there is no grain diameter larger than about 0.2 mm. Since the network models use a regular grid where pore bodies neither overlap nor are missing, the grid spacing is set to this value of 0.2 mm. A direct consequence is that the maximum pore body size is set to 0.1 mm. Thus, two of the fitting parameters are already set.

The remaining parameters that determine pore space are minimum and mean pore body radius and minimum, maximum and mean pore throat radius. These can be found by fitting porosity and permeability, respectively. Measured porosity of the Zeijen sand is 38.1%. Its permeability is $3 \cdot 10^{-12}$ m$^2$.

Although pore throat volume is taken into account in the determination of porosity, it plays a minor role herein. Permeability, however, is determined by the pore
Chapter 6. Determination of $\tau$

throat dimensions only. Thus, porosity is fitted by changing pore body sizes, permeability by changing pore throat sizes.

As a measure of pore throat size, $d_{10}$ or $d_{15}$ from a grain size distribution can be chosen. This information is used to determine the order of magnitude of the pore throat radii size. To keep the assumption valid that the volume of pore throats is much less than that of pore bodies, the radii should not be chosen too large.

Due to small variances, porosity is not exactly constant for networks of different sizes, when all parameters except the number of nodes is varied. Permeability is even more sensitive to the variation of network size. Finding a perfect fit to both porosity and permeability is impossible. Nevertheless, the fit was performed as good as possible. The found pore space parameters are listed in table 6.1.

When determining the REV size, these data will be used as pore space parameters. The only variable is the number of pore bodies. When the REV size has been determined, porosity and permeability is checked again.

6.1.2 Initial and boundary conditions

Two series of drainage simulations are performed: quasi-static and dynamic simulations. In all drainage simulations, the network is initially filled with wetting fluid, except for the top boundary layer. The top boundary layer of the network acts as an infinite nonwetting fluid reservoir. The initial pressure in the network is 0 kPa.

The boundary conditions are of Dirichlet type. The initial pressure in the network

Figure 6.1: Grain size distribution of the Zeijen sand. This sand is used to set up the pore space parameters in the performed simulations.
6.1 Virtual experimental set up

Table 6.1: Lattice network parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice dimensions variable</td>
<td>variable&lt;sup&gt;1&lt;/sup&gt;</td>
</tr>
<tr>
<td>Coordination number</td>
<td>6</td>
</tr>
<tr>
<td>Lattice spacing ((10^{-3} , m))</td>
<td>0.2</td>
</tr>
<tr>
<td>Min pore body radius ((10^{-3} , m))</td>
<td>0.08</td>
</tr>
<tr>
<td>Max pore body radius ((10^{-3} , m))</td>
<td>0.10</td>
</tr>
<tr>
<td>Mean pore body radius ((10^{-3} , m))</td>
<td>0.09</td>
</tr>
<tr>
<td>Min pore throat radius ((10^{-3} , m))</td>
<td>0.001</td>
</tr>
<tr>
<td>Max pore throat radius ((10^{-3} , m))</td>
<td>0.05</td>
</tr>
<tr>
<td>Mean pore throat radius ((10^{-3} , m))</td>
<td>0.0125</td>
</tr>
<tr>
<td>Standard deviation of distribution ((10^{-3} , m))</td>
<td>1.0</td>
</tr>
</tbody>
</table>

<sup>1</sup> see tables 6.5 and 6.6

is 0 kPa. Throughout all simulations, pressure at the wetting fluid reservoir is kept constant at 0 kPa. Pressure at the nonwetting fluid reservoir is different for the quasi-static and dynamic drainage experiments. The quasi-static simulations are performed with the model described in Chapter 3, the dynamic simulations with the one described in Chapter 4.

Table 6.2: Boundary conditions of the quasi-static simulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure wetting reservoir ((Pa))</td>
<td>0</td>
</tr>
<tr>
<td>Starting pressure nw reservoir ((Pa))</td>
<td>1000</td>
</tr>
<tr>
<td>Pressure step ((Pa))</td>
<td>50</td>
</tr>
<tr>
<td>End pressure nw reservoir ((Pa))</td>
<td>10000</td>
</tr>
</tbody>
</table>

In the quasi-static experiments, pressure at the nonwetting fluid boundary is initially 1 kPa. This value increases with increments of 50 Pa every time equilibrium between the two fluid phases has been achieved, until the end value of 10 kPa is reached. This value is high enough to have all mobile wetting fluid displaced out of the network. Increasing the boundary pressure further would not give a smaller irreducible wetting fluid saturation.

In the dynamic experiments, pressure at the nonwetting fluid boundary is constant throughout the drainage procedure. Drainage is performed with pressures 10, 15, 20 and 25 kPa in the nonwetting fluid reservoir. These boundary conditions are listed in tables 6.2 and 6.3.
Chapter 6. Determination of \( \tau \)

Table 6.3: Boundary conditions of the dynamic simulations

| Pressure wetting reservoir (Pa) | 0   |
| Pressure nw reservoir (Pa)     | 10000 |
|                                | 15000 |
|                                | 20000 |
|                                | 25000 |

6.1.3 Fluid properties

The fluid properties are given in table 6.1.3. Nonwetting fluid viscosity is set to 0 Pa·s for the first simulations to avoid unstable displacement. Unstable displacement is unfavorable to the chosen modelling approach, as explained in Section 5.2. Since gravity is neglected in the pore-scale models, densities of the fluids are redundant.

Table 6.4: Fluids’ parameters

| Contact angle \(^{\circ}\) | 0.0 |
| Interfacial tension \((kg \cdot s^{-2})\) | 0.0475 |
| Wetting fluid viscosity \((kg \cdot m^{-1} \cdot s^{-2})\) | 0.001 |
| Nonwetting fluid viscosity \((kg \cdot m^{-1} \cdot s^{-1})\) | 0.010 |

6.2 Determination of Representative Elementary Volume

In this section, the size of a Representative Elementary Volume (REV) is determined. This is done in two ways: by comparing capillary pressure-saturation curves and by comparing porosity and permeability data. The comparison of capillary pressure-saturation curves is done based on results from the quasi-static network model which is described in Chapter 3. In this model, fluid flow is not computed explicitly. Therefore, permeability cannot be computed to determine the REV size. In the dynamic network model described in Chapter 4, fluid flow is computed. When interpreting the model as a single-phase model, permeability data can be computed and used to determine the size of the REV. Since the network generator in both models is identical, both the quasi-static and the dynamic pore-scale network model can be used to fit porosity data.
6.2 REV determination

6.2.1 Comparing capillary pressure-saturation data

The REV-size determination is done with the quasi-static pore-scale network model that is described in Chapter 3. A set of networks is constructed with identical pore and throat distribution, but with different lattice size, as listed in Table 6.5.

| Table 6.5: Lattice dimensions for REV size determination |
|-----------------------------------|----------------------------------|
| length and width determination    | height determination             |
| 5×5×100                           | 30×30×10                         |
| 10×10×100                         | 30×30×20                         |
| 20×20×100                         | 30×30×30                         |
| 30×30×100                         | 30×30×40                         |
| 40×40×100                         | 30×30×50                         |
| 50×50×100                         |                                  |

First, the width and length of the REV is determined. The height of the network is fixed at 100 nodes, and width and length of the network is varied from 5 to 50 nodes. Capillary pressure-saturation curves are computed for each of these networks. These curves are given in Figure 6.2. From this graph, it can be seen that the capillary pressure curves start to converge when width and length are 30 nodes.

Having determined width and length, these are used to find a proper height of the network. Height of the network is varied from 10 to 50 nodes. The resulting capillary pressure-saturation curves are shown in Figure 6.3. From this graph, it can be concluded that 40 nodes is a reasonable height of the required REV.

In both Figures 6.2 and 6.3, drainage doesn’t start from wetting fluid saturation equal to 1. The reason for this is, that in these computations, wetting fluid saturation is determined for the whole network, including the nonwetting fluid boundary nodes. This does not influence the conclusions drawn in this section, as will be shown in Section 6.2.2.

6.2.2 Comparing permeability and porosity

In this section, two alternative methods for determining the size of an REV representing Zeijen sand is proposed. The first one considers permeability, the second porosity. Permeability convergence must be investigated using the dynamic pore-scale network model, since fluid flow is not computed in the quasi-static model. Porosity can be computed with the quasi-static as well as the dynamic pore-scale network model.

Permeability

To determine permeability of a network, the two-phase model is changed to a single-phase model. The single-phase flow computations in the two-phase network can be
Figure 6.2: Capillary pressure-saturation curves of a network with a height of 100 nodal layers and varying width and length

Figure 6.3: Capillary pressure-saturation curves of a network with a width and length of 30 nodes and varying height
simulated by setting both fluid viscosities to the same (wetting fluid) viscosity, and by setting fluid-fluid interfacial tension to zero. In this way, there are two fluids with exactly equal properties, that act as a single fluid.

The assumption that local capillary pressure equals zero is now beneficial, since only one fluid pressure is solved in the system of equations (see Section 4.2). When applying the two above-mentioned modifications, it appears that only one fluid occupies the pore space. Flow rate is then easily determined based on influx from the top reservoir.

For a single phase experiment, under the assumption that gravity can be neglected, Darcy’s law can be written as:

\[ q = k \frac{\mu}{\rho} \nabla P \]  

(6.1)

where \( q \) is darcy velocity \([m \text{ s}^{-1}]\), \( k \) is permeability \([m^2]\), \( \mu \) is dynamic viscosity \([kg \text{ m}^{-1} \text{ s}^{-1}]\), and \( P \) is pressure \([kg \text{ m}^{-1} \text{ s}^{-2}]\).

Permeability can then be determined from:

\[ k = \frac{q \mu L}{\Delta P} \]  

(6.2)

where \( L \) is the length of the sand column, and \( \Delta P \) is the pressure difference between top en bottom fluid reservoir.

In the network model, not Darcy velocity \( q \), but volumetric flux \( Q \) is computed. Therefore, the cross-sectional area of the porous medium sample has to be taken into account, too. Permeability is then determined following:

\[ k = \frac{Q \mu L}{A \Delta P} \]  

(6.3)

For the permeability determination, \( \Delta P \) is set to 10 kPa.

It should be noted, that permeability can only be determined in this way when Darcy’s law is valid, thus when flow is laminar. A measure for this requirement is the so-called Reynolds’ number for flow in porous media, \( Re \). This number should be smaller than a value between 1 and 10 [4]. Reynold’s number is given by:

\[ Re = \frac{qd}{\nu} \]  

(6.4)

where \( q \) is specific discharge, \( \nu \) is kinematic viscosity and \( d \) is a characteristic length of the porous matrix. As this Reynold’s number is based on that for flow in pipes, the characteristic length should be the length of the pore throats and bodies. In the dynamic model, grid spacing is then a good length to choose. The value of Reynold’s number in the REV is determined in Section 6.2.3.

Porosity

Porosity can be defined by the total interconnected void space that occupies a certain finite volume of solid material [4]. In the pore-scale network model, the total void
space is determined by accounting all fluid volume in the network. The finite volume of the porous medium is the cubic volume that surrounds the pore space. This volume is referred as $V_{\text{cube}}$. Thus, porosity is determined as:

$$n = \frac{V_{\text{nodes}} + V_{\text{throats}}}{V_{\text{cube}}}. \tag{6.5}$$

In table 6.6, the various network dimensions for the REV-determination based on permeability and porosity are given. The results of the single-phase experiments are given in figures 6.4 and 6.5. The results in figure 6.4 are consistent with those of figure 6.2. Porosity and permeability converge when the pore-scale network has a width and height of 30 nodes. From figure 6.5, it follows that the length of the REV can be 40 nodes, as found in Section 6.2.1. From the figures in this section, it follows that a network of 30$\times$30$\times$40 nodes is a reasonable REV.

| Table 6.6: Lattice dimensions for REV size determination |
|-----------------------------|-----------------------------|
| length and width determination | height determination |
| 5$\times$5$\times$100 | 30$\times$30$\times$5 |
| 10$\times$10$\times$100 | 30$\times$30$\times$10 |
| 15$\times$15$\times$100 | 30$\times$30$\times$15 |
| 20$\times$20$\times$100 | 30$\times$30$\times$20 |
| 25$\times$25$\times$100 | 30$\times$30$\times$25 |
| 30$\times$30$\times$100 | ... |
| 35$\times$35$\times$100 | ... |
| 40$\times$40$\times$100 | 30$\times$30$\times$85 |
| 45$\times$45$\times$100 | 30$\times$30$\times$85 |
| 50$\times$50$\times$100 | 30$\times$30$\times$90 |
| | 30$\times$30$\times$95 |
| | 30$\times$30$\times$100 |

For the 30$\times$30$\times$40 nodes network, distributions for pore body and pore throat sizes as well as a grid spacing are found that give that network a permeability of $5 \cdot 10^{-12}$ m$^2$ and a porosity of 39%. The permeability of Zeijen sand is determined to be $3 \cdot 10^{-12}$ m$^2$. Its porosity is 38%. The difference between the true and simulated properties is small enough to be ignored for this study. A further improvement in fit for permeability $k$ makes the fit in porosity worse.

The final pore throat distribution of the 30$\times$30$\times$40 node network is given in figure 6.6. In this figure, the truncated log-normal distribution is evident. The pore body distribution is given in figure 6.7. The variation in pore body radius is not large. On the used regular grid, pore bodies are not allowed to overlap, as pore throats must have a finite length. Thus, maximum porosity that can be reached with the spherical network model is that of a simple cubic packing of pore bodies:
Figure 6.4: Permeability and porosity of a NX×NY×100 network, where NX and NY are nodal width and length.

Figure 6.5: Permeability and porosity of a 30×30×NZ network, where NZ is nodal network height.
just below 48%. As Zeijen sand has a porosity of almost 40%, most pore bodies will have a radius that is not much smaller than the grid spacing.

Figure 6.6: Histogram of pore throat distribution of the 30×30×40 node network

Figure 6.7: Histogram of pore body distribution of the 30×30×40 node network
6.3 Determination of damping coefficient $\tau$

It should be noted, that pore throat volume is taken into account in the computation of porosity. It is neglected when determining macroscale saturation. The error made by ignoring pore throat volume in the computation of macroscale saturation is about 2%, as is explained in Appendix A.

6.2.3 Flow regime

In this section, Reynold’s number $Re$ is determined for the found REV with dimension $30 \times 30 \times 40$ nodes. For completeness, the Reynold’s number is also computed based on grain size properties, as is often done in laboratory [4]. Proposed lengths are $d_{10}$, $d_{50}$. Collins [15] retrieves the characteristic length from permeability and porosity as: $d = (k/n)^{1/2}$. Ward [67] relates the characteristic length to permeability only: $d = k^{1/2}$. It is clear, that the maximum value in for $Re$ in the drainage simulations is given by:

$$Re_{\text{max}} = \frac{q_{\text{max}} d_{\text{max}}}{\nu_{\text{min}}}$$

(6.6)

where $d_{\text{max}}$ is the maximum characteristic length, $\nu_{\text{min}}$ is wetting fluid kinematic viscosity and $q_{\text{max}}$ is evaluated at the beginning of the drainage procedure. In table 6.7, a set of possible characteristic lengths that occur in the network model are listed. From this table, it follows that $Re_{\text{max}}$ equals 3.27, which is well inside the proposed limits. Thus, flow in the REV is laminar.

<table>
<thead>
<tr>
<th>Characteristic length $d$</th>
<th>Reynold’s number $Re$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(k/n)^{1/2}$ (Collins)</td>
<td>0.06</td>
</tr>
<tr>
<td>$k^{1/2}$ (Ward)</td>
<td>0.04</td>
</tr>
<tr>
<td>mean $r_{\text{throat}}$</td>
<td>0.20</td>
</tr>
<tr>
<td>mean $r_{\text{body}}$</td>
<td>1.47</td>
</tr>
<tr>
<td>mean $l_{\text{throat}}$</td>
<td>0.38</td>
</tr>
<tr>
<td>grid spacing</td>
<td>3.27</td>
</tr>
</tbody>
</table>

6.3 Determination of damping coefficient $\tau$

Based on the results in previous section, the $30 \times 30 \times 40$ network is selected to determine the damping coefficient $\tau$. The procedure to compute $\tau$ is an extended version of the one introduced in Chapter 2. For certain values of average wetting fluid saturation, the difference between the quasi-static pressure and each of the dynamic capillary pressures is measured (as e.g. in figure 6.8(a)). For the same saturations, its rate of change is determined for all dynamic curves (as e.g. in figure 6.8(b)).
Chapter 6. Determination of $\tau$

Next, the difference in capillary pressure $\Delta P^c$ is plotted against the saturation rate of change $\frac{dS_w}{dt}$ for a given value of wetting fluid saturation. The value of damping coefficient $\tau$ can be determined from the slope of the obtained curves. There is a value for $\tau$ for each of the chosen average wetting fluid saturations. In figure 6.9, quasi-static and dynamic capillary pressure curves of the $30 \times 30 \times 40$ node network are given. The irreducible wetting fluid saturation of the quasi-static capillary pressure curve is larger than that of the dynamic curves. This is a result of trapping of the wetting fluid. The slowly increasing boundary conditions in a quasi-static drainage experiment give more possibilities and opportunities for bypassing. Pockets of wetting fluid can then become disconnected from its reservoir.

The irreducible wetting fluid saturation in the dynamic capillary pressure curves is not the same, either. For high boundary pressure conditions, the nonwetting fluid front will move more like a piston through the network than for low boundary pressures. The displacement of wetting fluid is more efficient for high boundary pressures, yielding lower irreducible wetting fluid saturation. This behaviour confirms flow-rate dependent irreducible wetting fluid saturation, as investigated by Wildenschild et al. [70]. Another effect that can be observed in figure 6.9 is that the capillary pressure curves are more smooth for high boundary conditions. This is also due to the more effective piston displacement.

Figure 6.10 shows the wetting fluid saturation as a function of time for the dynamic drainage experiments. In this figure, the effect of boundary pressure conditions on irreducible wetting fluid saturation is clearly visible. The kink that occurs in each graph, just before irreducible wetting fluid saturation has been reached is caused by the special boundary condition treated in Section 4.4. When nonwetting fluid enters a pore throat adjacent to the wetting fluid reservoir, that pore throat’s
**6.3 Determination of damping coefficient $\tau$**

![Quasi-static and dynamic capillary pressure-saturation curves from the 30×30×40 node network given in table 6.1.](image)

Fluid conductivity is set to zero. As the interface is more stable for high boundary conditions than for low ones, the transition from moving interface to blocked, immobile interface will be much sharper for high boundary pressures.

In figure 6.11, the difference between dynamic and quasi-static capillary pressure is plotted against saturation rate of change. Each graph shows these data for a chosen wetting fluid saturation. There are four data points in each graph, one for each dynamic capillary pressure (listed in table 6.3). To find the slopes of these curves, a straight line is drawn through the data points. The linearisation of the relationship between $\Delta P^c$ and $-\frac{\partial S_w}{\partial t}$ then takes the form

$$\Delta P^c = P^c_{dyn} - P^c_{static} = -\tau \frac{\partial S_w}{\partial t} + \beta. \quad (6.7)$$

A similar approach has been followed by Dahle et al. [17]. In relationship (6.7), $\beta$ is the intersect at the vertical axis in figure 6.11. Damping coefficient $\tau$ is now computed based on relationship (6.7). It is calculated as the linear fit of the slope of the curves given in figure 6.11. The intersect at the vertical axis is left unspecified, which gives the linear fit where $\beta \neq 0$.

At first sight, $\beta$ is required to be zero, since $\Delta P^c$ should diminish as the saturation rate of change goes to zero. Then, both fluids are at equilibrium, and the dynamic capillary pressure curve should coincide with the quasi-static curve. However, as $\frac{\partial S_w}{\partial t}$ goes to zero, behaviour of damping coefficient $\tau$ might be nonlinear.

In the results shown in this section, coefficient $\beta$ is negative. Then, damping coefficient $\tau$ is higher than in the case where $\beta$ is forced to be zero. The difference
between a linear fit with and without vertical axis intersect is very small. The offset on the vertical axis varies between about -70 Pa and -1600 Pa. On average, the offset is about -470 Pa.

The slopes of the curves in figure 6.11 are not equal, which indicates a dependence of damping coefficient $\tau$ on wetting fluid saturation. This dependence is shown in figure 6.12, where coefficient $\beta$ in equation 6.7 is not restricted. Damping coefficient $\tau$ ranges from about 3850 Pa s at wetting fluid saturation $S^w = 0.9$ to about 39000 Pa s at $S^w = 0.3$. Damping coefficient $\tau$ cannot be determined for lower wetting fluid saturation values, since $\Delta P^c$ is then undetermined.

The shape of the curves suggests that damping coefficient $\tau$ goes to zero when wetting fluid saturation equals 1. This is in good agreement of observations made by Manthey et al. [47, 46].

### 6.4 Summary and conclusions

In this chapter, damping coefficient $\tau$ is determined. The pore-scale network models, described in Chapter 3 and 4, are employed to simulate quasi-static and dynamic primary drainage. Properties of the pore-scale network models correspond to those of model Zeijen sand. A Representative Elementary Volume (REV) is determined with which dynamic and quasi-static capillary pressure-saturation curves are constructed. Dimensions of this REV are $30 \times 30 \times 40$ pore bodies.

The dynamic and quasi-static capillary pressure-saturation curves are related
6.4 Summary and conclusions

Figure 6.11: $\Delta P_c$ as function of $-dS_w/dt$ for different wetting fluid saturations, where $\Delta P_c$ is the difference between dynamic and quasi-static capillary pressure.

Figure 6.12: Damping coefficient $\tau$ as function of wetting fluid saturation from the $30 \times 30 \times 40$ node network given in table 6.1.
through a so-called damping coefficient $\tau$. This coefficient is shown to depend on wetting fluid saturation. At high wetting fluid saturation, damping coefficient $\tau$ goes to zero. For decreasing wetting fluid saturation (as drainage proceeds), $\tau$ increases to about 40 kPa s, at wetting fluid saturation $S^w$ equal to 0.3.
Chapter 7

Numerical pore-scale experiments: Investigation of $\tau$-dependencies

In this chapter, the relationship suggested by Stauffer [65, 66] for damping coefficient $\tau$ is investigated by performing numerical experiments with the circular network models. In Sections 7.3 and 7.4, the effect of fluid viscosity on damping coefficient $\tau$ is discussed. In Section 7.5, the effect of averaging domain size on damping coefficient $\tau$ is investigated.

The virtual experimental set up is basically the same as that stated in Chapter 6. To save computational time, however, the dimensions of the applied pore-scale network model are reduced. For the computations regarding the effect of fluid viscosity on damping coefficient $\tau$, the network consists of $15 \times 15 \times 40$ nodes. It is shown that for the current purposes this model size suffices. For the computations regarding the effect of averaging domain size on $\tau$, a $10 \times 10 \times 100$ node network is applied.

7.1 Analysis of Stauffer’s formula

In the late 1970’s, Stauffer [65, 66] investigated one-dimensional two-phase flow during drainage of homogeneous porous media, where air and water were the two fluid phases. Measurements of capillary pressure and water content under different flow conditions revealed that the relationships between capillary pressure, water content and fluid conductivity depend on the flow conditions. He refers to this dependency as the *dynamic* effect in unsaturated flow. In work by Celia, Dahle and Hassanizadeh [10, 36, 17], the difference between quasi-static (or equilibrium) and dynamic capillary pressure is described by a *damping coefficient*. This work is treated in Chapter 1.

Stauffer investigates dynamic effects in the capillary pressure-saturation relation-
ships through laboratory experiments concerning unsaturated flow. In these experiments, air is the nonwetting fluid, and water is the wetting fluid. Air is taken to be at constant atmospheric pressure. With atmospheric pressure as reference value, capillary pressure is negative water pressure. Based on his experiments, Stauffer proposes the following dynamic capillary pressure:

\[ P_{\text{dyn}} = P_{\text{static}} - \tau \frac{\partial S^w}{\partial t}. \]  

(7.1)

In this relationship, Stauffer suggested following dependencies for coefficient \( \tau \):

\[ \tau = \frac{\alpha \epsilon \mu}{\lambda k} \left( \frac{P^d}{\rho w g} \right)^2 \]  

(7.2)

where \( \tau \) is the damping coefficient, \( \alpha \) is a constant, \( \epsilon \) is porosity, \( \mu \) is dynamic water viscosity, \( \lambda \) is Brooks-Corey parameter, \( k \) is permeability, \( P^d \) is entry capillary pressure, \( \rho w \) is water density and \( g \) is gravitational force. The term \( \frac{P^d}{\rho w g} \) is a characteristic length scale of the porous medium. It should be noted that this term is a yet undefined intrinsic length scale. Entry capillary pressure is a measure for the pore throat radius, and \( \rho w g \) is the specific weight of the wetting fluid. As such, the fraction of entry capillary pressure over gravity forces does not have a direct physical basis, but it has dimension of length.

In the formulation of equation (7.2), damping coefficient \( \tau \) is a combination of fluid and soil properties. Some parameters are fluid properties \((\mu, \rho)\), some are soil properties \((\epsilon, \lambda, k)\), and some are both \((P^d)\). Stauffer’s damping (or dynamic) coefficient is considered to be constant, regardless of the wetting fluid content in the porous medium, as all variables in equation (7.2) are constants. For example, dynamic viscosity \( \mu \) is water viscosity. Air viscosity is 2 orders of magnitude smaller than that of water. Thus, regardless of the water content, water viscosity is dominant in the system.

In Chapter 6, damping coefficient \( \tau \) was found to depend on wetting fluid saturation \( S^w \) for the oil-water system under investigation. In this chapter, Stauffer’s formulation of damping coefficient \( \tau \) as in equation (7.2) is used to investigate the dependency on viscosity \( \mu \) and length scale \( L \). From equation (7.2), it can be seen that damping coefficient \( \tau \) varies linearly with fluid viscosity \( \mu \) and quadratically with \( L \) (through \( \frac{P^d}{\rho w g} \)).

### 7.2 Virtual experimental setup

In this chapter, two lattices are used that are smaller than the 30\( \times \)30\( \times \)40 node network used in Chapter 6. For the study into the effect of fluid viscosity on damping coefficient \( \tau \) (Section 7.3 and 7.4), a 15\( \times \)15\( \times \)40 nodes network is applied. Initial and boundary conditions, as well as fluid properties are the same as in Chapter 6, where a 30\( \times \)30\( \times \)40 node network is applied. The pressure gradients that are imposed on these networks are comparable, since the number of nodes in vertical direction is 40.
7.2 Virtual experimental setup

for both. The used lattice parameters are given in Table 7.1. Only the lateral size of
the pore-scale network model differs from that in Chapter 6.

For the investigation of the effect of averaging domain size on damping coefficient
\( \tau \) (Section 7.5), a network with \( \times 10 \times 10 \times 100 \) nodes is employed.

Table 7.1: Lattice network parameters of the two networks

<table>
<thead>
<tr>
<th>Lattice dimensions</th>
<th>( \times 15 \times 40 )</th>
<th>( \times 10 \times 10 \times 100 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coordination number</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>Lattice spacing (( 10^{-3} ) m)</td>
<td>0.2</td>
<td>0.3</td>
</tr>
<tr>
<td>Min pore body radius (( 10^{-3} ) m)</td>
<td>0.08</td>
<td>0.016</td>
</tr>
<tr>
<td>Max pore body radius (( 10^{-3} ) m)</td>
<td>0.10</td>
<td>0.15</td>
</tr>
<tr>
<td>Mean pore body radius (( 10^{-3} ) m)</td>
<td>0.09</td>
<td>0.086</td>
</tr>
<tr>
<td>Min pore throat radius (( 10^{-3} ) m)</td>
<td>0.001</td>
<td>0.002</td>
</tr>
<tr>
<td>Max pore throat radius (( 10^{-3} ) m)</td>
<td>0.05</td>
<td>0.03</td>
</tr>
<tr>
<td>Mean pore throat radius (( 10^{-3} ) m)</td>
<td>0.0125</td>
<td>0.016</td>
</tr>
<tr>
<td>Standard deviation of distribution</td>
<td>1.0</td>
<td>0.25</td>
</tr>
</tbody>
</table>

The volume-averaged fluid pressures and saturation are determined based on
internal nodes only, using the method described in Section 4.3.6. The resulting
capillary pressure curves for the case where viscosity ratio \( M \) equals 10 are shown in
figure 7.1.

Contrary to the capillary pressure curves in Chapter 6, drainage starts from
wetting fluid saturation equal to 1 in this figure. The peculiar shape of the dynamic
curves near irreducible wetting fluid saturation is due to the fact that at the end
of drainage, very little volume of continuous wetting fluid is left inside the porous
medium. Averaging over such a small volume leads to the observed non-smoothness
in the dynamic capillary pressure curve.

For the results of this study, the problems with averaging over the wetting fluid
phase near irreducible wetting fluid saturation has no effect, since the difference
between the dynamic and quasi-static capillary pressures can only be determined for
the saturation range of the quasi-static curve. The quasi-static capillary pressure
curve has a larger irreducible wetting fluid saturation than the dynamic ones due to
enclosure of wetting fluid by bypassing nonwetting fluid. Since there are no corners
and crevices in the pore throats (and pore bodies), wetting fluid is not allowed to
be displaced once it has been disconnected from its fluid reservoir. This mechanism
has also been illustrated in Chapter 5.

In figure 7.2, the damping coefficient \( \tau \) is plotted as a function of the wetting
fluid saturation \( S^w \) for the \( 30 \times 30 \times 40 \) and \( 15 \times 15 \times 40 \) node networks, where
viscosity ratio \( M \) equals 10. From this figure, it is clear that although the REV
needs to be 30 by 30 nodes wide (see Chapter 6), a pore-scale network of 15 by 15
nodes gives similar results. For the investigation of \( \tau \)-dependencies in this chapter, the 15×15×40 node network is used.

### 7.3 Dependency on viscosity ratio

To investigate the effect of viscosity ratio on damping coefficient \( \tau \), a set of four dynamic drainage experiments is performed. Dirichlet boundary condition for the nonwetting fluid reservoir is 10 kPa, for the wetting fluid 0 kPa. Initially, the network is filled with wetting fluid at pressure 0. In these experiments, only stable displacement (\( M > 1 \)) is considered. Viscosity ratios are 20, 10, 5 and 2.5.

For each of the four viscosity ratios, damping coefficient \( \tau \) is determined with the same procedure as in Chapter 6. For a number of wetting fluid saturation values, the difference between dynamic and quasi-static capillary pressure is plotted as a function of saturation rate of change at that saturation level. Damping coefficient \( \tau \) is determined as the slope of the linear fit of each of these curves, following

\[
P_{\text{dyn}}^c - P_{\text{stat}}^c = -\tau \frac{\partial S_w}{\partial t} + \beta.
\]  

(7.3)

Vertical axis intersect \( \beta \) is not restricted.

In figure 7.3, damping coefficient \( \tau \) is plotted as a function of wetting fluid saturation for different values of viscosity ratio \( M \). From this figure, it follows that

![Dynamic and quasi-static capillary pressure curves for the 15×15×40 node network given in table 7.1. Viscosity ratio \( M \) equals 10.](image)
7.3 Dependency on viscosity ratio

Figure 7.2: Damping coefficient $\tau$ as function of wetting fluid saturation for the 15x15x40 and the 30x30x40 node network. Viscosity ratio $M$ equals 10.

Figure 7.3: Damping coefficient $\tau$ as function of wetting fluid saturation, plotted for different values of viscosity ratio $M$. 
the value of damping coefficient $\tau$ is linearly proportional to viscosity ratio $M$. For example, when $M$ doubles from 5 to 10, damping coefficient $\tau$ doubles, too.

Thus, figure 7.3 suggests that the coefficient $\tau$ is a function of wetting fluid saturation and viscosity ratio: $\tau = \tau(S^w, M)$. To see, whether this relationship fully describes coefficient $\tau$, or whether more factors play a role, the data set can be simplified through the following transformation: $\tau/M = f(S^w)$. The resulting relationship should be a single line, when coefficient $\tau$ is completely described by relationship $\tau = \tau(S^w, M)$. The simplified relationship $\tau/M$ as function of wetting fluid saturation $S^w$ is shown in figure 7.4. In this figure, it is clear that the curves are more or less parallel, but not the same. Thus, $\tau/M$ is not a unique function of wetting fluid saturation.

![Figure 7.4: Lumped parameter $\tau/M$ as function of wetting fluid saturation.](image)

### 7.4 Dependency on average fluid viscosity

In Section 7.3, the dependency of damping coefficient $\tau$ on fluid viscosity ratio $M$ is investigated. This dependency does not explain the wetting fluid saturation dependency that has been observed in Chapter 6. This is to be expected, since viscosity ratio is a parameter that doesn’t take interaction between two fluids into account. In dynamic drainage experiments as studied here, wetting and nonwetting fluid interact. Since the two fluid phases show a pressure gradient under flow conditions, they have an effect on the pressure field inside the system. Through this pressure field, the two fluid phases are coupled.
A more useful approach in considering the two fluid viscosities is by introducing an average fluid viscosity. This should be a saturation-weighted fluid viscosity, defined as

\[ \mu_{\text{avg}} = S_w \mu_w + (1 - S_w) \mu_n. \]  

(7.4)

As such, the wetting fluid dependency of damping coefficient \( \tau \) that has been observed in Chapter 6 might be resolved.

As mentioned before, Stauffer found no explicit dependency on wetting fluid saturation \( S_w \). All variables in equation (7.2) are constant. When an average fluid viscosity is employed as in relationship 7.4, an adaptation of Stauffer’s formulation might still be used, while a dependency on \( S_w \) can be introduced. Then, the adapted formulation takes the form:

\[ \tau = \frac{\alpha \epsilon \mu_{\text{avg}}}{\lambda k} \left( \frac{P_d}{\rho_w g} \right)^2. \]  

(7.5)

In the drainage experiments performed in this work, only stable displacement is considered. The nonwetting fluid front moves as a piston through the network. Thus, the average fluid viscosity formulation (7.4) can be easily determined from fluid viscosity ratio and average saturation. In figure 7.5, damping coefficient \( \tau \) is shown as function of average fluid viscosity \( \mu_{\text{avg}} \) based on the data in figure 7.3. A linear trend line is included. In figure 7.5, damping coefficient \( \tau \) and average fluid viscosity \( \mu_{\text{avg}} \) are related as:

\[ \tau = 3.9 \cdot 10^6 \mu_{\text{avg}} + 2.1 \cdot 10^5. \]  

(7.6)

This value is in reasonable agreement with the value observed in the laboratory for Zeijen sand. The factor \( \frac{\alpha \epsilon}{\lambda k} \left( \frac{\mu_n}{\rho_g} \right)^2 \), which consists of porous medium properties only, is evaluated at \( 8 \cdot 10^8 \).

From figure 7.5 and equation (7.6), it appears that damping coefficient \( \tau \) is an unique function of average fluid viscosity \( \mu_{\text{avg}} \). The wetting fluid dependency of \( \tau \) which has been observed in Chapter 6 is taken into account in the definition of average fluid viscosity (7.4). To investigate whether the description of the wetting fluid dependency of \( \tau \) is fully captured by the introduction of average fluid viscosity, the data in figure 7.3 were replotted in figure 7.6, i.e. \( \tau/\mu_{\text{avg}} \) as a function of \( S_w \). In the adapted Stauffer formulation, lumped parameter \( \tau/\mu_{\text{avg}} \) is expected to be a constant, equal to

\[ \frac{\tau}{\mu_{\text{avg}}} = \frac{\alpha \epsilon}{\lambda k} \left( \frac{P_d}{\rho_w g} \right)^2. \]  

(7.7)

However, from figure 7.6, it is clear that the the lumped parameter \( \tau/\mu_{\text{avg}} \) is still a function of wetting fluid saturation. Since the parameter is a function of

\[ ^1 \text{This approach is the same as Dahle and Celia [16] apply at the pore scale in their dynamic network model.} \]
wetting fluid saturation, introducing $\mu_{avg}$ into Stauffer’s original formulation does not describe the wetting fluid dependency completely.

This is to be expected, since at wetting fluid saturation $S_w$ equal to 1, average fluid viscosity $\mu_{avg}$ equals $\mu_w$. According to equation (7.6), damping parameter $\tau$ is then equal to $\tau = 3.9 \cdot 10^6 \mu_w$, which is not zero. However, according to figure 6.12, damping coefficient $\tau = 0$ at $S_w = 1$. The description of $\tau$–dependencies is therefore yet incomplete.

### 7.5 Dependency on averaging domain size

To investigate the effect of averaging domain size on damping coefficient $\tau$, a $10 \times 10 \times 100$ nodes network is constructed. The averaging domains are always in the center of the network. Their size is determined by the number of layers from the top and bottom of the network that is discarded in the averaging procedure. This is sketched in figure 4.6. The number of layers to be skipped from the boundary varies from 0 to 25. Capillary pressure and wetting fluid saturation are determined from the remaining averaging domain.

Viscosity ratio $M$ equals 10 for the simulations shown in this section. The Dirichlet boundary conditions for the quasi-static simulation are 0 kPa for the wetting fluid reservoir and 3 to 10 kPa with increments of 50 Pa for the nonwetting fluid reservoir. In the dynamic simulation, Dirichlet boundary conditions are 0 kPa for the wetting fluid reservoir and 10 kPa for the nonwetting fluid reservoir.
7.5 Dependency on averaging domain size

Figure 7.6: Lumped parameter $\frac{\tau}{\mu_{avg}}$ as function of wetting fluid saturation. The lumped parameter is a function of wetting fluid saturation.

Figure 7.7 shows the quasi-static capillary pressure curves for three different averaging domain sizes. When all layers are included in the averaging domain, saturation is less than unity, since the nonwetting fluid reservoir is taken into account as well.

The capillary pressure curves in figure 7.7 are practically horizontal. This is due to a combination of factors. First, the Zeijen sand, on which the geometrical properties are based, is a very homogeneous, fine sand. Second, a bottle-neck effect has been observed in the drainage experiment. The lateral dimension of $10 \times 10$ nodes is apparently too small to avoid this effect. Extending width and length of the network was no option because of computer memory issues.

In figure 7.8, capillary pressure-saturation curves of the dynamic drainage experiment are shown. Because of the irregular shape of the curves, a moving median filter has been applied. The filter length is set to 20. The first 20 data points are read, and the median value is determined. This value is assigned to the 10th data point. For the second filtered point, data points 11 through 30 are used. Thus, the filter is moved half its length for each new data point. This procedure is repeated until all capillary pressure-saturation points have been filtered.

What is evident, is that the dynamic capillary pressure increases for increasing averaging domain size. This is due to the chosen fluid properties in combination with the Dirichlet boundary conditions. Most of the pressure drop over the network will be in the nonwetting fluid as it is much more viscous. An increase of nonwetting boundary pressure will therefore affect the average nonwetting fluid pressure more
than the average wetting fluid pressure. Thus, capillary pressure will increase for increasing boundary conditions.

In figure 7.9, saturation versus time is shown for the different averaging domain sizes. It is clear that saturation rate of change $\frac{\partial S_w}{\partial t}$ is larger for the smaller averaging domains. Under the imposed boundary conditions, the nonwetting fluid moves as a stable front through the network, as the nonwetting fluid is much more viscous. As a consequence, a small domain is drained faster than a large domain.

The irreducible saturation of the quasi-static capillary pressure curve (figure 7.9) is larger than that in the dynamic capillary pressure curves of figure 7.8. The explanation for this is that the lower boundary conditions during quasi-static drainage give more possibilities for bypassing. This increases the chance of wetting fluid becoming trapped or disconnected from its reservoir. The trapped fluid contributes to the irreducible wetting fluid saturation.

Even without computing damping coefficient $\tau$ explicitly, one can see from figures 7.8 and 7.9 that the value of $\tau$ increases with increasing averaging domain size. Firstly, the difference between the dynamic and the quasi-static capillary pressure curve increases. Secondly, the rate of change of saturation $\frac{\partial S_w}{\partial t}$ decreases. Both changes contribute to an increase of damping coefficient $\tau$.

As a first quantitative analysis of the data, the difference between dynamic and quasi-static capillary pressure is determined for various values of wetting fluid saturation. The average capillary pressure difference was then plotted against saturation

Figure 7.7: Quasi-static capillary pressures against saturation from the $10 \times 10 \times 100$ node network. The data are filtered with a moving median method, using filter length 20.
7.5 Dependency on averaging domain size

![Graph showing dynamic capillary pressure against wetting fluid saturation for different averaging domain sizes: 100 layers, 70 layers, and 50 layers. Each curve is labeled with the corresponding number of layers and is shown against a wetting fluid saturation axis and a dynamic capillary pressure axis.]

Figure 7.8: Capillary pressure against saturation from the $10 \times 10 \times 100$ node network. The data are filtered with a moving median method, using filter length 20.

![Graph showing time-saturation curves for the same network and averaging domain sizes as in figure 7.8. Each curve is labeled with the corresponding number of layers and is shown against a time axis and a wetting fluid saturation axis.]

Figure 7.9: Time-saturation curves for the same network and averaging domain sizes as in figure 7.8. These data are also filtered with the moving median filter.
rate of change to find damping coefficient $\tau$. This has been done for the three averaging domain sizes under investigation. Thus, for each of the three averaging domain sizes, a value for damping coefficient $\tau$ is retrieved. A fourth point can be added to the data set. At very small length scale, say an interface, there is only one capillary pressure. Therefore, $\tau$ must be zero for small length scale, yielding the origin as fourth data point.

In figure 7.10, the relationship between averaging domain size and damping coefficient $\tau$ is shown. Although it can be discussed whether three (or four, since the origin can be included) data points suffice to identify a dependency, two fits are made to the data points. The found relationships are given by

\[
\tau = \alpha x \quad (7.8)
\]
\[
\tau = \beta x^2 + \gamma x \quad (7.9)
\]

where $x$ is the number of layers in the averaging domain and

\[
\alpha = 831.6 \pm 86.2 \quad (7.10)
\]
\[
\beta = 6.4 \pm 0.0006 \quad (7.11)
\]
\[
\gamma = 295.6 \pm 0.05 \quad (7.12)
\]

The quadratic relationship clearly matches the data point best. This behaviour is confirmed in laboratory experiments and numerical simulations [47, 46].

Figure 7.10: Damping coefficient $\tau$ as function of the averaging domains used to create figures 7.7 through 7.9
7.6 Summary and conclusions

In this chapter, various parameters that damping coefficient $\tau$ depends on are investigated. Geometrical properties of the employed network model are the same as in Chapter 6. Lattice dimensions of the network model are reduced to $15 \times 15 \times 40$ nodes. Although this network is smaller than the REV which is determined in Chapter 6, the computed damping coefficient $\tau$ is similar for the two network lattice dimensions.

It is shown that $\tau$ varies linearly with viscosity ratio $M = \frac{\mu_n}{\mu_w}$. A more practical relationship is that between $\tau$ and saturation-weighted average fluid viscosity $\mu_{avg} = S_w \mu_w + S_n \mu_n$. For the porous medium and fluids under investigation in this study, this relationship is given by $\tau = 3 \cdot 10^6 \mu_{avg}$. Thus, fluid viscosities play a more important role in two-phase flow than quasi-static models assume.

Through average fluid viscosity, a dependency of damping coefficient $\tau$ on wetting fluid saturation as seen in Chapter 6 can be introduced. However, the saturation-dependency of damping coefficient $\tau$ is not entirely governed by average fluid viscosity $\mu_{avg}$.

The dependency on length scale is studied by investigating a pore-scale network model that consist of $10 \times 10 \times 100$ nodes. Damping coefficient $\tau$ is determined for various averaging domain sizes. Each of these averaging domain sizes acts as an REV of certain dimensions. From the results, it follows that $\tau$ varies quadratically with averaging domain size, or length scale.
Chapter 7. Investigation of $\tau$-dependencies
Chapter 8

Summary, conclusions, and recommendations

This dissertation describes the research that has been carried out in the framework of the research program "Upscaling Flow and Transport Processes in Porous Media: From Pore to Core" funded by the Dutch Science Council (NWO/ALW), under grant number 809.62.010.

8.1 Summary and conclusions

In Chapter 1, a short introduction is given on two-phase flow in porous media. Attention is paid to the definition of capillary pressure. Traditionally, capillary pressure is determined under equilibrium conditions. The resulting capillary pressure-saturation relationship is referred to as the quasi-static capillary pressure-saturation curve. Next, an extended definition of capillary pressure which is also valid under nonequilibrium conditions is presented. This capillary pressure is referred to as the dynamic capillary pressure. Dynamic and quasi-static capillary pressure are assumed to be linearly dependent through saturation rate of change. The linear relationship is governed by a so-called damping coefficient \( \tau \). This coefficient is subject of this dissertation.

In Chapter 2, a pore-scale network model with elements (pore bodies and pore throats) of rectangular cross section is presented. The shape of the elements allows two immiscible fluids (wetting and nonwetting) to reside in the same network element at the same time. This model is referred to as the angular pore-scale network model.

In principle, the angular pore-scale network model is developed to handle both dynamic and quasi-static drainage. However, when simulating quasi-static and dynamic drainage, numerical problems occurred which made it technically impossible to simulate performed laboratory experiments at the same scale. For a smaller porous
medium sample, an indication of the behaviour of damping coefficient $\tau$ could be given.

Preliminary results show that $\tau$ is a function of wetting fluid saturation. Results in this chapter also indicate that averaging over the area of fluid-fluid interfaces gives a better representation of capillary pressure than averaging over fluid phase volumes. The strong advantage of this model is its weak point at the same time: because of its angular geometry, it can simulate two-phase flow in a more realistic way than the traditional (circular) ball-and-stick models. However, this angular geometry allows countercurrent imbibition, with lead to uncontrolled oscillations.

In Chapter 3, a quasi-static pore-scale network model is presented. In this model, pore bodies are spheres and pore throats are cylinders. Pore throats are considered to have no volume with respect to the pore bodies.

The displacement procedure is similar to that in percolation theory: based on boundary conditions (external capillary pressure) and accessibility and allowability (through entry capillary pressure of connected pore throats), nonwetting fluid drains the porous medium. Since the fluid pressure field does not have to be solved, the required amount of computational time is very small.

Partially filled pore bodies do not exist in this model. The error created by ignoring partially filled pore bodies when comparing quasi-static capillary pressure with dynamic capillary pressure is marginal, as shown in Appendix B.

In Chapter 4, the dynamic circular pore-scale network model is presented. The network generation is identical to that in the quasi-static model that is presented in Chapter 3. Pore bodies are spheres and pore throats are cylinders. Pore throats are considered to have no volume with respect to the pore bodies. The pore throats do govern hydraulic resistance to flow.

Dirichlet boundary conditions are applied to the top and bottom layer of pore bodies, which act as infinite nonwetting and wetting fluid phase reservoirs, respectively.

The displacement procedure in the dynamic pore-scale network model differs from the displacement procedure in the quasi-static model. Since transient displacement is computed here, the fluid pressure field has to be solved every time step in each node in the network. Based on the fluid content and pressure difference between two adjacent pore bodies, displacement of fluids is computed. To solve the fluid pressures numerically, an IMPES-schedule is applied. Fluid pressure is computed implicitly, while saturation is solved explicitly. Within a pore body, capillary pressure is assumed to be zero. Therefore, only a single fluid pressure has to be solved from the system of equations.

In Chapter 5, the dynamic pore-scale network model from Chapter 4 is tested on its possibilities and limitations. Attention is paid to the effect of viscosity ratio $M = \frac{\mu_w}{\mu_n}$ on the displacement of the two fluids. This ratio affects the pressure field in the nodes of in the network, and therefore plays a role in the displacement of the fluids.
8.1 Summary and conclusions

From the tests performed with the dynamic pore-scale network model, it must be concluded that the model is limited to simulating stable drainage only. This means, that viscosity ratio must be larger than unity. The applied method of volume averaging does not give reliable results when the nonwetting fluid front becomes unstable.

When nonwetting fluid reaches the bottom layer of pore bodies, which represents the reservoir with wetting fluid, the imposed Dirichlet boundary condition (constant pressure) is changed to a no-flow Neumann condition (no-flow boundary). This change does not affect the results for stable displacement. For unstable displacement, the change in boundary condition type has a significant effect on both irreducible wetting fluid saturation and (average) capillary pressure.

In Chapter 6, damping coefficient $\tau$ is determined. The pore-scale network models, described in Chapter 3 and 4, are employed to simulate quasi-static and dynamic primary drainage. Properties of the pore-scale network models correspond to those of model Zeijen sand. A Representative Elementary Volume (REV) is determined with which dynamic and quasi-static capillary pressure-saturation curves are constructed. Lattice dimensions of this REV are $30 \times 30 \times 40$ pore bodies.

The dynamic and quasi-static capillary pressure-saturation curves are related through a so-called damping coefficient $\tau$. This coefficient is shown to depend on wetting fluid saturation. At high wetting fluid saturation, damping coefficient $\tau$ goes to zero. For decreasing wetting fluid saturation (as drainage proceeds), $\tau$ increases to about $40 \text{ kPa} \cdot \text{s}$, at wetting fluid saturation $S_w 0.3$.

In Chapter 7, various parameters that damping coefficient $\tau$ depends on are investigated. Geometrical properties of the employed network model are the same as in Chapter 6. Lattice dimensions of the network model are reduced to $15 \times 15 \times 40$ nodes. Although this network is smaller than the REV which is determined in Chapter 6, the computed damping coefficient $\tau$ is similar for the two network lattice dimensions.

It is shown that $\tau$ varies linearly with viscosity ratio $M = \frac{\mu_n}{\mu_w}$. A more practical relationship is that between $\tau$ and saturation-weighted average fluid viscosity $\mu_{\text{avg}} = S_w \mu_w + S_n \mu_n$. For the porous medium and fluids under investigation in this study, this relationship is given by $\tau = 3 \times 10^6 \mu_{\text{avg}}$. Thus, fluid viscosities play a more important role in two-phase flow than quasi-static models assume.

Through average fluid viscosity, a dependency of damping coefficient $\tau$ on wetting fluid saturation as seen in Chapter 6 can be introduced. However, the saturation-dependency of damping coefficient $\tau$ is not entirely governed by average fluid viscosity $\mu_{\text{avg}}$.

The dependency on length scale is studied by investigating a pore-scale network model that consist of $10 \times 10 \times 100$ nodes. Damping coefficient $\tau$ is determined for various averaging domain sizes. Each of these averaging domain sizes acts as an REV of certain dimensions. From the results, it follows that $\tau$ varies quadratically with averaging domain size, or length scale.
8.2 Recommendations

In this section, some recommendations are made to improve the dynamic pore-scale network models that are developed in the framework of this research.

8.2.1 Pore space representation

The pore-scale network models that are developed for this research are created, such that the centerpoint of each pore lies on a regular grid. The resulting pore-space representation is therefore also regular, with coordination number is six for all internal pore bodies. Although the constructed grid is regular, varying sizes of pore bodies and pore throats yield a certain irregularity. An improved construction of pore space can be achieved when the pore-scale networks are built with true irregular geometry. That is, with varying coordination number for pore bodies. By allowing this, the pore-space representation is better than in the regular case.

A second improvement in pore-space geometry can be obtained for the shapes of the pore bodies and pore throats. The pore bodies and pore throats in the pore-scale network models that are developed for this dissertation have either angular or circular cross section. For the determination and investigation of damping coefficient $\tau$, only the quasi-static and dynamic models with spherical pore bodies and cylindrical pore throats are employed. In reality, pore structure is neither spherical/cylindrical nor cubical/angular. The network models can be improved to also allow other shapes for pore bodies and/or pore throats. For example, cross section of pore throats could be either circular, hexagonal, angular or hexagonal. This will improve the representation of actual pore structure in the network model.

8.2.2 Boundary conditions

Applied boundary conditions to the pore-scale network models are of Dirichlet type. Pressure is held fixed at the top and bottom layer of pore bodies to simulate drainage in a pressure cell. The models are in principle constructed such, that Neumann conditions (constant flow rate at the boundaries) can be applied as well. This option has not been investigated in the current work. Since dynamic effects are also visible in steady-state or flow-through experiments, it is worthwhile to test the possibilities of implementing Neumann boundary conditions. This will create opportunities to simulate a larger range of laboratory experiments.

8.2.3 Solution procedure

In the angular pore-scale network model in Chapter 2, an IMPES scheme is used to solve the system of equations. The pressure field is solved implicitly, while the saturation is solved explicitly. As a result of this, there is a discrepancy between the pressure field and the saturation, which may lead to the observed oscillations. An improvement of the angular model could be to solve the set of equations by means of a fully implicit scheme.
A second way that helps to avoid oscillatory behaviour in the current angular pore-scale network model, is to immobilize wetting fluid adjacent to a pore body that is drained to (local) irreducible wetting saturation. The immobilization of wetting fluid is basically the same as replacing the angular pore throat by a pore throat of circular cross section with the same dimension. However, a disadvantage of this procedure is that the physically more realistic nature of pore throats is lost.

### 8.2.4 Pore-scale description of parameters

Capillary pressure is interfacial property. It is therefore sensible to simulate it as such. In the circular pore-scale network models of Chapters 3 and 4, local capillary pressure is not considered. Local capillary pressure can be introduced, similar to the local capillary pressure in the angular pore-scale model. This could be done as indicated in table 8.1. When local capillary pressure is introduced in the circular pore-scale network model, it is better to switch from the IMPES scheme used in this work to a fully implicit scheme for reasons mentioned in Section 8.2.3.

<table>
<thead>
<tr>
<th>Domain</th>
<th>$S^w$</th>
<th>$P^c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>II</td>
<td>$1 &gt; S^w &gt; 0.5$</td>
<td>$\frac{2\sigma}{R_{body}}$</td>
</tr>
<tr>
<td>III</td>
<td>$0.5 &gt; S^w &gt; 0$</td>
<td>$\frac{2\sigma}{R_{body}} &lt; P^c &lt; \frac{2\sigma}{r_{thr, min}}$</td>
</tr>
<tr>
<td>IV</td>
<td>0</td>
<td>$\frac{2\sigma}{r_{thr, min}}$</td>
</tr>
</tbody>
</table>

$R_{body}$ is pore body radius, $r_{thr, min}$ is radius of the smallest pore throat adjacent to $R_{body}$.
Bibliography


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Summary

Dynamic effect in two-phase flow in porous media: a pore-scale network approach

This dissertation describes the research that has been carried out in the framework of the research program "Upscaling Flow and Transport Processes in Porous Media: From Pore to Core" funded by the Dutch Science Council (NWO/ALW), under grant number 809.62.010.

In Chapter 1, a short introduction is given on two-phase flow in porous media. Attention is paid to the definition of capillary pressure. Traditionally, capillary pressure is determined under equilibrium conditions. The resulting capillary pressure-saturation relationship is referred to as the quasi-static capillary pressure-saturation curve. Next, an extended definition of capillary pressure which is also valid under nonequilibrium conditions is presented. This capillary pressure is referred to as the dynamic capillary pressure. Dynamic and quasi-static capillary pressure are assumed to be linearly dependent through saturation rate of change. The linear relationship is governed by a so-called damping coefficient $\tau$. This coefficient is subject of this dissertation.

In Chapter 2, a pore-scale network model with elements (pore bodies and pore throats) of rectangular cross section is presented. The shape of the elements allows two immiscible fluids (wetting and nonwetting) to reside in the same network element at the same time. This model is referred to as the angular pore-scale network model.

In principle, the angular pore-scale network model is developed to handle both dynamic and quasi-static drainage. However, when simulating quasi-static and dynamic drainage, numerical problems occurred which made it technically impossible to simulate performed laboratory experiments at the same scale. For a smaller porous medium sample, an indication of the behaviour of damping coefficient $\tau$ could be given.

Preliminary results show that $\tau$ is function of wetting fluid saturation. Results in this chapter also indicate that averaging over the area of fluid-fluid interfaces gives a better representation of capillary pressure than averaging over fluid phase volumes.

The strong advantage of this model is its weak point at the same time: because of its angular geometry, it can simulate two-phase flow in a more realistic way than the
traditional (circular) ball-and-stick models. However, this angular geometry allows countercurrent imbibition, with lead to uncontrolled oscillations.

In Chapter 3, a quasi-static pore-scale network model is presented. In this model, pore bodies are spheres and pore throats are cylinders. Pore throats are considered to have no volume with respect to the pore bodies.

The displacement procedure is similar to that in percolation theory: based on boundary conditions (external capillary pressure) and accessibility and allowability (through entry capillary pressure of connected pore throats), nonwetting fluid drains the porous medium. Since the fluid pressure field does not have to be solved, the required amount of computational time is very small.

Partially filled pore bodies do not exist in this model. The error created by ignoring partially filled pore bodies when comparing quasi-static capillary pressure with dynamic capillary pressure is marginal, as shown in Appendix B.

In Chapter 4, the dynamic circular pore-scale network model is presented. The network generation is identical to that in the quasi-static model that is presented in Chapter 3. Pore bodies are spheres and pore throats are cylinders. Pore throats are considered to have no volume with respect to the pore bodies. The pore throats do govern hydraulic resistance to flow.

Dirichlet boundary conditions are applied to the top and bottom layer of pore bodies, which act as infinite nonwetting and wetting fluid phase reservoirs, respectively.

The displacement procedure in the dynamic pore-scale network model differs from the displacement procedure in the quasi-static model. Since transient displacement is computed here, the fluid pressure field has to be solved every time step in each node in the network. Based on the fluid content and pressure difference between two adjacent pore bodies, displacement of fluids is computed. To solve the fluid pressures numerically, an IMPES-schedule is applied. Fluid pressure is computed implicitly, while saturation is solved explicitly. Within a pore body, capillary pressure is assumed to be zero. Therefore, only a single fluid pressure has to be solved from the system of equations.

In Chapter 5, the dynamic pore-scale network model from Chapter 4 is tested on its possibilities and limitations. Attention is paid to the effect of viscosity ratio $M = \frac{n^w}{n^w}$ on the displacement of the two fluids. This ratio affects the pressure field in the nodes of in the network, and therefore plays a role in the displacement of the fluids.

From the tests performed with the dynamic pore-scale network model, it must be concluded that the model is limited to simulating stable drainage only. This means, that viscosity ratio must be larger than unity. The applied method of volume averaging does not give reliable results when the nonwetting fluid front becomes unstable.

When nonwetting fluid reaches the bottom layer of pore bodies, which represents the reservoir with wetting fluid, the imposed Dirichlet boundary condition (constant
pressure) is changed to a no-flow Neumann condition (no-flow boundary). This change does not affect the results for stable displacement. For unstable displacement, the change in boundary condition type has a significant effect on both irreducible wetting fluid saturation and (average) capillary pressure.

In Chapter 6, damping coefficient $\tau$ is determined. The pore-scale network models, described in Chapter 3 and 4, are employed to simulate quasi-static and dynamic primary drainage. Properties of the pore-scale network models correspond to those of model Zeijen sand. A Representative Elementary Volume (REV) is determined with which dynamic and quasi-static capillary pressure-saturation curves are constructed. Lattice dimensions of this REV are $30 \times 30 \times 40$ pore bodies.

The dynamic and quasi-static capillary pressure-saturation curves are related through a so-called damping coefficient $\tau$. This coefficient is shown to depend on wetting fluid saturation. At high wetting fluid saturation, damping coefficient $\tau$ goes to zero. For decreasing wetting fluid saturation (as drainage proceeds), $\tau$ increases to about 40 kPa s, at wetting fluid saturation $S_w 0.3$.

In Chapter 7, various parameters that damping coefficient $\tau$ depends on are investigated. Geometrical properties of the employed network model are the same as in Chapter 6. Lattice dimensions of the network model are reduced to $15 \times 15 \times 40$ nodes. Although this network is smaller than the REV which is determined in Chapter 6, the computed damping coefficient $\tau$ is similar for the two network lattice dimensions.

It is shown that $\tau$ varies linearly with viscosity ratio $M = \frac{\mu_n}{\mu_w}$. A more practical relationship is that between $\tau$ and saturation-weighted average fluid viscosity $\mu^{avg} = S_w \mu_w + S_n \mu_n$. For the porous medium and fluids under investigation in this study, this relationship is given by $\tau = 3 \cdot 10^6 \mu^{avg}$. Thus, fluid viscosities play a more important role in two-phase flow than quasi-static models assume.

Through average fluid viscosity, a dependency of damping coefficient $\tau$ on wetting fluid saturation as seen in Chapter 6 can be introduced. However, the saturation-dependency of damping coefficient $\tau$ is not entirely governed by average fluid viscosity $\mu^{avg}$.

The dependency on length scale is studied by investigating a pore-scale network model that consist of $10 \times 10 \times 100$ nodes. Damping coefficient $\tau$ is determined for various averaging domain sizes. Each of these averaging domain sizes acts as an REV of certain dimensions. From the results, it follows that $\tau$ varies quadratically with averaging domain size, or length scale.
Samenvatting

Het dynamisch effect in tweefasenstroming in poreuze media: een porieschaal netwerk benadering

Dit proefschrift beschrijft het onderzoek dat is uitgevoerd in het kader van het onderzoeksprogramma ”Upscaling Flow and Transport Processes in Porous Media: From Pore to Core” van de Stichting voor Nederlands Wetenschappelijk Onderzoek (NWO/ALW), onder nummer 809.62.010.

In Hoofdstuk 1 wordt een korte introductie gegeven over tweefasenstroming in poreuze media. Hierin wordt aandacht besteed aan de definitie van capillaire druk in poreuze media. Capillaire druk wordt traditioneel bepaald onder evenwichtscondities. De capillaire druk-saturatie relatie die hieruit volgt, wordt quasi-statische capillaire druk-saturatie relatie genoemd. Tevens wordt een uitgebreidere definitie die ook geldig is onder niet-evenwichtscondities, gepresenteerd. Deze capillaire druk wordt dynamische capillaire druk genoemd. Er is een verband tussen de quasi-statistische en de dynamische capillaire druk, dat lineair wordt verondersteld. De coefficient die het lineaire gedrag beschrijft wordt dempingscoëfficiënt $\tau$ genoemd. Deze coefficient is het onderwerp van studie in dit proefschrift.

In Hoofdstuk 2 wordt een porieschaal netwerk model gepresenteerd, waarvan de elementen (porielholtes en poriën) een rechthoekige doorsnede hebben. Door de vorm van deze elementen is het mogelijk dat de twee niet-mengende vloeistoffen (een bevochtigende en een niet-bevochtigende vloeistof) zich tegelijkertijd in hetzelfde element bevinden. Dit model is het hoekige porieschaal netwerk model genoemd.

Dit hoekige porieschaal netwerk model is in principe ontwikkeld om zowel dynamische als quasi-statistische drainage te kunnen simuleren. Tijdens simulaties van quasi-statistische en dynamische drainage kwamen echter numerieke problemen naar boven, die het technisch onmogelijk maakten om uitgevoerde laboratoriumexperimenten op dezelfde schaal na te bootsen. Het bleek wel mogelijk om voor een poreus medium dat kleiner was dan bij de laboratoriumexperimenten, indicatief gedrag van dempingscoëfficiënt $\tau$ te bepalen.

Eerste resultaten van het hoekige model tonen aan dat $\tau$ afhankelijk is van het gehalte aan bevochtigende vloeistof in het poreus medium. Resultaten in dit hoofdstuk tonen tevens aan, dat middeling over het oppervlak van de menisci tussen de

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twee niet-mengende vloeistoffen een betere beschrijving van capillaire druk oplevert dan middeling over de volumes van de twee vloeistoffen.

Het sterkste punt van het hoekige model is tevens haar zwakste: vanwege de hoekige geometrie van de elementen kan het tweefasenstroming realistischer benaderen dan met de traditionele 'ball-and-stick' modellen. Deze geometrie leidt echter ook tot tegenstroomse imbietie, hetgeen ongecontroleerde oscillaties tot gevolg heeft.


De procedure waarmee het vloeistofgrensvlak verplaatst wordt is hetzelfde als in percolatietheorie: op basis van de randvoorwaarden (extern opgelegde capillaire druk) en toegankelijkheid van verbonden porieën (door intree-capillaire druk), draaint niet-bevochtigende vloeistof het poreuze medium. Omdat de druktoestand in de vloeistoffen niet in ieder knooppunt numeriek opgelost hoeft te worden is de benodigde rekentijd erg klein.

Gedeeltelijk gevulde porieholtes bestaan niet in dit model. De fout in gehalte van bevochtigende vloeistof in het poreus medium, die ontstaat door het niet opnemen van gedeeltelijk gevulde porieholtes wanneer quasi-statische capillaire druk vergeleken wordt met dynamische capillaire druk is marginaal, zoals aangegeven in Appendix B.


Aan de boven- en onderlaag van de porieholtes, die staan voor oneindige reservoors van respectievelijk niet-bevochtigende en bevochtigende vloeistof, worden Dirichlet randvoorwaarden opgelegd.

De verplaatsingsprocedure in het dynamisch porieschaal netwerk model verschilt van de procedure in het quasi-statisch model. Omdat in het dynamisch netwerk model tijdsafhankelijke verplaatsing wordt berekend, wordt het drukveld in de vloeistoffen voor iedere tijdstap opnieuw berekend in ieder knooppunt van het netwerk. Op basis van de vloeistofinhoud en het drukverschil tussen twee met elkaar verbonden porieholtes wordt de vloeistofverplaatsing berekend. Om de vloeistofdruk in ieder knooppunt te berekenen wordt gebruik gemaakt van een zogenoemd IMPES-schema. Vloeistofdruk wordt impliciet berekend, terwijl gehalte aan bevochtigende vloeistof expliciet wordt berekend. In een porieholte is de capillaire druk gelijk aan nul. In een porieholte is de druk van de bevochtigende vloeistof dus gelijk aan de druk van de niet-bevochtigende vloeistof, en hoeft er slechts een van
Samenvatting

De twee vloeistofdrukken opgelost te worden.

In Hoofdstuk 5 wordt het dynamisch porieschaal netwerk model uit Hoofdstuk 4 getest op haar mogelijkheden en beperkingen. Er wordt voornamelijk gekeken naar het effect van de viscositeitsratio \( M = \frac{\mu_n}{\mu_w} \) op de verplaatsing van de twee vloeistoffen. Deze ratio is van invloed op het drukveld in de knooppunten in het netwerk, en speelt daarmee een rol in de verplaatsing van de twee vloeistoffen.

Uit de uitgevoerde tests blijkt, dat het model beperkt is tot het simuleren van stabiele drainage. Dit houdt in, dat de viscositeitsratio zoals hierboven opgenomen, groter moet zijn dan 1. De methode van middeling over vloeistofvolumes geeft geen betrouwbare resultaten wanneer het front tussen de twee vloeistoffen onstabiel wordt.

Wanneer niet-bevochtigende vloeistof bij de onderste laag knooppunten aankomt, die het reservoir met bevochtigende vloeistof voorstelt, wordt de Dirichlet randvoorwaarde (constante druk) vervangen door een no-flow Neumann randvoorwaarde (ondoorlatende rand). Dit heeft geen invloed op de resultaten bij stabiele verplaatsing. Bij onstabiele verplaatsing heeft de verandering in type randvoorwaarde een significant effect op zowel residuele saturatie van niet-bevochtigende vloeistof en (gemiddelde) capillaire druk.

In Hoofdstuk 6 wordt dempingscoëfficiënt \( \tau \) bepaald. De porieschaal netwerk modellen die beschreven worden in Hoofdstukken 3 en 4 worden gebruikt om quasi-statische en dynamische primaire drainage te simuleren. De eigenschappen van de netwerk modellen komen overeen met die van model Zeijen zand. Een Representative Elementary Volume (REV) wordt vastgesteld waarmee dynamische en quasi-statische capillaire druk-saturatie curves worden bepaald. De afmetingen van dit REV zijn 30×30×40 porieholtes.

De dynamische en quasi-statische capillaire druk-saturatie curves zijn aan elkaar gekoppeld door een zogenoemde dempingscoëfficiënt \( \tau \). Er wordt aangetoond, dat deze coefficient afhankelijk is van de saturatie van de bevochtigende vloeistof. Bij hoge saturatie van bevochtigende vloeistof gaat de waarde van dempingscoëfficiënt \( \tau \) naar nul. Bij afnemende saturatie van bevochtigende vloeistof (bij voortschrijdende drainage) neemt \( \tau \) toe tot circa 40 kPa s, bij saturatie van bevochtigende vloeistof \( S_w 0,3 \).

In Hoofdstuk 7 worden verschillende parameters onderzocht waar dempingscoëfficiënt \( \tau \) van afhankelijk is. Geometrische eigenschappen van het gebruikte netwerk model zijn dezelfde als in Hoofdstuk 6. De afmetingen van het netwerk model zijn teruggebracht tot 15×15×40 knooppunten. Hoewel dit model zo kleiner is dan het REV dat in Hoofdstuk 6 bepaald is, is de berekende dempingscoëfficiënt vergelijkbaar voor de beide netwerkafmetingen.

Er wordt aangetoond, dat \( \tau \) lineair afhangt van viscositeitsratio \( M = \frac{\mu_n}{\mu_w} \). Een in de praktijk bruikbaardere relatie is die tussen \( \tau \) en saturatie-gewogen gemiddelde vloeistofviscositeit \( \mu_{avg} \). Voor het in deze studie onderzochte systeem geldt, dat deze relatie gegeven wordt door \( \tau = 3 \cdot 10^6 \mu_{avg} \). Zo speelt vloeistofviscositeit een
belangrijkere rol in tweefasenstroming dan quasi-statische modellen doen vermoeden.

Door gemiddelde vloeistofviscositeiten kan de afhankelijkheid van $\tau$ op saturatie, zoals in Hoofdstuk 6 ingebouwd worden. De saturatie-afhankelijkheid van $\eta$ is echter niet volledig bevat in gemiddelde vloeistofviscositeit.

De afhankelijkheid van $\tau$ van lengteschaal is onderzocht door te kijken naar een enkele drainage in een netwerk model dat bestaat uit $10 \times 10 \times 100$ knooppunten. Verschillende middelings“domeinen” worden gebruikt. Elk van deze domeinen wordt gezien als een REV met een bepaalde afmeting. Uit de resultaten blijkt, dat $\tau$ kwadratisch met middelingslengte varieert.
About the author

Twan Willem Jacobus Gielen was born on January 6, 1975 in Tegelen, the Netherlands. He grew up in the little village of America, which lies in the South-East part of The Netherlands. In 1993, he graduated from the St. Willibrord Gymnasium (pre-academic secondary education) in Deurne. In the same year, he started his academic education at Utrecht University, The Netherlands, where he studied Geophysics. In 1999, he earned his M.Sc. degree in Theoretical Geophysics. Topic of his thesis was the adaptation of a numerical solute-transport model to simulate heat transfer in porous media.

In 1999, he started his Ph.D. research in the Hydrology and Ecology Section in the Civil Engineering Department of Delft University of Technology. As part of his research, he visited the Civil and Environmental Engineering Department at Princeton University, USA, and the Matematisk Institutt in Universitetet i Bergen, Norway, to work on the development of the dynamic pore-scale network models described in this dissertation.

Since December 2005, he is working as geohydrological advisor at Tauw, an engineering company in Deventer, the Netherlands. Currently, he is working on issues related to thermal energy storage in groundwater.

In his spare time, Twan is principal euphonium player in the renowned wind orchestra based in his native village.
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Last but not least, I would like thank my parents, family and friends. To all of you: Thanks!

Utrecht, March 5, 2007

Twan Gielen
Appendix A

Error neglecting pore throat volume

One of the assumptions in our network model is the neglecting of pore throat volume in the computation of fluid saturations. Fluid saturation is defined as:

\[ S^\alpha = \frac{V^\alpha}{V^{tot}} \]  

(A-1)

where \( V^\alpha \) is volume of phase \( \alpha \) in the pore bodies and \( V^{tot} \) is total averaging volume. In our network model, this total averaging volume is defined as the sum of all fluid phase volumes:

\[ V^{tot} = \sum_{\alpha=n,w} V^\alpha \]  

(A-2)

Following above presented formulation, it is clear that pore throat volume is neglected. Key advantage of this formulation is that the equations that describe flow of two phases in our network model form a set of linear equations in \( P \), where \( P \) is the fluid pressure inside a pore body. These linear equations can be solved with relatively straightforward numerical methods. When volume of (and therefore, fluid mass in) pore throats is explicitly taken into account, these equations become nonlinear. This is due to the fact that fluid conductivities in the throats depend on throat saturation, which in turn depends on phase pressures inside the pore throats. Therefore, phase pressure inside pore throats must be determined as well as phase pressure in pore bodies.

A second advantage of ignoring the volume of pore throats in our mass balance is that fluid phase pressures only have to be solved in the pore bodies, not in the pore bodies and throats. This is also a considerate aid in determining upscaled parameters of our network as volume-averaged phase pressures and saturations. Average phase pressures are computed based on local (pore-scale) phase saturation and pressure. These parameters are thus averaged over the volume where they are evaluated. It is possible to determine average phase pressure when including phase volume inside
Appendix A. Error neglecting pore throat volume

pore throats, but this is much more complex. Under flow conditions, phase pressure cannot be assumed to be constant over the phase inside a pore throat. This makes upscaling of phase pressures to the macro-scale much more involved.

However, pore throat volume is accounted for in the computation of porosity. The pore throats offer hydraulic resistance to flow based on their radius and length. For that, they do have volume. The pore throats are part of the void space that represents pores in a porous medium.

Thus, we have the situation where pore throat volume is ignored when determining fluid saturation and accounted for when determining porosity. This appendix provides a justification of that, at first glance contradictory, assumption.

To test the validity of this assumption, we use data from the $30 \times 30 \times 40$ nodes network as used in Chapter 6, see table A.1. These data are input to the network realisation routine. The $30 \times 30 \times 40$ nodes network that is used in Chapter 5 is thus constructed. This network has the following geometrical properties:

<table>
<thead>
<tr>
<th>Table A.1: Lattice input parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice dimensions</td>
</tr>
<tr>
<td>Coordination number</td>
</tr>
<tr>
<td>Lattice spacing ($10^{-3}$ m)</td>
</tr>
<tr>
<td>Min pore body radius ($10^{-3}$ m)</td>
</tr>
<tr>
<td>Max pore body radius ($10^{-3}$ m)</td>
</tr>
<tr>
<td>Mean pore body radius ($10^{-3}$ m)</td>
</tr>
<tr>
<td>Min pore throat radius ($10^{-3}$ m)</td>
</tr>
<tr>
<td>Max pore throat radius ($10^{-3}$ m)</td>
</tr>
<tr>
<td>Mean pore throat radius ($10^{-3}$ m)</td>
</tr>
<tr>
<td>Standard deviation of distribution</td>
</tr>
</tbody>
</table>

Thus, 98% of the void pore space is occupied by pore bodies. Discarding pore throat volumes in the determination of fluid phase saturations has therefore minor effect. The assumption to neglect pore throat volume in the determination of
fluid phase saturations and to account for them in the determination of porosity is therefore valid.
Appendix B

Comparison of quasi-static models

The quasi-static pore-scale network model that is introduced in Chapter 3 provides the capillary pressure curves that are used in the computation of damping coefficient $\tau$. To compute damping coefficient $\tau$, quasi-static capillary pressure is subtracted from dynamic capillary pressure for a given value of wetting fluid saturation.

However, an error is made in this procedure. The displacement procedures of this quasi-static model and the dynamic model are slightly different. In the quasi-static model, pore bodies are drained completely when entry pressure of an adjacent pore throat is overcome. Partially filled pore bodies do not exist. In the dynamic pore-scale network model, partially drained pore bodies do exist. Therefore, the dynamic and quasi-static capillary pressure that are computed at a certain saturation, might actually belong to two different saturation states.

The dynamic pore-scale network model that is described in Chapter 4 is also capable of performing quasi-static drainage simulations. Such a static simulation is in fact a series of sequential dynamic drainage experiments. Capillary pressure is then evaluated when equilibrium between the two fluids has been achieved.

To investigate the effect of partially filled pore bodies, a quasi-static drainage simulation is run with the quasi-static network model and the dynamic model. The used network is the same as in Section 3.5.2, see table 3.2. Initial and boundary conditions are given in table 3.1. The resulting quasi-static capillary pressure curves are shown in figure B.1. From this figure, it can be seen that the effect of partially filled pore bodies becomes visible for wetting fluid saturation less than 0.5. The effect on capillary pressure value is very small, since the porous medium under consideration is very homogeneous.

Most significant effect of using the quasi-static network model is that it shortens the range over which damping coefficient $\tau$ can be computed.
Figure B.1: Quasi-static capillary pressure curves, retrieved with the sequential dynamic pore-scale network model and the quasi-static model
Appendix C

Average phase pressures during motion of an interface in a single tube

C-1 Introduction

In this text, the algebraic solutions are presented for the motion of a fluid-fluid interface through a single tube for different viscosity ratios. Viscosity ratio $M$ is defined as $M = \frac{\mu_n}{\mu_w}$. Only drainage is considered. The nonwetting fluid displaces the wetting fluid from the left. Thus, fluid left of the interface is nonwetting fluid, fluid right of the interface is wetting fluid. Following assumptions are made in this text:

- fluids are incompressible
- gravity is neglected
- flow is laminar
- tube radius $R$ is constant
- tube length is constant
- tube is perfectly wetting ($\theta = 0$)
- The pressure drop at the interface is given by the Young-Laplace equation.

The pressure field is imposed by applying Dirichlet boundary conditions on both sides of the tube, see figure C.1. Fluid pressure at the nonwetting fluid boundary is $P$, fluid pressure at the wetting fluid boundary is 0. Three different viscosity ratios are considered in this text:
Appendix C. Average phase pressures during motion I

Figure C.1: Schematic representation of a tube with radius $R$ and length $L$. Dirichlet boundary conditions are applied. Pressure reference level is set at right side of the tube.

- $M = 1$
- $M = 10$
- $M = 0.1$

At the end, formulations for average phase pressures and capillary pressure are derived for a general viscosity ratio $\xi$.

C-2 Local phase pressures

The fluid pressure distribution depends on viscosity ratio, the pressure drop at the interface, the chosen boundary conditions and the location of the interface. In figure C.2, a schematic pressure field is shown. The pressure drop at the interface is constant.

Figure C.2: A sketch of a pressure field in the tube. The interface is at position $x$. Pressure at the left side of the tube is $P$, at the right side 0. Pressure drop at the interface is constant.
constant, and given by:
\[ P^c = \frac{2\sigma \cos \theta}{R} \quad (C-1) \]
The pressure gradients in the nonwetting and wetting phase are a function of viscosity ratio.

**Viscosity ratio equals 1**

When M = 1, the pressure gradients left and right of the interface are equal. The fluid pressures as a function of interface location \( x \) can be seen to be given by:
\[ P^n = -\frac{P - P^c}{L} x + P \quad (C-2) \]
\[ P^w = -\frac{P - P^c}{L} x + P - P^c \quad (C-3) \]
where \( P^n \) is the fluid pressure left of the interface and \( P^w \) is the fluid pressure right of the interface.

**Viscosity ratio equals 10**

When M = 10, the pressure drop in the nonwetting phase is 10 times as high as the pressure drop in the wetting phase. The fluid phase pressures as function of interface location \( x \) become:
\[ P^n = \frac{P^c - P}{0.9x + 0.1L} x + P \quad (C-4) \]
\[ P^w = \frac{P^c - P}{0.9x + 0.1L} (x - L) \quad (C-5) \]

**Viscosity ratio equals 0.1**

When M = 10, the pressure drop in the wetting phase is 10 times as high as the pressure drop in the nonwetting phase. The fluid phase pressures as function of interface location \( x \) become:
\[ P^n = \frac{P^c - P}{9x - 10L} x + P \quad (C-6) \]
\[ P^w = \frac{P^c - P}{9x - 10L} x + 10 \frac{P^c - P}{9x - 10L} L \quad (C-7) \]

**C-3 Average phase pressures**

The local average phase pressures can be used to determine the average phase pressures and the average capillary pressure. Since the pressure drop in each phase is linear, average phase pressure can be determined by evaluating local fluid pressure at the center of the phase. When the interface is at \( x = l \), and the tube length
is \( L \), then the average nonwetting phase pressure is the fluid pressure at \( x = l/2 \)
and the average wetting phase pressure is the fluid pressure at \( x = L - (L - l)/2 \)
(or \( x = l/2 + L/2 \)). For example: when the interface is at \( 0.4L \), average nonwetting phase pressure equals the local fluid pressure at \( x = 0.2L \). The average wetting phase pressure is the fluid pressure at \( x = 0.7L \). Thus, fluid phase pressures are volume-averaged.

Average capillary pressure is defined as the difference between the average nonwetting fluid phase pressure and the average wetting fluid phase pressure. As such, capillary pressure is a volume-averaged quantity, too. It should be noted that this volume-averaged capillary pressure is evaluated at different interface locations, where the fluids are not at equilibrium. It is therefore a dynamic capillary pressure. A static capillary also exists in the same system, which is identified as the entry capillary pressure of the tube.

\section*{C-4 Results}

\subsection*{Input}

The prevailing problem was coded in Fortran, using the input that is given in table C.1.

\begin{table}[h]
\centering
\begin{tabular}{ll}
\hline
R (m) & \( 1 \cdot 10^{-3} \) \\
L (m) & \( 1 \cdot 10^{-2} \) \\
\( \sigma \) (kg s\(^{-2}\)) & 0.0475 \\
\( \theta \) (-) & 0.0 \\
P (kg m\(^{-1}\)s\(^{-2}\)) & 1000 \\
Pc (kg m\(^{-1}\)s\(^{-2}\)) & 95 \\
\hline
\end{tabular}
\caption{Input parameters}
\end{table}

\subsection*{Output}

In figure C.3, the pressure field in the tube is shown for the case where the interface is at \( x = 0.004 \) m, when 40\% of the tube is drained. Also shown is the pressure field for a single-fluid case, which is a straight line.

\subsection*{Viscosity ratio equals 1}

In figure C.4, local pressure fields are shown for various interface positions. The pressure gradients left and right of the interface are equal. The difference between the two average phase pressures, average capillary pressure, is therefore constant and equal to the pressure drop at the interface. For isoviscous fluids, static and dynamic capillary pressure are equal.
Figure C.3: The pressure field in the tube when the interface is at $x = 0.004$ m. Shown are the pressure fields for a single fluid and for two fluids with viscosity ratios $M = 1$, 10 and 0.1, respectively.

Figure C.4: Pressure field in the tube when viscosity ratio $M = 1$. Shown is the pressure field with the interface at different locations in the tube. The pressure gradients are equal on either side of the interface.
Appendix C. Average phase pressures during motion I

Figure C.5: Plot of average pressures in the tube as function of the interface location in the tube. Average capillary pressure is 547.5 Pa.

Viscosity ratio equals 10

In figure C.6, local pressure fields are shown for various interface positions. The pressure gradient in the nonwetting phase is 10 times higher than the gradient in the wetting phase. Average phase pressures are plotted versus interface location in figure C.7. From this, it can be seen, that average capillary pressure is constant during the drainage of the tube. Capillary pressure is found to be 547.5 Pa. This is higher than the entry capillary pressure of the tube, which is 95 Pa.

Viscosity ratio equals 0.1

In figure C.8, local pressure fields are shown for various interface positions. The pressure gradient in the wetting phase is 10 times higher than the gradient in the nonwetting phase. Average phase pressures are plotted versus interface location in figure C.9. From this, it can be seen, that average capillary pressure is constant during the drainage of the tube. Capillary pressure is determined to be 547.5 Pa. This is equal to the average capillary pressure for the case where viscosity ratio M equals 10.
Figure C.6: Pressure field in the tube when viscosity ratio $M = 10$. Shown is the pressure field with the interface at different locations in the tube.

Figure C.7: Plot of average pressures in the tube as function of the interface location in the tube. Average capillary pressures is 547.5 Pa, where entry capillary pressure is 95 Pa.
Figure C.8: Pressure field in the tube when viscosity ratio $M = 0.1$. Shown is the pressure field with the interface at different locations in the tube.

Figure C.9: Plot of average pressures in the tube as function of the interface location in the tube. Average capillary pressures is 547.5 Pa, where entry capillary pressure is 95 Pa.
Figure C.10: Schematic representation of a tube with radius R and length L. Dirichlet boundary conditions are applied. Pressure on the left of the interface is referred to as $P_L$, pressure on the right as $P_R$. Pressure drop at the interface is $P_c$. The pressure gradients on either side of the interface may differ due to viscosity differences.

C-5 Average fluid pressures for general viscosity ratio $\xi$

As the results for average capillary pressure are the same for the three used viscosities, we decided to investigate the system in a more general manner. The used configuration is shown in figure C.10. Dirichlet conditions are used, with $P = P_1$ at the left side of the tube and $P = P_2$ on the right side of the tube. The tube is drained from left to right. Viscosity ratio between the wetting and nonwetting fluid is taken to be $\xi$, where $\xi$ can be any positive number.

The general pressure field is given by:

\[
P_L = -a_1 x + b_1 \quad \text{for } x < l
\]
\[
P_R = -a_2 x + b_2 \quad \text{for } x > l
\]
\[
P_c = P_L - P_R \quad \text{for } x = l
\]

(C-8)

Coefficients $b_1$ and $b_2$ can directly be determined from the boundary conditions:

\[
b_1 = P_1
\]
\[
b_2 = P_2 + a_2 L
\]

(C-9) (C-10)

With these, the equations for the pressure in the tube become:

\[
P_L = -a_1 x + P_1 \quad \text{for } x < l
\]
\[
P_R = a_2 (L - x) + P_2 \quad \text{for } x > l
\]
\[
P_c = P_L - P_R \quad \text{for } x = l
\]

(C-11) (C-12) (C-13)

The abovementioned system has three equations and four unknowns. The system can be completed by viscosity ratio $\xi$, since the pressure gradients in the tube sections are a linear function of viscosity ratio.

\[
M = \xi \rightarrow a_1 = \xi a_2
\]

(C-14)
The pressure equations can now be rewritten as:

\[ P_L = -\xi a_2 x + P_1 \quad \text{for } x < l \]  
\[ P_R = a_2 (L - x) + P_2 \quad \text{for } x > l \]  
\[ P_i^c = P_L - P_R \quad \text{for } x = l \]

Using the interface condition C-17, coefficient \( a_2 \) can now be determined:

\[ a_2 = \frac{P_2 - P_1 + P_i^c}{((1 - \xi)(l - L))} \]

With this, the pressure field in the tube is given by:

\[ P_L = -\xi \frac{P_2 - P_1 + P_i^c}{((1 - \xi)(L - l))^2} x + P_1 \quad \text{for } x < l \]  
\[ P_R = \frac{P_2 - P_1 + P_i^c}{((1 - \xi)(l - L))} (L - x) + P_2 \quad \text{for } x > l \]  
\[ P_i^c = P_L - P_R \quad \text{for } x = l \]

Since the local phase pressures are linear, average phase pressures can be found to evaluate the local phase pressure at the center of the phase:

\[ \langle P^n \rangle = P_L \quad \text{at } x = l/2 \]  
\[ \langle P^w \rangle = P_R \quad \text{at } x = l/2 + L/2 \]

Average capillary pressure is given by:

\[ \langle P^c \rangle = \langle P^n \rangle - \langle P^w \rangle \]
\[ = -\xi a_2 \frac{l}{2} + P_1 - \left[ a_2 \left( L - \frac{l}{2} - \frac{L}{2} \right) + P_2 \right] \]
\[ = \frac{1}{2} ((1 - \xi)(l - L)) a_2 + P_1 - P_2 \]  
\[ = \frac{1}{2} ((1 - \xi)(l - L)) \frac{P_2 - P_1 + P_i^c}{((1 - \xi)(l - L))} + P_1 - P_2 \]
\[ = \frac{1}{2} (P_1 - P_2 + P_i^c) \]

**C-6 Conclusions**

In a single cylindrical tube, volume-averaged capillary pressure does not depend on viscosity ratio, length of the tube or location of the interface. Capillary pressure only depends on the Dirichlet boundary pressures and the entry capillary pressure of the tube, which is given by Young-Laplace equation.
Appendix D

Average phase pressures during motion of an interface in a tube-ball-tube configuration

D-1 Introduction

In this text, the algebraic solutions are presented for the motion of a single interface through a configuration that consist of two vertical tubes connected by a ball, see figure D.1. Only drainage is considered. The nonwetting fluid displaces the wetting fluid from the top.

The assumptions are the same as in the pore-scale network model:

- fluids are isoviscous and incompressible
- gravity is neglected
- flow is laminar
- all resistance is in the tubes
- \( R >> r_1, r_2 \)
- local capillary pressure in the ball is zero

We distinguish three time periods for each of which the unknown pressure in the ball, \( P_b \), has to be found. These are:

1. interface location is in tube 1;
2. interface location is in ball;
Appendix D. Average phase pressures during motion I

\[ P_{\text{n}} = P \]
\[ r_1 / P_{c1} \]
\[ r_2 / P_{c2} \]
\[ r_4 \]
\[ L \]
\[ L \]
\[ P_{w} = 0 \]

\[ \text{Figure D.1: Configuration of the tubes and ball, including dimensions and boundary conditions} \]

3. Interface location is in tube 2.

The corresponding pressures in the ball will be referred to as \( P_{Ib}^l \), \( P_{IIb}^l \) and \( P_{IIIb}^l \).

D-2 Interface position and filling times

Interface in tube 1

**Determination of \( P_{b}^l \)**

To determine \( P_{b}^l \), we balance the volumetric fluxes entering and leaving the system:

\[
\frac{\pi r_1^4}{8 \mu L} (P - P_{b}^l - P_c^l) = \frac{\pi r_2^4}{8 \mu L} (P_{b}^l) \quad (D-1)
\]
\[
r_1^4 (P - P_{b}^l - P_c^l) = r_2^4 P_{b}^l \quad (D-2)
\]
\[
P_{b}^l = \frac{r_1^4}{r_1^4 + r_2^4} (P - P_c^l) \quad (D-3)
\]
\[
P_{b}^l = f_1 (P - P_1^c) \quad (D-4)
\]

where we define

\[
f_1 = \frac{r_1^4}{r_1^4 + r_2^4} \quad (D-5)
\]
\[
f_1 + f_2 = 1 \quad (D-6)
\]
\[
f_2 = \frac{r_2^4}{r_1^4 + r_2^4} \quad (D-7)
\]

**Determination of interface position \( l \) and filling time of tube 1**

We know that the velocity of the interface is the volumetric flux divided by the
cross-sectional area. The interface velocity is also equal to \( \frac{dl}{dt} \). We can then identify the location of the interface in time as follows:

\[
q = \frac{dl}{dt} \quad (D-8)
\]

\[
q = \frac{r_2^2}{8\mu L} (P - P_{b}^l - P_c) \quad (D-9)
\]

\[
q = \frac{r_2^2}{8\mu L} f_2 (P - P_{1}^c) \quad (D-10)
\]

\[
l = \frac{r_2^2}{8\mu L} f_2 (P - P_{1}^c) t \quad (D-11)
\]

Knowing \( l \) as a function of \( t \), we can see that the filling time of tube 1 equals:

\[
t_{\text{fill}} = \frac{8\mu L^2}{r_2^2 f_2 (P - P_{1}^c)} \quad (D-12)
\]

**Interface in ball**

**Determination of** \( P_{b}^{\text{II}} \)

To determine \( P_{b}^{\text{II}} \), we again balance the volumetric fluxes entering and leaving the system:

\[
\frac{\pi r_1^4}{8\mu L} (P - P_{b}^{\text{II}}) = \frac{\pi r_2^4}{8\mu L} (P_{b}^{\text{II}}) \quad (D-13)
\]

\[
r_1^4 (P - P_{b}^{\text{II}}) = r_2^4 P_{b}^{\text{II}} \quad (D-14)
\]

\[
P_{b}^{\text{II}} = \frac{r_4^4}{r_1^4 + r_2^4} (P) \quad (D-15)
\]

\[
P_{b}^{\text{II}} = f_1 P \quad (D-16)
\]

**Determination filling time of the ball**

For this case, we can use the volume of the ball, \( \frac{4}{3}\pi R^3 \), and one of the fluid fluxes, to find the filling time directly. It is not necessary to know the interface location exactly, since we assume zero local capillary pressure in the ball. Knowing the flux in tube 2 and the volume of the ball, the filling time of the ball is easily seen to be:

\[
t_{\text{fill}} = \frac{V_b}{Q} = \frac{4}{3}\pi R^3 = \frac{32\mu L R^3}{3r_2^2 f_1 P} \quad (D-17)
\]

**Interface in tube 2**

**Determination of** \( P_{b}^{\text{III}} \)

Balancing the volumetric fluxes again, we find:

\[
\frac{\pi r_2^4}{8\mu L} (P_{b}^{\text{III}} - P_c) = \frac{\pi r_1^4}{8\mu L} (P - P_{b}^{\text{III}}) \quad (D-18)
\]
Appendix D. Average phase pressures during motion I

\[ r_2^4 P_{b}^{III} - r_2^4 P_c^2 = r_1^4 P - r_1^4 P_c^{III} \] \hspace{1cm} (D-19)

\[ P_b^{III} = \frac{r_1^4 P + r_2^4 P_c^2}{r_1^4 + r_2^4} \] \hspace{1cm} (D-20)

\[ = f_1 P + f_2 P_c^2 \] \hspace{1cm} (D-21)

This equation can be rewritten as:

\[ P_b^{III} = f_1 (P - P_c^2) + f_1 P_1^c + f_2 P_2^c \] \hspace{1cm} (D-22)

**Determination of interface position \( l \) and filling time of tube 2**

The velocity of the interface in tube 2 is given by:

\[ q = \frac{r_2^2}{8 \mu L} (P_b^{III} - P_c^2) \] \hspace{1cm} (D-23)

\[ = \frac{r_2^2}{8 \mu L} (f_1 (P - P_c^2) + f_1 P_1^c + f_2 P_2^c - P_c^2) \] \hspace{1cm} (D-24)

\[ = \frac{r_2^2}{8 \mu L} (f_1 (P - P_c^2) + f_1 (P_c^c - P_c^2)) \] \hspace{1cm} (D-25)

\[ l = \frac{r_2^2}{8 \mu L} f_1 (P - P_c^2) t \] \hspace{1cm} (D-26)

Knowing \( l \) as a function of \( t \), we can see that the filling time of tube 2 equals:

\[ t_{fill} = \frac{8 \mu L^2}{r_2^2 f_1 (P - P_c^2)} \] \hspace{1cm} (D-27)

**D-3 Local average phase pressures**

Knowing the location of the interface in the time, we can determine the volumes and the average pressures of both fluid phases in the tubes and the ball.

**Interface in tube 1**

The average nonwetting and wetting phase pressure in tube 1 are given by:

\[ \langle p^n \rangle = \frac{-l P - P_1^l - P_1^c}{2} \] \hspace{1cm} (D-28)

\[ \langle p^w \rangle = \frac{P_1^l + P - \left(\frac{P_1^l - P_c}{L}\right)}{2} \] \hspace{1cm} (D-29)

This can be rewritten as:

\[ \langle p^n \rangle = P - \frac{l f_2}{2L} (P - P_1^c) \] \hspace{1cm} (D-30)

\[ \langle p^w \rangle = \frac{1}{2} \left( P + P_b^l + P_c^2 \right) - \frac{l}{2L} (P - P_b - P_1^c) \] \hspace{1cm} (D-31)
Interface in ball

\[
\langle p^n \rangle = P_{b}^{II} = f_1 P
\]
(D-32)

\[
\langle p^w \rangle = P_{b}^{II} = f_1 P
\]
(D-33)

Interface in tube 2

The average nonwetting and wetting phase pressure in tube 2 are given by:

\[
\langle p^n \rangle = P_{b}^{III} - \frac{l}{2} \frac{P_{b}^{III} - P_c^e}{L}
\]
(D-34)

\[
\langle p^w \rangle = \frac{P_{b}^{III}}{2} - \frac{l}{2} \frac{P_{b}^{III} - P_c^e}{L} - \frac{P_c^e}{2}
\]
(D-35)

Rewriting yields:

\[
\langle p^n \rangle = f_1 P + f_2 P_c^e - \frac{l f_1}{2L} (P - P_c^e)
\]
(D-36)

\[
\langle p^w \rangle = \frac{f_1 (L - l)}{2L} (P - P_c^e)
\]
(D-37)

D-4 Global average phase pressures

The local average phase pressures can be used to determine the global average phase pressures and the global capillary pressure. To arrive at the global average pressures, the local pressures are weighted with their volume. Since the pressure gradient in the tubes is linear, the local average pressure can be used for this.
Appendix D. Average phase pressures during motion I

Figure D.3: Pressure field in tube 2 when interface is present

Interface in tube 1

\[
\langle P^w \rangle = P - \frac{l f_2}{2L} (P - P_1^c) \\
v_1^w = \pi r_1^2 (L - l) \\
v_b^w = \frac{4}{3} \pi R^3 \\
v_2^w = \pi r_2^2 L \\
\langle p_1^w \rangle = \frac{1}{2} f_1 (P - P_1^c) + \frac{l}{2L} f_2 (P - P_1^c) - \frac{1}{2} P_1^c \\
\langle p_b^w \rangle = f_1 (P - P_1^c) \\
\langle p_2^w \rangle = \frac{1}{2} f_1 (P - P_1^c) \\
\langle P^w \rangle = \frac{\langle p_1^w \rangle v_1^w + \langle p_b^w \rangle v_b^w + \langle p_2^w \rangle v_2^w}{v_1^w + v_b^w + v_2^w}
\]

Interface in ball

\[
v_1^w = \pi r_1^2 L \\
v_b^w = \pi r_2^2 f_1 P \\
v_b^w = \frac{4 \pi R^3}{3} - \frac{\pi r_2^2 f_1 P}{8 \mu L} dt \\
dt = 0 \text{ to } \frac{32 \mu L R^3}{3 \pi r_2^2 f_1 P} \\
v_2^w = \pi r_2^2 L \\
\langle p_1^w \rangle = \frac{1}{2} (1 + f_1) P
\]
\begin{align*}
\langle p^n_1 \rangle &= f_1 P 
(D-52) \\
\langle p^n_w \rangle &= f_1 P 
(D-53) \\
\langle p^w_2 \rangle &= \frac{1}{2} 
(D-54) \\
\langle P^n \rangle &= \frac{\langle p^n_1 \rangle v^n_1 + \langle p^n_b \rangle v^n_b}{v^n_1 + v^n_b} 
(D-55) \\
\langle P^w \rangle &= \frac{\langle p^w_b \rangle v^w_b + \langle p^w_2 \rangle v^w_2}{v^w_b + v^w_2} 
(D-56)
\end{align*}

**Interface in tube 2**

The average nonwetting and wetting phase pressure in tube 2 are given by:

\begin{align*}
v^n_1 &= \pi r_1^2 L 
(D-57) \\
v^n_b &= \frac{4}{3} \pi R^3 
(D-58) \\
v^n_2 &= \pi r_2^2 l 
(D-59) \\
v^w_2 &= \pi r_2^2 (L - l) 
(D-60) \\
\langle p^n_1 \rangle &= \frac{1}{2} [(1 + f_1) P + f_2 P_c^2] 
(D-61) \\
\langle p^n_b \rangle &= f_1 P + f_2 P_c^2 
(D-62) \\
\langle p^n_2 \rangle &= f_1 P + f_2 P_c^2 - \frac{l}{2L} f_1 (P - P_c^2) 
(D-63) \\
\langle p^w_2 \rangle &= \frac{1}{2} f_1 (P - P_c^2) - \frac{l}{2L} f_1 (P - P_c^2) 
(D-64) \\
\langle P^n \rangle &= \frac{\langle p^n_1 \rangle v^n_1 + \langle p^n_b \rangle v^n_b + \langle p^n_2 \rangle v^n_2}{v^n_1 + v^n_b + v^n_2} 
(D-65) \\
\langle P^w \rangle &= \frac{1}{2} f_1 (P - P_c^2) - \frac{l}{2L} f_1 (P - P_c^2) 
(D-66)
\end{align*}

**D-5 Results**

**Input**

The prevailing problem was coded in Fortran, using the input that is given in table D.1.

**Output**

The results are given in the two figures below. Figures D.4 and D.5 show both the dynamic and the static \( P^c - S^w \) curves for the system with the input from table D.1.

Figure D.6 shows the individual average dynamic phase pressures, as well as the resulting (dynamic) \( P^c - S^w \) curve as a function of average wetting fluid saturation.
Appendix D. Average phase pressures during motion I

Figure D.4: Dynamic and static $P_c - S_w$ curves for the system under consideration

Figure D.5: Dynamic and static $P_c - S_w$ curves for the system under consideration, zoomed
D-6 Insights from limit cases

To gain insight into the behaviour, some limit cases have been considered. These are:

- $R >> r_1 >> r_2$
- $R >> r_2 >> r_1$
- $R >> r_{1,2}, r_1 = r_2$

When $r_1$ is much larger than $r_2$, $f_1 = 1$ and $f_2 = 0$. When $r_2$ is much larger than $r_1$, $f_2 = 1$ and $f_1 = 0$. When $r_2$ equals $r_1$, $f_1$ and $f_2$ are both $\frac{1}{2}$.

The averages are determined by the ball, and the influence of the throats is negligible, except when the considered phase is residing only in a tube. For example, when the oil-water interface is in tube 1, the average nonwetting fluid pressure is the average oil pressure in the tube, and the average wetting fluid pressure is the pressure in the ball.

The average phase pressures in the tubes are determined as the average between the phase pressures on entry and exit of the tube. This is illustrated in figure D.7 as an example. When the interface enters tube 1, the nonwetting phase pressure at the interface is $P$. When the interface exits the tube, the pressure is $P_{b}^{I} + P_{b}^{c}$. The average nonwetting phase pressure in tube 1 is therefore given by $\langle P^{n} \rangle = \frac{1}{2} (P + P_{b}^{I} + P_{b}^{c})$. The average wetting phase pressure is the wetting pressure in the ball.

When the interface is in tube 2, the average wetting fluid pressure is determined in a similar way, see figure D.8.

To increase the accessibility to the equations, a formulation with both $P_{b}$ and $f_{1}$ is used.

**Case $R >> r_1 >> r_2$**

When the interface is in tube 1, we have:

$$P_{b}^{I} = f_{1} (P - P_{1}^{c}) = P - P_{1}^{c}$$  \hspace{1cm} (D-67)
Appendix D. Average phase pressures during motion 1

Figure D.6: Individual average dynamic phase pressures and capillary pressure as function of average wetting fluid saturation

\[ \frac{1}{2}(P+P_b+P_c) \]

Figure D.7: Average nonwetting fluid pressure in tube 1 for the limit cases

\[ \frac{1}{2}(P_b - P_c) \]

Figure D.8: Average wetting fluid pressure in tube 2 for the limit cases
\[ \langle P^n \rangle = \frac{1}{2} (P + P_b + P_i^c) = \frac{1}{2} (P + P - P_1^c + P_1^c) = P \] (D-68)

\[ \langle P_w \rangle = P_b = P_1^c \] (D-69)

\[ \langle P_c^c \rangle = P_1^c \] (D-70)

When the interface is in the ball, we have:

\[ P_{bII} = f_1 P = P \] (D-71)

\[ \langle P^n \rangle = P \] (D-72)

\[ \langle P_w \rangle = P \] (D-73)

\[ \langle P_c \rangle = 0 \] (D-74)

When the interface is in tube 2, we have:

\[ P_{bIII} = P \] (D-75)

\[ \langle P^n \rangle = P_{bIII} = P \] (D-76)

\[ \langle P_w \rangle = \frac{1}{2} (P_b - P_2^c) = \frac{1}{2} (P - P_2^c) \] (D-77)

\[ \langle P_c^c \rangle = \frac{1}{2} (P + P_2^c) \] (D-78)

\[ \langle P^c \rangle = \frac{1}{2} (P + P_2^c) \] (D-79)

**Case** \( R >> r_2 >> r_1 \)

When the interface is in tube 1, we have:

\[ P_b^I = 0 \] (D-80)

\[ \langle P^n \rangle = \frac{1}{2} (P + P_b + P_i^c) = \frac{1}{2} (P + P_1^c) \] (D-81)

\[ \langle P_w \rangle = P_b^I = 0 \] (D-82)

\[ \langle P^c \rangle = \frac{1}{2} (P + P_1^c) \] (D-83)

When the interface is in the ball, we have:

\[ P_{bII} = f_1 P = 0 \] (D-84)

\[ \langle P^n \rangle = 0 \] (D-85)

\[ \langle P_w \rangle = 0 \] (D-86)

\[ \langle P_c \rangle = 0 \] (D-87)

When the interface is in tube 2, we have:

\[ P_{bIII}^I = P_2^c \] (D-88)

\[ \langle P^n \rangle = P_{bIII}^I = P_2^c \] (D-89)

\[ \langle P_w \rangle = \frac{1}{2} (P_b - P_2^c) = 0 \] (D-90)

\[ \langle P^c \rangle = P_2^c \] (D-91)
Case $R >> r_{1,2}, r_1 = r_2$

When the interface is in tube 1, we have:

$P^I_b = f_1(P - P^c_1) = \frac{1}{2}(P - P^c_1)$ \hspace{1cm} (D-92)

$\langle P^n \rangle = \frac{1}{2} \left( P + \frac{1}{2}P - \frac{1}{2}P^c_1 + P^c_1 \right) = \frac{3}{4}P + \frac{1}{4}P^c_1$ \hspace{1cm} (D-93)

$\langle P_w \rangle = \frac{1}{2}(P - P^c_1)$ \hspace{1cm} (D-94)

$\langle P^c \rangle = \frac{1}{4}P + \frac{3}{4}P^c_1$ \hspace{1cm} (D-95)

When the interface is in the ball, we have:

$P^II_b = \frac{1}{2}P$ \hspace{1cm} (D-96)

$\langle P^n \rangle = \frac{1}{2}P$ \hspace{1cm} (D-97)

$\langle P_w \rangle = \frac{1}{2}P$ \hspace{1cm} (D-98)

$\langle P_c \rangle = 0$ \hspace{1cm} (D-99)

When the interface is in tube 2, we have:

$P^III_b = \frac{1}{2}(P + P^c_2)$ \hspace{1cm} (D-100)

$\langle P^n \rangle = \frac{1}{2}(P + P^c_2)$ \hspace{1cm} (D-101)

$\langle P_w \rangle = \frac{1}{2}(P^{III}_b - P^c_2) = \frac{1}{4}(P - P^c_2)$ \hspace{1cm} (D-102)

$\langle P^c \rangle = \frac{1}{4}P + \frac{3}{4}P^c_2$ \hspace{1cm} (D-103)

D-7 Conclusions

From sections D-4 and D-5, it can be concluded that dynamic capillary pressure can be less than static capillary pressure in case of drainage! This is the case when the assumptions of the pore-scale network model are used in combination with isoviscous fluids. When viscosity ratio equals 1, the displacement front is neutrally stable.

From section D-6, it can be seen, that the average capillary pressure is zero when the interface is in the ball for all three configurations. This is an indication of the flat interface assumption.

The average capillary pressure results for the $R >> r_1 >> r_2$ and $R >> r_1 >> r_2$ cases are similar. When the interface is in the largest tube, average capillary pressure equals $P^c_i$, where $i$ identifies the largest tube. When the interface is in the smallest tube, average capillary pressure equals $\frac{1}{2}(P + P^c_j)$, where $j$ denotes the largest tube.
When \( R >> r_{1,2}, \) \( r_1 = r_2, \) average capillary pressures are equal when the interface is in the tubes, and zero when the interface is in the ball. This can be expected based on symmetry of the configuration.