Non-linearities and Upscaling in Porous Media

The average equilibrium capillary pressure-saturation relationship in two-phase flow in porous media

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Chapter 1

Introduction

Two-phase flow is of importance in many natural and industrial porous media. For example, in groundwater contamination problems, often Non-Aqueous Phase Liquids (NAPLs) are released. These are hazardous organic liquids that are immiscible with water and form a visible, separate oily phase in the subsurface (Mayer and Hassanzadeh, 2005). Another example of two-phase flow in the subsurface occurs in oil reservoirs. During secondary oil recovery, gas, air, or water is injected into an oil reservoir in order to mobilize oil and increase reservoir production. In industrial porous media, two-phase flow occurs for example during the drying process of paper and foods, in absorbing materials like diapers, in oil filters, and fuel cells.

The examples of two-phase flow in porous media given above illustrate its importance in many aspects of daily life, from environmental problems to industrial processes. Therefore, the correct description of two-phase flow in porous media is very important.

Two-phase flow in porous media is the simultaneous flow of two immiscible fluids or phases through a porous medium. Immiscible fluids are fluids that share a distinct fluid-fluid interface, and cannot be mixed together. A two-phase flow system in a porous medium consists of three phases, being the porous medium itself, which is a solid, and two fluid phases, which can be either a liquid or a gas. Typically, one of the fluid phases wets the solid grains of the porous medium more than the other, giving rise to the concept of wettability.

The flow processes in two-phase flow in porous media can be described with a conceptual model. This conceptual model can be expressed in the form of a mathematical model, which attempts to capture the physical processes in mathematical expressions. In order to do this, usually several assumptions regarding the conceptual model are needed for simplification. In the case of two-phase flow in porous media, some of these assumptions are:

- Flow velocity of the fluids is low, so that it can be assumed that inertial forces in the Navier-Stokes equations are negligible. As a result Darcy’s law can be used to describe the flow of the fluids through the porous medium.
- The variables in the mathematical expressions are macroscale variables, i.e. they are upscaled version of their microscale equivalents.

The mathematical model of a two-phase flow system in a porous medium consists of equations for the conservation of mass for each phase, in combination with a momentum equation for each phase (Darcy’s law). Moreover, supplementary equations are needed to close the system of governing equations. These supplementary equations are the constitutive relationships between relative permeability, capillary pressure, and saturation. The constitutive relationships are the most important fluid-rock properties in systems where two-phase flow occurs, as for example enhanced oil recovery or remediation of groundwater and soil.

Commonly, the capillary pressure-saturation relationship is determined in the laboratory as it cannot be derived directly from physical considerations. It is desirable and often assumed that the capillary pressure-saturation relationship obtained in laboratory experiments is an intrinsic property of the soil, and therefore is independent of the experimental conditions under which
it was obtained. Moreover, often these laboratory determined Pc-Sw curves are applied in the numerical modelling of situations outside the laboratory, usually at a much larger scale and under conditions very different from the laboratory conditions. In these numerical models, the Pc-Sw curve obtained in the laboratory is used as local capillary pressure-saturation relationship. This means the pressure and saturation for each node or element in the numerical domain are derived from this curve. However, a laboratory sample in general contains micro-heterogeneities, each having its own Pc-Sw relationship (see Figure 1.1). Therefore, the obtained sample-scale Pc-Sw curve represents an average curve over these micro-heterogeneities. Nonetheless, this sample-scale Pc-Sw curve is used to represent ‘the’ Pc-Sw relationship for the porous medium in the modelling of large-scale domains, as is illustrated in Figure 1.1.

Note that it is desirable to obtain an average Pc-Sw relationship for micro-heterogeneities, because then they do not need to be discretised separately. For instance, in the assessment and remediation of contamination by DNAPLs in the subsurface, often macro-scale simulations are used (Braun et al., 2005). These simulations require parameters for the macroscale in order to avoid the detailed discretisation of geological structures. It is impossible to collect all the information about the geological heterogeneities on the small scale, and representing them discretely in the numerical model. Therefore upscaled effective parameters (e.g. the constitutive relationships) are needed. However, these parameters should represent the
influence of the lower scale heterogeneities on two-phase flow behaviour at the scale on which the simulation takes place.

This thesis investigates the sample-scale equilibrium $P_c-S_w$ relationship. The main aim is to investigate whether the sample-scale equilibrium $P_c-S_w$ curve truly is an intrinsic property of the porous medium, or whether it depends on other factors, such as for instance measurement methods. This is done by performing numerical simulations of a primary drainage experiment. The numerical simulations are performed with either a numerical model provided by dr. ir. C. Berentsen, or with the model MUFTE-UG from Universität Stuttgart.

The first step in this thesis is to investigate the influence of the averaging method used to obtain the sample-scale equilibrium $P_c-S_w$ relationship in a numerical simulation. The sample-scale equilibrium $P_c-S_w$ curve can be obtained by averaging the pressures and saturations obtained during a simulation for each node in the numerical domain. These pressures and saturations are derived from the local $P_c-S_w$ curve specified in the model for the porous medium. However, there are several ways of averaging saturation and pressure. Using the correct averaging method thus is of importance in upscaling the $P_c-S_w$ curve from the local to the sample-scale or macroscale.

Initially, a simple homogeneous one-dimensional domain will be used to perform a simulation representing a primary drainage process. For this domain, the analytical sample-scale equilibrium $P_c-S_w$ curve is known, as it should be equal to the local scale equilibrium $P_c-S_w$ relationship that is specified in the model. Thus, the obtained average equilibrium $P_c-S_w$ relationships can be compared to the local $P_c-S_w$ relationship, and a correct averaging method will be the one that results in a $P_c-S_w$ curve equal to the local curve.

As a second step, heterogeneities are introduced in a two-dimensional domain. Again, simulations representing a drainage process will be performed. The heterogeneities will be simple, so that an ‘analytical’ macroscale $P_c-S_w$ relationship can be obtained based on the assumption of capillary equilibrium. Subsequently, sample-scale equilibrium $P_c-S_w$ relationships obtained using an averaging method can be compared to this analytical solution. This will show the influence of small-scale heterogeneities on the average equilibrium $P_c-S_w$ curve.

As a last step, the traditional measurement of the $P_c-S_w$ relationship is investigated. Particularly, attention will be given to the use of a hydrophilic membrane in laboratory determination of the $P_c-S_w$ curve. This membrane prevents the nonwetting phase from leaving the sample, which could have an effect on the obtained sample-scale equilibrium $P_c-S_w$ curve. Ideally, this effect should be non-existent as it is always assumed that the obtained $P_c-S_w$ curve is an intrinsic property of the porous medium.

The research objectives of this thesis are:

1) To investigate different averaging methods that can be used to determine an average sample-scale equilibrium capillary pressure-saturation relationship in a homogeneous domain.

2) To investigate the effect of small-scale heterogeneities on the sample-scale equilibrium capillary pressure-saturation relationship.

3) To investigate the effect of a hydrophilic membrane that is often used in the laboratory determination of the static capillary pressure-saturation relationship.

The thesis has the following structure. Chapter 2 provides an introduction into the concepts underlying the classical theory of two-phase flow in porous media. In Chapter 3, the numerical models used in this thesis are described. In Chapter 4, a set of numerical simulations is discussed that are used to obtain preliminary information for the simulations that will be performed in Chapter 5, 6, and 7. In Chapter 5, averaging of the equilibrium...
capillary pressure-saturation relationship for a homogeneous domain is investigated, while in Chapter 6 the same is done for a heterogeneous domain. Chapter 7 deals with the effect of boundary conditions on the equilibrium capillary pressure-saturation relationship, and investigates the effect of the hydrophilic membrane often used in laboratory experiments to determine the static capillary pressure-saturation relationship. Finally, in Chapter 8 the results presented in this thesis are summarized, and the main conclusions are presented. The chapter finishes with remarks and suggestions for future work.
Chapter 2

Theory of two-phase flow

In this chapter, the physical-mathematical model for two-phase flow will be introduced. Both microscale and macroscale concepts will be discussed.

2.1 Concepts of two-phase flow in porous media

Two-phase flow in porous media is the simultaneous flow of two immiscible fluids through a porous medium. A two-phase flow system in a porous medium consists of three phases. These are the porous medium itself, and two fluid phases, which can be either a liquid or a gas. A porous medium is a solid phase permeated by a network of pore spaces. These pore spaces can be occupied by one or more fluids. The pore space is quantified by the porosity, which is the volume of pores divided by the total volume:

\[ n = \frac{V_{\text{pores}}}{V_{\text{total}}} \]  

(2.1)

In order to enable flow, the pores in a porous medium need to be interconnected. The fraction of the porous medium consisting of interconnected pores can be described by the effective porosity:

\[ n_{\text{eff}} = \frac{V_{\text{connected}}}{V_{\text{total}}} \]  

(2.2)

When considering two-phase flow, it is important to consider the scale on which the flow is to be modelled or observed. It is possible to develop equations that describe fluid-fluid interfaces and flow at the pore scale, or microscale. However, these equations are microscale equations and can only be applied at this scale. When equations are needed for a larger scale (the macroscale), it is not correct to simply use the microscale equations. A rigorous averaging procedure should be applied to transform the microscale equations to equations that are valid at the macroscale.

2.1.1 Microscale concepts of two-phase flow

At the microscale or pore scale, two immiscible fluids in a porous medium share a distinct fluid-fluid interface. In addition, the two fluids both share a fluid-solid interface with the porous medium grains. This is illustrated in Figure 2.1. In case of two-phase flow, there will be one fluid-fluid interface, two fluid-solid interfaces and one contact line where the two fluids and the solid are in contact. The interface between the two fluids is sharp. The fluids are phases, meaning they are a volume bounded by an area. Within this volume, no jumps in the chemical composition and physical properties occur.
Typically, one of the fluids in a two-phase flow system wets the solid grain surface more than the other. This observation reflects the concepts of interfacial tension and wettability (Mayer and Hassanizadeh, 2005). Interfacial tension is the result of the difference between the inward attraction of the molecules in the interior of each phase and those at the surface of contact. Within a substance, there are only attractive forces between molecules of the same substance. These forces are called cohesive forces, and these are the forces that keep a substance together. At an interface however, there are also adhesive forces. These are attractive forces between the molecules of one substance and the molecules of the other substance. Adhesive forces are manifested as a tendency of the fluids to cling to each other (Bear, 1972). A molecule situated far away from the interface will only experience cohesive forces, and is uniformly attracted by the surrounding molecules. However, a molecule at the interface experiences both cohesive and adhesive forces, and the attraction by molecules from the same substance can be different from the attraction by molecules from the other substance. This is illustrated in Figure 2.2 for an air-water system.

Figure 2.1: NAPL trapped in a porous medium. The red substance is the NAPL, the white are the porous medium grains, and the blue are the pores not yet occupied by NAPL (source: www.zeroppm.org)

Figure 2.2: imbalance of cohesive forces at the interfaces between two immiscible phases, in this case air and water (from Mayer and Hassanizadeh, 2005).
As a result, there is a net imbalance of forces. When considering the molecule in Figure 2.2, it experiences a net downward force as the cohesive forces are stronger than the adhesive forces. This means that, in order to bring a molecule to the interface, work needs to be done to overcome the net downward force that governs at this interface. Therefore, molecules at the interface will possess additional energy compared to molecules inside the bulk phase. This excess surface energy between the two phases is also known as interfacial tension, which describes the amount of work that needs to be done to separate a unit area of substance $\alpha$ from substance $\beta$:

$$\sigma_{\alpha\beta} = \frac{\partial W}{\partial A_{\alpha\beta}}$$

(2.3)

where $\sigma_{\alpha\beta}$ is the interfacial tension, $\partial W$ is the change in work, and $\partial A$ is the change in surface area between phase $\alpha$ and $\beta$. A surface that possesses free energy will contract when it has the chance, and therefore the free interfacial energy is called interfacial tension. Note that this force acts tangential to the interface. For a two-phase system, three interfacial tensions are present, being the interfacial tension between the solid and nonwetting phase ($\sigma_{sn}$), between the solid and wetting phase ($\sigma_{sw}$), and between the wetting and nonwetting phase ($\sigma_{nw}$).

Figure 2.3 shows two immiscible fluids that are in contact with a solid phase, as would be the case with two-phase flow inside a porous medium. In the figure, $\theta$ is the angle between the interface and the solid surface, and is also called the contact angle. This contact angle is usually measured through the fluid with the highest affinity for the solid grains. When the fluids are in equilibrium with the solid surface, the following equation holds:

$$\sigma_{f_1f_2}\cos\theta = \sigma_{sf_1} - \sigma_{sf_2} \quad \text{or} \quad \cos\theta = \frac{\sigma_{sf_1} - \sigma_{sf_2}}{\sigma_{f_1f_2}}$$

(2.4)

Where $\sigma_{f_1f_2}$ is the interfacial tension between two fluids, $\sigma_{sf_1}$ is the interfacial tension between the solid and the first fluid, and $\sigma_{sf_2}$ is the interfacial tension between the solid and the second fluid.

Figure 2.3: Two immiscible fluids in contact with a solid, the direction of the interfacial tension is shown as well (from Bear, 1972).
Equation (2.4) is also known as Young’s equation, and only can be used if the forces working on the interfaces are in equilibrium (i.e. when the interfaces do not move anymore). Young’s equation follows from a balance of forces that act horizontal to the solid surface. Thus, it only considers equilibrium of force components along the tangent to the solid surface, assuming the forces acting in other directions to be negligible. Note that if

$$\frac{\sigma_{sf_1} - \sigma_{sf_2}}{\sigma_{fs_i}} > 1$$ \hspace{1cm} (2.5)$$
equilibrium is not possible and the liquid $f_2$ will spread out indefinitely between liquid $f_1$ and the solid phase.

In general, one of the fluids will show a stronger preference for the solid phase. Therefore, the two fluids are often defined by their preference towards the solid phase. The wetting fluid is the fluid that shows the greatest preference towards contact with grain particles, while the nonwetting fluid is the fluid that shows the least preference towards contact with the grain particles (Mayer and Hassanizadeh, 2005). This means that if a fluid has a contact angle $>90^\circ$, it is the nonwetting fluid, while if it has a contact angle of $< 90^\circ$, it is the wetting fluid.

![Figure 2.4: Typical wettability preferences for combinations of water, NAPL and air (from Mayer and Hassanizadeh, 2005)](image)

Figure 2.4 shows different fluids in contact with a solid surface. As can be seen, in case of air and water, water will be the wetting phase while air is the nonwetting phase. In case of NAPL and air, NAPL is the wetting phase while air is the nonwetting phase. In case of NAPL and water, water is the wetting phase, while NAPL is the nonwetting phase.

The term wettability is used to describe the tendency of one phase being attracted to the grain particles in preference to another phase (Mayer and Hassanizadeh, 2005). Note that wettability only has a relative meaning, because the order of wetting depends on the chemical composition of the fluids and the solid. For instance, as is shown in Figure 2.4, a NAPL can be wetting in case of a NAPL-air system, but is nonwetting in case of a NAPL-water system. Another important remark is that interfacial tension and wettability may be different when a fluid-fluid interface is advancing or receding on a solid surface (Bear, 1972). This phenomenon is called contact angle hysteresis, and will be discussed further in Section 2.2.3. Note that a contact angle can only be defined if the interface is in equilibrium and does not move or deform. If the interface is not in an equilibrium state, a unique contact angle can not be defined. That is because a range of contact angles can be possible when the interface is not in an equilibrium state (Hassanizadeh and Gray, 1993a).
2.1.2 Microscale capillary pressure
When two immiscible fluids are in contact within a pore, the interface between them will develop a curvature as a result of balance of forces, which is the combined effect of cohesive and adhesive forces. Across the interface, a pressure difference exists. This is because the pressures in the phases on each side of the interface are not equal, and the pressure in the nonwetting phase will be larger than the pressure in the wetting phase.

The capillary pressure is defined as the pressure difference between the nonwetting and wetting phase:

$$p_c = p_n - p_w$$  \hspace{1cm} (2. 6)

where $p_n$ is the pressure of the nonwetting phase and $p_w$ is the pressure of the wetting phase (Fetter, 1999). The difference in pressure is caused by interfacial forces across the fluid-fluid surface, which are able to balance a pressure difference between the phases on each side. If the pressure difference becomes too large, the interfacial forces can no longer balance the pressure difference and the interface will start to move (i.e. the contact line is displaced). Thus, the local capillary pressure is balanced by interfacial forces, which is described by the Young-Laplace equation:

$$p_c = \frac{2\sigma}{R}$$  \hspace{1cm} (2. 7)

where $R$ is the mean curvature of the surface, and $\sigma$ is the interfacial tension. This equation is valid for a meniscus of general shape.

![Figure 2.5: cross section of a capillary tube containing a wetting and nonwetting phase. $\Theta$ is the contact angle, $R$ is the radius of curvature of the fluid-fluid interface, $r$ is the radius of the tube, $P_w$ is the wetting phase pressure, and $P_n$ is the nonwetting phase pressure.](image)

When a spherical meniscus is considered in a vertical tube with a circular cross section or radius $r$, the equation becomes:
where $\sigma$ is the interfacial tension, $\theta$ is the contact angle and $r$ is the radius of the tube (see Figure 2.5). The contact angle depends on chemical composition of the fluid and the solid, and the surface roughness of the solid. In addition, it can also shown to be dependent on the history of the drainage process in the sample, as will be discussed in Section 2.2.3.

Important to note is that the capillary pressure as defined in Equations (2.7) and (2.8) only will be equal to the capillary pressure as defined in Equation (2.6) when the interface is in an equilibrium state. When the interface is not in an equilibrium state, the pressure difference between the two phases across the interface will not be equal to $2\sigma/R$. Thus:

\[
\sigma = \frac{2\sigma \cos \theta}{r}
\]  

(2.8)

Only when the interface is not moving, the pressure difference across the interface is balanced by the interfacial tension of the interface (Hassanizadeh and Gray, 1993a).

Equation (2.8) indicates that in order for an interface to move through a pore, a certain pressure has to be overcome. Only when the interfacial forces can no longer balance the pressure difference between the two phases, the interface will start to move. The difference in phase pressures thus has to become larger than $2\sigma/R$. Equation (2.8) indicates that this so called threshold pressure becomes larger with decreasing pore size.

The equations given above for capillary pressure only apply at the microscale, as $p_c$ depends locally on $\sigma$ and $R$. Therefore, the capillary pressure depends on the geometry of the void space, on the nature of the solids and liquids, and on the degree of saturation. However, in natural porous media, the geometry of the void space is very irregular and complex, so it is difficult if not impossible to describe it analytically (Bear, 1972). This makes it difficult to find a mean radius of curvature $R$ for an area larger than the pore. One could assume an idealized representation of a porous medium, for instance by assuming that the porous medium can be represented by capillary tubes (e.g. Dahle et al., 2005). Then a relation $P_c = P_c(S_w)$ can be derived for this idealized porous medium structure. However, this will never result in a macroscopic relation $P_c = P_c(S_w)$ for the actual porous medium. The only way to derive this macroscopic equation has been to perform laboratory experiments.

2.1.3 Macroscale relations

If we want to study flow and transport in porous media, equations are needed that are valid at a larger scale than the microscale. This is because it is not possible to deal with fluid distributions and flow at the pore scale. The larger scale is called the macroscale or continuum scale, and the variables at this scale are averages over the neighbourhood of the position of interest (Hassanizadeh and Gray, 1993a). This neighbourhood is called a Representative Elementary Volume (REV). An REV is that volume over which you have to average a medium property so that it is no longer dependent on pore-scale fluctuations. This is illustrated in Figure 2.6. Note that at larger volumes $V$, heterogeneities can start to play a role so that the medium property no longer is a constant. The REV should be large enough so that
pore-scale variations are not of importance, but small enough to avoid influences due to heterogeneities.

![Figure 2.6](image)

Figure 2.6: the concept of REV explained for the property porosity. The REV is the volume over which one has to average so that microscopic effects no longer influence the variable and the variable becomes constant (from Bear, 1972)

At the macroscale, a consideration of the continuum is assumed. This means that the phases are assumed to have a continuous distribution within space, and that they can be described by a set of state variables that are continuous and differentiable functions of space and time (Helmig and Cunningham, 2006). In the macroscopic continuum, discontinuities which can be recognized at the microscale can no longer be identified. Note that also at the microscale a continuum is assumed, as the pore scale already represents an average over the molecular consideration. At the microscale, it is assumed that each phase is a continuum, separated by interfaces (discontinuities) from the other phases. The different scales are illustrated in Figure 2.7.

![Figure 2.7](image)

Figure 2.7: Scales: going from microscale to macroscale to local scale to field scale (from Helmig and Cunningham, 2006)

Thus, at the macroscale, it is no longer possible to distinguish between separate phases. Only the ratio of phases can be described and measured. This ratio is also known as the saturation, and is defined as:
2.1.4 Qualitative description of two-phase flow

Starting from a porous medium that is fully saturated with wetting fluid, a description can be given of what will happen as a nonwetting fluid starts displacing the wetting fluid. First of all, before the nonwetting fluid can enter the porous medium, the entry pressure (or threshold pressure) should be overcome. Thus, a capillary pressure must build up at the interface between the two fluids before drainage of the wetting fluid can start (Bear, 1972). When the entry pressure is reached, the nonwetting fluid will start to displace the wetting fluid. The nonwetting fluid will start to occupy the largest pores first, while the wetting fluid will continue to occupy the smaller pores. As the wetting fluid leaves the pore space, the largest pores are being drained first. The larger pores can not support the pressure difference between the two phases, and as a result release the wetting fluid. As the drainage process continues, and the nonwetting phase pressure increases, more and more small pores are drained as their entry pressure is being reached. At some point, the wetting phase saturation becomes so low that the wetting phase forms rings called ‘pendular rings’ around the grain contact points (Figure 2.8).

\[
S_\alpha = \frac{\text{volume of fluid phase } \alpha \text{ within REV}}{\text{volume of pore space within REV}} = \frac{V_\alpha}{V_{\text{pore}}} \quad \alpha = w, n
\]

with

\[
S \in [0, 1] \quad \text{and} \quad \sum S_\alpha = 1
\]

Note that the saturation is a medium property that only occurs at the macroscale. It does not exist at the microscale because on this scale, the separate phases can be recognized. Other medium properties that only occur at the macroscale are porosity and permeability. Porosity describes the ratio of pore volume to total volume of a porous medium (Equation (2.1)). Permeability describes the ability of a porous medium to transmit fluids.
The pendular rings are isolated and do no longer form a continuous water phase, except for a very thin film of water of nearly molecular thickness on the grains’ surfaces (Bear, 1972). At this point, flow of the wetting phase is no longer possible, because there is no continuous connection. The wetting fluid in this case is said to be in its pendular state, and the water pressure applied at a certain position can no longer be transferred to other positions due to the discontinuity of the wetting fluid. Now, when the water saturation would be increased again (i.e. imbibition), the pendular rings will expand until a continuous wetting fluid phase is formed. When the wetting fluid is continuous and able to flow, it is said to be funicular. As the water saturation is further increased, finally the nonwetting fluid phase will no longer be a continuous phase, as it will break into individual globules that occupy the centre of the larger pores. A globule of the nonwetting phase then can only move if the surrounding wetting phase applies a pressure difference which is large enough to squeeze the globule through the pore throat. The globules of nonwetting phase are said to be insular. Depending on the pore size distribution, the transition from pendular to funicular wetting fluid does not have to take place at the same moment throughout the porous medium. It is possible that at low saturation, part of the wetting fluid forms a continuous phase, while the rest is in the pendular state. As saturation increases, there will be a gradual transition as more wetting fluid becomes funicular (Bear, 1972).

2.1.5 The traditional theory of two-phase flow

The traditional theory for two-phase flow is based on a macroscale equation that was initially proposed by Henry Darcy in 1856, now 150 years ago. Darcy empirically derived this equation for the case of slow flow of a single-phase fluid in an isotropic porous medium. Darcy’s equation is commonly written in the following form:

\[ q = -\frac{K}{\mu} (\nabla P - \rho g) \]  

(2.12)

where \( q \) is the Darcy velocity vector, \( K \) is the intrinsic permeability tensor, \( \mu \) is the fluid viscosity, \( P \) is the phase pressure, \( \rho \) is the fluid density and \( g \) is the gravitational acceleration vector. In this equation, the pressure and gravitational forces constitute the driving forces, whereas the viscous forces constitute the resistive forces (Mayer and Hassanizadeh, 2005). The Darcy equation thus is based on the balance between pressure, gravitational and viscous forces. Inertia forces are assumed to be negligible for flow in porous media. Through the years, the Darcy equation has been extended and applied to more and more complicated systems, such as two-phase flow. The extended Darcy equation for two phase flow becomes:

\[ q_\alpha = -\frac{k_{ra}}{\mu_\alpha} K (\nabla P_\alpha - \rho_\alpha g) \]  

\( \alpha = w, n \)  

(2.13)

where \( \alpha \) refers to the fluid phase under consideration, and \( k_{ra} \) is the relative permeability of phase \( \alpha \). This extension has been done by assuming that just as for single-phase flow, the driving forces in two-phase flow are pressure and gravitational forces. New in this equation is the relative permeability \( k_{ra} \), which scales the saturated intrinsic permeability such that the influence on flow of one phase due to the presence of the other phase is taken into account.
The extended form of Darcy’s law can now be used in the conservation equation for fluid $\alpha$, which is given by:

$$\frac{\partial nS_{\alpha}P_{\alpha}}{\partial t} + \nabla \cdot \left( q_{\alpha} \rho_{\alpha} \right) = 0 \quad \alpha = w, n$$

(2.14)

in the absence of sources and sinks. Equation (2.14) simply states that the change in mass of fluid $\alpha$ through time should be equal to the fluxes flowing in or out of the volume under consideration.

Now substituting the extended form of Darcy’s equation into Equation (2.14) gives the mass balance equation for fluid $\alpha$:

$$\frac{\partial nS_{\alpha}P_{\alpha}}{\partial t} - \nabla \cdot \left( \rho_{\alpha} \frac{k_{\alpha}}{\mu_{\alpha}} \nabla P_{\alpha} - \rho_{\alpha} g \right) = 0$$

(2.15)

Note that in Equation (2.15), it is assumed that the solid matrix does not deform and thus that the solid grains do not move.

Equation (2.15) results in a total of 8 equations, as there is a mass balance equation for each phase, and the Darcy equation consists of three components for each phase as well. However, there are 14 unknowns:

$$(q_{\alpha}), \rho_{\alpha}, P_{\alpha}, k_{\alpha \alpha}, S_{\alpha} \quad i = 1,2,3 \quad \alpha = 1,2$$

(2.16)

Therefore, 6 additional equations are required in order to completely describe the system. The density of the wetting and nonwetting phase can be described by the equation of state, which is an empirical relation describing the dependence of density on temperature and pressure:

$$\rho_w = \rho_w(P_w, T) = \rho_{w,0} e^{-\alpha(T-T_0)} \beta(P-P_0)$$

(2.17a)

$$\rho_n = \rho_n(P_n, T) = \rho_{n,0} e^{-\alpha(T-T_0)} \beta(P-P_0)$$

(2.17b)

where $\rho_{w,0}$ and $\rho_{n,0}$ are the wetting and wetting phase densities at $T=T_0$ and $P=P_0$, $\alpha$ is the thermal expansion coefficient, and $\beta$ is the compressibility. The remaining 4 equations can be obtained from laboratory determination of the relative permeability and capillary pressure as function of saturation (Gray and Hassanizadeh, 1991):

$$k_{rw} = k_{rw}(S_w)$$

(2.18a)

$$k_{rn} = k_{rn}(S_w)$$

(2.18b)

$$P_c = P_c(S_w)$$

(2.19)

The capillary pressure is defined as:
Note that Equations (2.18) and (2.19) are hysteretic functions of $S_w$. This means that for a particular value of $S_w$, the function can have different values, depending on the history of the sample. This will further be discussed in Section 2.2.3.

The last equation that is needed describes the relation between the two saturations:

$$S_w + S_n = 1$$

Thus, the pair of partial differential equations for simultaneous flow of two immiscible phases as given in Equation (2.15) can be coupled by introducing the saturation condition, the relative permeability-saturation relations, and the capillary pressure-saturation relation. In addition, fluid and medium properties such as density and porosity need to be specified (Mayer and Hassanizadeh, 2005).

**2.2 Constitutive relationships**

The capillary pressure-saturation relationship and the relative permeability-saturation relationship are so-called constitutive relationships. As was shown in Section 2.1.5, these relationships are needed to close the set of governing equations describing two-phase flow in porous media.

**2.2.1 The capillary pressure-saturation relationship**

There is no physically derived theory that can be used to determine capillary-pressure saturation relationships. Therefore, such curves need to be determined empirically through laboratory experiments. Figure 2.9 shows the general shape of these experimentally derived $P_c-S_w$ curves. The $P_c-S_w$ relationships are obtained from a column that is filled with the porous medium under consideration. Initially, this porous medium is fully saturated with wetting fluid. Then, the nonwetting phase is forced into the column from one side, and the nonwetting phase will start to displace the wetting phase. Nonwetting phases usually are air or NAPLs, while the wetting phase usually is water. As a result of the displacement, on the other side of the column the wetting fluid will start to flow out. The displacement will reduce the wetting phase saturation $S_w$, and in addition the capillary pressure will increase. This process is called a drainage process, and the curve describing the relation between the capillary pressure and saturation during this process is called a drainage curve. When starting from an initially fully saturated sample, the resulting curve is called the primary drainage curve. However, before the nonwetting phase can enter the fully saturated column, first a certain pressure has to be reached at the interfaces between wetting and nonwetting phase before the interfaces will start to move and drainage of the wetting phase will initiate. The minimum pressure that is needed for the nonwetting phase to enter the porous medium is called the displacement or entry pressure (Bear, 1972). As the drainage process takes place, more and more wetting phase is displaced by the nonwetting phase. Eventually, no more wetting phase will be displaced, even with further increase in capillary pressure. The wetting phase saturation at which this happens is known as the irreducible or residual wetting phase saturation (Fetter, 1999).
When this saturation is reached, the wetting fluid does not flow anymore, due to phase fragmentation or strong wetting phase attachment to the grain particles. The wetting phase thus has reached the funicular state, and its relative permeability has become zero. When now the nonwetting fluid is displaced by forcing the wetting phase back into the sample, a main imbibition or wetting curve is obtained. With decreasing capillary pressure, more and more nonwetting phase is displaced by the wetting phase. When zero capillary pressure is reached however, some of the nonwetting phase will remain in the sample. The saturation related to this is called the residual nonwetting phase saturation. At this saturation, the nonwetting phase has become insular. As can be seen in Figure 2.9, the drainage and imbibition curves do not follow the same paths in the $P_c-S_w$ plane. This is because the pores in a porous medium wet and drain differently. This phenomenon is also known as hysteresis. Hysteresis causes the capillary pressure-saturation relationship to be non-unique. This means that the history of the sample influences the relationship. Depending on the moment the drainage or imbibition process is reversed, an infinite number of scanning curves can be formed within the region enveloped by the main drainage and imbibition curves (Mayer and Hassanizadeh, 2005). Hysteresis will be further discussed in Section 2.2.3.

The experimental capillary pressure-saturation relationships that are obtained from laboratory experiments are often parameterized for further use. Several approaches have been suggested for this, but the two most widely used models are those of Brooks and Corey and van Genuchten. Brooks and Corey derived their model in 1964. This model contains two parameters: the entry pressure $P_d$ and the pore size distribution index, $\lambda$. Their model is stated as follows:
\[ S_e = \left( \frac{P_d}{P_c} \right)^{\lambda} \quad \text{when } P_c > P_d \]

\[ S_e = 1 \quad \text{when } P_c < P_d \]  \hfill (2.22)

where \( P_d \) is the entry pressure, and \( \lambda \) is the Brooks-Corey pore size distribution index. \( S_e \) is the effective saturation, defined as:

\[ S_e = \frac{S_w - S_{wr}}{1 - S_{wr} - S_{nr}} \]  \hfill (2.23)

where \( S_w \) is the wetting phase saturation, \( S_{wr} \) is the residual wetting phase saturation, and \( S_{nr} \) is the residual nonwetting phase saturation. The pore size distribution index \( \lambda \) is related to the slope of the \( P_c-S_w \) curve, as is illustrated in Figure 2.10. As can be seen, the larger the pore size distribution index (and thus the more uniform the sand is, i.e. more sorted), the sharper the capillary pressure-saturation curve becomes. Moreover, finer sand will have a higher wetting phase saturation at a certain capillary pressure than coarser sand. This means that the finer sand can hold more wetting phase at a certain capillary pressure. Also, the finer sand has a higher entry pressure, as would be expected as the pores in a fine sand are smaller.

![Figure 2.10: a) typical capillary pressure-saturation curves for a uniform and a non-uniform sand, showing the influence of the pore-size distribution index \( \lambda \) on the slope of the \( P_c-S_w \) curve; b) capillary pressure-saturation curves for different types of sand (from Helmig and Cunningham, 2006)]
In 1980, van Genuchten proposed the following model:

\[
S_v = \left[1 + (\alpha h_c)^n\right]^{-m}
\]  \hspace{1cm} (2.24)

where \(h_c\) is the capillary pressure head:

\[
h_c = \frac{P_c}{\rho_w g}
\]

and \(\alpha\), \(n\), and \(m\) are fitting parameters. The Brooks-Corey model and the van Genuchten model both can be used to parameterize the experimental capillary pressure-saturation relationship. However, a major difference between the two models occurs near full wetting phase saturation. Near full wetting phase saturation, the Brooks-Corey model is discontinuous, while the van Genuchten model is continuous. The Brooks-Corey model assumes a finite entry pressure while the van Genuchten model assumes a smooth transition from zero capillary pressure. Figure 2.11 illustrates this difference. From the physical point of view, it seems reasonable that a porous medium has a finite entry pressure, especially if that porous medium has a narrow pore size distribution. However, for porous media that have a more mixed pore size distribution, a smooth transition might be more appropriate (Mayer and Hassanizadeh, 2005).

![Figure 2.11: The Brooks-Corey and van Genuchten models. The Brooks-Corey model is discontinuous at \(S_w = 1\), and requires an entry pressure to be reached before the nonwetting phase can enter the porous medium. The van Genuchten model on the other hand is continuous, and increases gradually from \(S_w = 1\) (from Helmig and Cunningham, 2006).](image)

### 2.2.2 The relative permeability-saturation relationship

The second constitutive relationship needed in the theory of two-phase flow in porous media is the relative permeability-saturation relationship. This relationship is needed to account for the presence of two fluids in a porous medium. When two fluids are present in a porous
media, part of the pore space will be occupied by either one of the fluids, and the fluids will influence each other during flow. When the flow of one of the fluids at a point is being considered, part of the pore space near this point will be occupied by another fluid, and the permeability for this fluid will be reduced. This permeability is called relative permeability, and is dependent on saturation. It has been shown that, just as the capillary pressure-saturation relationship, the relative permeability-saturation relationship also suffers from hysteresis, although this is less pronounced (Hassanizadeh et al., 2002)

Relative permeability is defined as the ratio of the permeability of a phase at a given saturation to the intrinsic permeability of the porous medium:

$$k_{r\alpha} = \frac{k_{\alpha}}{K} \quad 0 \leq k_{\alpha} \leq K \text{ and } 0 \leq k_{r\alpha} \leq 1$$  \hspace{1cm} (2.25)

Figure 2.12 shows typical relative permeability curves for a pair of immiscible fluids. The shape of the relative permeability-saturation relationship is dependent on the specific porous medium, and on whether the fluid under consideration is wetting or nonwetting to the solid matrix.

As can be seen from the Figure 2.12, both $k_r$-$S_w$ curves begin at unity when the porous medium is fully saturated by the fluid under consideration. When the saturation of the fluid decreases, the relative permeability decreases. When the residual saturation is reached, the fluid has become discontinuous and flow is no longer possible. The relative permeability then has become zero. Thus, the wetting fluid phase will only start to flow above the irreducible wetting phase saturation, and the nonwetting fluid phase will only start to flow above the residual nonwetting phase saturation (Mayer and Hassanizadeh, 2005).

Figure 2.12 also shows that the relative permeability of the wetting phase at the residual nonwetting phase saturation is less than the relative permeability of the nonwetting phase at the irreducible wetting phase saturation. This is because the residual nonwetting phase is present as globules in the middle of the larger pores, and as such causes more obstruction to
flow than the wetting phase at the irreducible wetting phase saturation. At the irreducible wetting phase saturation, the wetting phase is present in small pores and therefore is a lesser obstacle to flow of the nonwetting phase. In addition, it can be noted that at equal phase saturations, \( k_{rw} > k_{nw} \) (Mayer and Hassanizadeh, 2005). This is due to wettability effects. Because the wetting phase fluid coats the solid grains, it acts as lubrication for the nonwetting phase, so that the resistance to flow for the nonwetting phase is reduced. Finally, the figure shows that the sum of the two relative permeabilities for the two fluids is less than 1, i.e. \( k_{rw} + k_{nw} < 1 \). This is the result of the interference of the flow of one fluid with the flow of the other fluid, due to differences in fluid viscosities (Mayer and Hassanizadeh, 2005).

As was mentioned above, the relative permeability is a function of saturation. This function can be determined from laboratory measurements directly, but more often the relative permeability-saturation relationship is simply derived from the experimentally determined capillary pressure-saturation relationship. This can be done because the capillary pressure-saturation curves also possess information on the pore size distribution of the porous medium. Two well known models that are often used are those of Mualem (1976) and Burdine (1953). These two models can be applied to either the Brooks-Corey or the van Genuchten model for the capillary pressure-saturation relationship. If for example the Burdine model is used in conjunction with the Brooks-Corey model, one would get:

\[
\begin{align*}
    k_{rw} &= S_e^{2+\frac{3\lambda}{2}} \\
    k_{nw} &= (1 - S_e)^3 \left(1 - S_e^{2+\frac{3\lambda}{2}} \right)
\end{align*}
\]

### 2.2.3 Hysteresis

As was mentioned before, the \( P_c-S_w \) relationship and to a lesser extent the \( k_r-S_w \) relationship experience hysteresis. There have been many suggestions through the years that try to explain hysteresis. One suggestion that has been done is related to “Haines Jumps”. With Haines Jumps, during a drainage process, the interfaces can suddenly jump instead of moving constantly through a pore. This results in higher capillary pressure during drainage than during imbibition. However, Hassanizadeh and Gray (1993a) doubt this explanation for hysteresis, as there is no substantial proof for it. Actually, there are several experiments that show that the jumps of the interfaces do cause small fluctuations in the capillary pressure, but these fluctuations are much smaller than the difference measured between drainage and imbibition curves in a hysteresis loop at a certain saturation (Hassanizadeh and Gray, 1993a).

Another explanation for hysteresis in the macroscale capillary pressure-saturation relationship is the contact angle. The contact angle is a function of the direction of displacement (Bear, 1972). Note that this is a process that takes place at the microscale. Figure 2.13 shows the curvature of a surface between nonwetting and wetting fluid as it moves within a capillary tube. As was mentioned before in Section 2.1.1, the contact angle can have different values when the equilibrium state of the interface is not yet reached, depending on whether the interface is advancing or receding over a solid surface. From Figure 2.13 it becomes clear that when a nonwetting fluid is displacing the wetting fluid during drainage, the contact angle will be smaller than the equilibrium value. This equilibrium value is the value that can be calculated with the Young-Laplace equation. When the wetting fluid is displacing the nonwetting fluid during imbibition, the contact angle will be smaller than the equilibrium value. Sometimes, this effect also is called the raindrop effect, as the front of a raindrop that
moves over a sloped surface will have a contact angle related to imbibition, while the back of the raindrop has a contact angle that is related to drainage. This is illustrated in Figure 2.14.

**Figure 2.13:** Contact angle hysteresis in a capillary tube for a) stationary state; b) displacement of wetting fluid by nonwetting fluid; c) displacement of nonwetting fluid by wetting fluid. As can be seen, $\theta_2 < \theta < \theta_1$ (after Bear, 1972).

Another mechanism that is thought to be causing hysteresis in the capillary pressure-saturation relationship is the so-called ‘ink-bottle effect’. This effect is due to the geometry of the pore space in a porous medium, which usually has many bottle necks. This mechanism is illustrated in Figure 2.15. As can be seen, for the same capillary pressure, during drainage and imbibition the pore space has different fluid distributions as a result of the non-symmetric
geometry of the pore space. This thus would result in different saturations during drainage and imbibition at the same capillary pressure.

Finally, a fourth mechanism that could be causing hysteresis comprises so-called trapping effects. Trapping effects influence the residual saturation in a porous medium during the several imbibition and drainage cycles that take place. The residual saturation that will occur in a porous medium depends on the pore geometry, the heterogeneity and also the displacement process. In addition, as Figure 2.16 shows, the number of drainage and imbibition cycles influences the residual saturation as well. In the figure, during the first drainage cycle, the NAPL phase reaches into the largest pore only. When drainage is ceased, a residual NAPL globule will be left behind in this pore as a result of trapping due to the higher entry pressure to the left of the NAPL globule than is present in the globule itself. Several cycles of imbibition and drainage so can result in different residual nonwetting phase saturations, and hysteresis of the $P_c-S_w$ curve.

Although the mechanisms described above all suggest different reasons for hysteresis, most researchers agree that hysteresis is related to the configuration and distribution of interfaces. For a given saturation, there are a number of different interface configurations and thus a range of interfacial areas that are possible for a given saturation. In Section 2.5, a new theory for two-phase flow will be described that includes interfacial area and is able to explain the observed hysteresis in the capillary pressure-saturation curve.
Finally note that the mechanisms described above all are microscale processes, taking place at the pore scale. However, at the larger scale the presence of heterogeneities could also be causing hysteresis (e.g. Ataie-Ashtiani et al., 2002).

![Figure 2.16: a) non-wetting fluid (darker) in a pore channel; b) capillary pressure-saturation relationship (from Multiphase Flow, Transport and Bioremediation in the Subsurface, short course reader, 2006).]

### 2.3 Traditional measurements of capillary pressure-saturation curves

#### 2.3.1 General method

As was mentioned before, there is no method to theoretically/physically derive a capillary pressure-saturation relationship for a particular porous medium. Therefore, capillary pressure-saturation curves need to be determined experimentally in the laboratory. There are several methods for determining the capillary pressure-saturation relationship in porous media. In general, these methods can be divided into two groups. The first group is the displacement methods, which are based on the establishment of successive states of hydrostatic equilibrium (Bear, 1972). The second group are the dynamic methods, which are based on the establishment of successive states of steady flow of a wetting and nonwetting fluid. Note that dynamic here does not refer to the dynamic effect, which only occurs under transient flow conditions. The most commonly used methods are the displacement methods. Examples of displacement methods are the ‘porous diaphragm method’ or ‘Welge restored state method’, the ‘mercury injection method’ and the ‘centrifuge method’. These methods will be discussed in more detail in Section 2.3.2.

In laboratory experiments, it is common practice to determine the capillary pressure-saturation curve under static or equilibrium conditions. A schematic of an experimental setup is shown in Figure 2.17. For example, for the determination of a drainage curve a soil sample fully saturated with wetting fluid is drained by increasing the capillary pressure with small increments. This can be done by applying a pressure to the nonwetting phase, or by applying a suction to the wetting phase. After each incremental increase in the applied capillary pressure, the sample is given sufficient time to reach equilibrium. This means the fluids in the sample
are given the time to redistribute and equilibrate to the new situation. After equilibrium is reached, the saturation of the wetting phase and both wetting and nonwetting phase pressures of the sample are measured, and these measurements then comprise one point on the equilibrium $P_c-S_w$ curve. The time needed to reach equilibrium after each incremental increase in applied capillary pressure can range from a few hours to several days. Generally, it takes weeks or longer to obtain a complete capillary pressure-saturation curve (Hassanizadeh et al., 2002). This is because when static equilibrium is approached, the pressure differentials decrease so that flow rates decrease rapidly as well.

![Diagram](image)

**Figure 2.17:** Simple experimental setup for determining the capillary pressure-saturation curve. In this setup, the capillary pressure is increased by increasing the distance $L$ between the two fluid levels (from Mayer and Hassanizadeh, 2005).

The procedure described above can be used to obtain a primary drainage curve. After the sample has been drained by increasing the capillary pressure with incremental steps to the residual wetting phase saturation, the sample can be rewetted again by incrementally decreasing the capillary pressure again. The values for capillary pressure and saturation at equilibrium conditions then will comprise the main imbibition curve. With these two curves, the envelope is obtained that describes the range of possible $P_c-S_w$ curves. Finally, there are several remarks that can be made considering the traditional method for obtaining capillary pressure-saturation curves:

- The capillary pressure-saturation curves are obtained under static conditions. However, the curves obtained this way may not be valid under dynamic or transient conditions. There is theoretical and experimental evidence that in that case the capillary pressure is not only a function of saturation, but also is a function of the rate of change of saturation. The dependence of capillary pressure-saturation curves on the rate of change of saturation is due to dynamic effects (Hassanizadeh et al., 2002). In Section 2.4, dynamic effects and experimental observations of these effects are described in more detail.

- Commonly, the laboratory experiments are performed by making use of hydrophobic and hydrophilic membranes at the inflow and outflow of the sample, respectively. With these membranes it is possible to obtain a capillary pressure-saturation relationship relatively fast. When a drainage experiment is performed, a hydrophilic membrane prevents the nonwetting phase from leaving the sample at the outflow, while a hydrophobic membrane prevents the wetting phase from leaking out of the sample at
2.3 TRADITIONAL MEASUREMENTS OF CAPILLARY PRESSURE-SATURATION CURVES

The inflow. As a result, when the nonwetting phase reaches the outflow of the sample after some time during a drainage experiment, it will start to accumulate. The hydrophilic and hydrophobic membranes thus may significantly influence the distribution of fluids in the sample, and therefore may have an effect on the traditionally measured capillary pressure-saturation relationship. The effect of the presence of membranes in laboratory experiments performed under static conditions is further investigated in Chapter 7, where numerical simulations of both static and steady-state experiments are performed.

- Usually, in the traditional measurement of capillary pressure-saturation curves, the fluid pressures are measured in the fluid reservoirs outside the sample, while the saturation is determined through volumetric or gravimetric methods. The average capillary pressure inside the sample then is simply determined by subtracting the pressure in the wetting phase fluid reservoir from the pressure in the nonwetting phase fluid reservoir. However, pressures measured outside the sample do not necessarily represent pressures inside the sample. This will only be the case if the fluids inside the sample are in contact with the fluid reservoirs, and if enough time is allowed for the pressures inside the sample to adapt to the imposed pressures in the fluid reservoirs. The measurement of outside fluid pressures will be discussed in more detail in Chapter 5, Section 5.6.

2.3.2 Laboratory methods for measuring $P_c$-$S_w$ relationship

Capillary pressure-saturation relationships need to be determined in various fields in which two-phase flow in porous media is of importance. For instance, in reservoir engineering, the determination of the water-oil capillary pressure-saturation relationship is needed to determine the connate water saturation in a reservoir, to determine the height of the transition zone (i.e. the zone where both water and oil are present), and to model oil displacement by free water imbibition and/or water injection. In remediation, the $P_c$-$S_w$ relationship is needed in modelling the evolution of different remediation strategies.

Over time, several standardized laboratory methods have been developed for measurement of the $P_c$-$S_w$ relationship. The most important ones are described below.

**Pressure cell**

This method is also known as the porous plate method or the porous diaphragm method, and is one of the most commonly used methods for determining $P_c$-$S_w$ relationships. With this method, a rock or soil sample is placed inside a chamber with one end in capillary contact with a porous plate. Depending on the type of experiment that is to be performed, i.e. drainage or imbibition, this porous plate will be wetting phase wet or nonwetting phase wet, respectively. As a result, the passage of one of the fluids is allowed while the outflow of the other fluid is prohibited. Initially the sample is fully saturated. However, by adjusting the capillary pressure, the liquid in the sample is expelled through the porous plate. The capillary pressure at the surface of the porous diaphragm that is in contact with the sample can be regulated either by adjusting the wetting phase pressure in the porous diaphragm or by adjusting the pressure of the fluid that surrounds the sample inside the chamber. After the capillary pressure at the barrier is adjusted, the sample is allowed to reach equilibrium, after which the saturation of the sample is determined by weighing the sample (gravimetric method) or by measuring the volume of wetting fluid that was discharged or imbibed (volumetric method). Figure 2.18 shows a schematic representation of a pressure cell.
In general, a procedure to determine a $P_c$-$S_w$ curve with a pressure cell starts with the saturation of the sample and diaphragm with the fluid to be displaced. Then the sample is placed in the pressure cell apparatus. When the chamber is closed, a pressure is applied, and the sample is allowed to reach static equilibrium. The applied pressure causes the outflow of the fluid in the sample through the porous diaphragm, and the inflow of the fluid surrounding the sample. The capillary pressure at each pressure stage is determined from (Corey, 1994):

$$P_c = \rho_{\text{liquid}} gh + P_{\text{applied}}$$

In addition, the saturation is determined volumetrically from the amount of liquid that has been removed from the sample, provided that the initial amount of fluid inside the sample is known.

When static equilibrium in the sample is reached, and the capillary pressure and saturation are determined, the applied pressure is increased with a small increment, and again the sample is allowed to reach static equilibrium, after which the capillary pressure and saturation are determined. This process continues until the desired saturation or capillary pressure is reached. Finally, the obtained capillary pressures and saturations can be plotted against each other to obtain the equilibrium capillary pressure-saturation relationship.

A disadvantage of the pressure cell is that it usually takes a long time for the sample to reach static equilibrium after a pressure increase. As a result, the determination of a complete $P_c$-$S_w$ curve can take over 40 days. In addition, the capillary pressure is not allowed to exceed the entry pressure of the porous plate or diaphragm, because then the infiltrating phase can leave the pressure cell through this diaphragm.

**Centrifuge methods**

Another common method used in both scientific and industrial environments is the centrifuge method. The concept of this method is to rotate a small sample that is initially saturated with a wetting phase at a fixed constant speed. Due to the centrifugal force, some of the liquid inside the sample is forced to flow out. The amount of liquid that is released from the sample at a certain rotation speed can be determined for instance by using a strobe light. This then can be used to calculate the saturation inside the sample. The capillary pressure can be derived from the speed of rotation through (Corey, 1994):
\[ P_c = \frac{1}{2} \Delta \rho \omega^2 (R^2 - r^2) \]  \hspace{1cm} (2.28)

Where \( \Delta \rho \) is the density difference between the wetting and nonwetting fluid, \( \omega \) is the angular velocity of the rotation, \( R \) is the radius at the outflow end of the sample, and \( r \) is the radius of a point inside the sample for which the capillary pressure has to be determined.

If the experiment is repeated for different speeds of rotation, the capillary pressure can be plotted as a function of saturation. On average, 10 different rotational speeds are needed to obtain a full capillary pressure curve. Figure 2.19 shows a schematical drawing of a centrifuge apparatus with a sample holder.

A disadvantage of the centrifuge method is that it can only be used for drainage. This is because it is difficult to let wetting phase imbibe into the sample during rotation (Corey, 1994). In addition, there is always a pressure gradient present along the sample due to the difference in rotation radii. This can cause problems in some cases.

**Mercury injection method**

In order to reduce the time needed to obtain a full capillary pressure-saturation curve, the mercury injection method was developed. Before the injection of mercury, the sample is placed inside a chamber that subsequently is evacuated. After this, mercury is forced into the sample applying a certain pressure. Mercury in this case is the nonwetting phase, and its saturation can be determined from the amount of mercury injected and the pore volume of the sample. Because the sample is evacuated, the capillary pressure is equal to the injection pressure. By injecting mercury at increasing pressures, each time waiting until the fluids inside the sample have reached a static equilibrium, a mercury capillary pressure-saturation curve can be obtained.

Advantages of this method are that it is very fast (only minutes), and there is no limitation on the pressures that can be applied, as there is for the pressure cell. However, the mercury injection capillary pressure-saturation curves are not representative for other fluid systems (e.g. an oil-water system). This is because these systems have different surface tensions. Thus,
the laboratory determined capillary pressure using mercury needs to be converted to the capillary pressure of the system of interest. This can be done by considering the Laplace equation for both systems:

$$p_{\text{lab}}^c = \frac{2\sigma_{\text{al}g} \cos \theta_{\text{al}g}}{r} \quad \text{gives} \quad r = \frac{2\sigma_{\text{al}g} \cos \theta_{\text{al}g}}{p_{\text{lab}}^c} \quad (2.29)$$

$$p_{\text{syst}}^c = \frac{2\sigma_{\text{ow}} \cos \theta_{\text{ow}}}{r} \quad \text{gives} \quad r = \frac{2\sigma_{\text{ow}} \cos \theta_{\text{ow}}}{p_{\text{syst}}^c} \quad (2.30)$$

Where $$\sigma_{\text{al}g}$$ is the surface tension of the vacuum-mercury system, $$\theta_{\text{al}g}$$ is the contact angle of the vacuum-mercury system, $$p_{\text{lab}}^c$$ is the capillary pressure determined from the mercury injection experiment, $$\sigma_{\text{ow}}$$ is the surface tension of the system for which the capillary pressure-saturation relationship is required, and $$\theta_{\text{ow}}$$ is the contact angle of the desired fluid system. Note that $$r$$ refers to the porous medium and thus is independent on the system of fluids, so that it is a constant value in both Equation (2.29) and (2.30). Therefore, these two equations can be rewritten and equated, which results in an expression for the capillary pressure of the fluid system we would like to have:

$$p_{\text{syst}}^c = \frac{2\sigma_{\text{ow}} \cos \theta_{\text{ow}}}{2\sigma_{\text{al}g} \cos \theta_{\text{al}g}} p_{\text{lab}}^c \quad (2.31)$$

If the contact angles are ignored, we get

$$p_{\text{syst}}^c = \frac{\sigma_{\text{ow}}}{\sigma_{\text{al}g}} p_{\text{lab}}^c \quad (2.32)$$

**Long column method**

The long column method can be used to determine $$p_{c^c_{\text{syst}}}$$-$$S_{w}$$ curves for air-water systems. With this method, a long column filled with a porous medium is put with its base in contact with a source of wetting fluid. The column then is allowed to drain in response to earth’s gravity field, until an equilibrium situation is reached. After the column has reached equilibrium, the saturation in the column is determined at several elevations from samples taken at these heights. In addition, the capillary pressure at the corresponding heights is determined from:

$$p_{c}(h) = (\rho_{\text{w}} - \rho_{\text{ow}})gh + P_{co} \quad (2.33)$$

where $$p_{c}$$ is the capillary pressure at an elevation $$h$$, and $$P_{co}$$ is the capillary pressure at a reference datum from which $$h$$ is measured (Corey, 1994).

Disadvantages of this method are that it can only be used for small capillary pressures, and that the time to reach equilibrium can be very long and uncertain. However, it is a very simple method, and it was the first method used for the determination of capillary pressure-saturation relationships.
Vapour Pressure
This method can only be used for determining capillary pressure-saturation relationships in a water-air system. A sample with a known amount of wetting phase fluid is put into a sealed chamber. Subsequently, the sample is allowed to reach equilibrium with the atmosphere inside the chamber. The capillary pressure inside the sample now can be determined from the vapour pressure of the wetting phase at equilibrium inside the chamber (Corey, 1994).

Dynamic methods
A method that is not often used is the dynamic method. With this method, simultaneous steady flow of both the nonwetting and wetting phase fluid is established in the sample. The pressure of the two fluids in the sample can be measured using special walled disks. Now the saturation in the sample is varied by changing the flow rate of one of the fluids. This will also result in an altered capillary pressure. By changing the flow rate of one of the fluids a number of times, a capillary pressure-saturation relationship can be obtained (Bear, 1972).

2.3.3 From the laboratory scale to the field scale
After the determination of the capillary pressure-saturation relationship in the laboratory, often some additional steps are needed to obtain a relationship representative of the reservoir or aquifer for which it will be used. This is because a laboratory sample is very small and thus may not be representative of the variation that can occur inside the reservoir. For instance, the permeability and porosity of the sample might not be representative for the average permeability and porosity of the entire reservoir (Ahmed, 2001).

To find a representative \( P_c-S_w \) relationship for the larger scale of a reservoir of aquifer, the Leverett J-function can be used. This relation was developed by Leverett in 1941, and combines all available capillary-saturation data from small samples into one dimensionless function that is valid for the whole reservoir or aquifer. The Leverett J-function is given by:

\[
J(S_w) = \frac{P_c}{\sigma \cos \theta} \sqrt{\frac{K}{n}} \tag{2.34}
\]

Where \( P_c \) is the capillary pressure, \( \theta \) is the contact angle, \( K \) is the intrinsic permeability, and \( n \) is the porosity. Originally, Leverett developed his function to convert all capillary pressure-saturation data into one single dimensionless curve. However, it has been shown that there are significant differences in the obtained J-function from reservoir to reservoir, and therefore a universal function cannot be found. Still, when the capillary pressure-saturation data of a single reservoir are converted using the Leverett J-function, a single dimensionless curve is obtained representing a common \( P_c-S_w \) relationship for the whole reservoir. Moreover, an obtained Leverett J-function curve for a certain reservoir can be used for a reservoir of the same rock type in absence of other data.

Combining the Leverett J-function for the whole reservoir and the one for a single sample and rewriting, an expression for the reservoir capillary pressure can be obtained:

\[
P_c^{\text{reservoir}} = P_c^{\text{lab}} \frac{\sigma_{\text{reservoir}}}{\sigma_{\text{lab}}} \sqrt{\frac{n_{\text{res}} K_{\text{core}}}{n_{\text{core}} K_{\text{res}}}} \tag{2.35}
\]
This expression relates the laboratory capillary pressure to the reservoir capillary pressure through the interfacial tensions, porosity, and permeability of both laboratory and reservoir (Ahmed, 2001).

2.3.4 Measuring saturation and capillary pressure

In the methods for measuring capillary pressure-saturation relationships that were described above, saturation is commonly determined gravimetrically, by observing the change in sample weight or by measuring the weight of the fluid flowing out of the sample. Also, saturation can be determined volumetrically, by determining the volume of fluid leaving the sample. Both of these methods give an average saturation for the whole sample. However, it is also possible to directly measure saturation inside the sample using a sensor, so that a local saturation is obtained. Though this is called ‘local’ saturation, it will still represent an average over the volume of the sample that is captured by the sensor. There are several methods for determining a local saturation. For example, gamma-ray attenuation can be used. With this measurement technique, the saturation inside the sample is related to the amount of attenuation of a beam of gamma-rays that penetrates the porous medium. Another method for the local measurement of saturation is Time Domain Reflectometry (TDR). This method is based on the determination of the permittivity of the soil, which is closely related to its water content (e.g. Heimovaara, 1993).

The measurement of the capillary pressure of a sample can be done in several ways. Usually, the capillary pressure is determined from sensors that are placed in the fluid reservoirs connected to the soil sample. The used sensors are Pore Pressure Transducers (PPT), and the capillary pressure of the sample follows from the difference between the pressure measured by the PPT in the nonwetting fluid reservoir and the pressure measured by the PPT in the wetting fluid reservoir. The capillary pressure-saturation relationship obtained is thus an average over the whole sample. However, Pore Pressure Transducers (PPT) make it also possible to determine local capillary pressure directly inside the sample, in stead of determination from pressures outside the sample (Oung and Bezuijen, 2003).

2.4 Dynamic effects

As described in Section 2.3, traditionally the capillary pressure-saturation relationship is measured under static conditions. However, the relationship that is determined this way is also applied to situations where there is a transient or dynamic flow. This approach however may not be appropriate as through the years several researchers have shown that the capillary pressure-saturation relationship obtained under dynamic flow conditions is different from the capillary pressure-saturation relationship obtained under static conditions (e.g. Topp et al., 1967, Stauffer, 1978). There is both theoretical and experimental evidence that under dynamic flow conditions, the capillary pressure is not only a function of saturation, but also is a function of the rate of change of saturation. This is thought to be due to so called ‘dynamic effects’.

2.4.1 Experimental observations of dynamic effects

During the past 50 years, several experimental works have been conducted that investigate dynamic effects. Almost all experiments however are performed for air-water systems. Some of the exceptions are the experiments presented by Kalaydjian et al. (1992b), which are performed for an oil-water system.
Kalaydjian et al. (1992b) performed two series of imbibition tests in two different kind of rock with a relatively homogeneous porosity: a limestone and a sandstone. More details of the experimental setup and procedure can be found in Kalaydjian et al. (1992b).

For both rock samples, three imbibition experiments were performed at flow rates of 15 cc/hr, 5 cc/hr and 1 cc/hr, respectively. The capillary pressure was calculated as the difference between the oil pressure and water pressure, which were measured with pressure transducer pairs at several heights in the column. It was found that the obtained capillary pressure-saturation curves are different for different flow rates, and that the difference is more pronounced in case of the limestone sample. This is though to be due to the less complex structure of the sandstone compared to the limestone, which has a double porosity. As the flow rate increases, the capillary pressure becomes higher for a certain oil saturation. Thus, as the experiment becomes more dynamic, the capillary pressure increases for a fixed saturation.

In addition to the capillary pressure, Kalaydjian et al. (1992b) also determined the relative permeabilities during the experiment for each flow rate. The obtained relative permeability-saturation curves show that the relative permeabilities are dependent on flow rate. As the flow rate increases, the endpoints of the relative permeabilities increase in value, while the curvature of the curves decreases. This means that for a given saturation, with higher flow rates the relative permeability of both the oil and water phase becomes higher. In addition, at high flow rates, the relative permeability almost becomes linear. This indicates that capillary forces become less important, and viscous forces dominate flow. When the curves are highly nonlinear, for instance at low flow rates, the relative permeability of the wetting phase will stay low even at higher wetting phase saturations. This is due to the domination of capillary forces over viscous forces, which counteract flow and therefore decrease the relative permeability. Actually, the relative permeability depends on the capillary number, which describes the ratio of viscous forces over capillary forces. A high capillary number means that viscous forces dominate, and the relative permeability curve as a result will be almost linear. At low capillary numbers, capillary forces dominate and the relative permeability curves will be highly non-linear.

In order to compare dynamic and static conditions, Kalaydjian et al (1992b) assumed that the static capillary pressure can be approached by the measurements performed for the low flow rate experiment of 1 cc/hr. In addition they suggest the following equation to describe the relation between the static and dynamic capillary pressure:

\[ P_{c,\text{dyn}} - P_{c,\text{stat}} = -\lambda \frac{\partial nS_o}{\partial t} \]  

(2.36)

where \( P_{c,\text{dyn}} \) is the capillary pressure measured at a flow rate of 5 or 15 cc/hr, \( P_{c,\text{stat}} \) is the capillary pressure measured for the flow rate of 1 cc/hr, \( \frac{\partial nS_o}{\partial t} \) is the time derivative of the oil saturation calculated at a flow rate 5 or 15 cc/hr, and \( \lambda \) is a coefficient.

In order to validate the dynamic expression of the capillary pressure-saturation relationship, the two higher flow rate experiments (5 cc/hr and 15 cc/hr) are compared to the low flow rate measurement (1 cc/hr), that is assumed to represent static conditions. Figure 2.20 shows the difference between the capillary pressure measured in the limestone sample between the two high flow rate experiments and the low flow rate experiment.
As can be seen, the difference between the dynamic and ‘static’ capillary pressure is largest for the highest flow rate experiment. This would indicate the dynamic effect becomes stronger at higher flow rates. Moreover, the figure shows that the difference between the dynamic and static capillary pressure is dependent on the water saturation. At low and high water saturations, the difference between the two capillary pressures becomes less. Figure 2.21 shows the difference between the time derivatives of saturation as a function of local saturation.

Figure 2. 20: The difference between capillary pressure curves measured in the three imbibition experiments for the limestone sample (from Kalaydjian et al., 1992b)

This figure shows that the change in water saturation with time is larger for the experiment with the higher flow rate of 15 cc/hr. In addition, the rate of change of saturation with time is dependent on the water saturation.

Figure 2. 21: Calculation of the factor $\lambda$ for the limestone sample (from Kalaydjian et al., 1992b)

Figure 2. 22: The difference between time derivatives of the local saturation in the three flow experiments, for the limestone sample (from Kalaydjian et al., 1992b)
Finally, Kalaydjian et al. (1992b) calculated the parameter $\lambda$ that occurs in Equation (2.36). This is shown in Figure 2.22, which plots $\lambda$ as a function of the water saturation. As can be seen, the parameter $\lambda$ seems to be dependent on saturation. Moreover, for the higher flow rate of 15 cc/hr, $\lambda$ on average is smaller than for the flow rate of 5 cc/hr. In other words, it seems that the parameter $\lambda$ is inversely related to flow rate. Thus, Kalaydjian et al. (1992b) show that the parameter $\lambda$ is dependent on saturations as well as on flow rate. However, they were not able to quantitatively describe this dependence.

Another paper that is often referred to when dynamic effects are considered is a paper written by Topp et al. in 1967. In this paper, water content-pressure head data obtained by either equilibrium, steady-state or unsteady-state methods are presented. Like many other researchers, Topp et al. consider an air-water system.

Topp et al. (1967) used a sandy soil sample with dimensions of 2.54 cm height $\times$ 1.0 cm width $\times$ 7.6 cm length. The water content in the sample was varied by varying the gas pressure in the sample. More details of the experimental setup and procedure can be found in Topp et al. (1967). They performed a series of drainage experiments on the column, and determined the drainage water content-pressure head relationship by static equilibrium, steady-state flow, or unsteady-state flow methods. Figure 2.23 shows the obtained water content-pressure head curves for various flow conditions.

For the static equilibrium curves, a series of equilibria was obtained by successively increasing the gas phase pressure, and then allowing equilibrium to be reached before taking a measurement. Equilibrium was assumed to be reached when the air-water interface in the horizontal outflow capillary no longer moved. Topp et al. (1967) observed that for intermediate water saturations, the time needed to meet the criterion was longest (4000-6000 minutes), while for low and high water saturations the time needed to reach equilibrium was fastest (1000-4000 minutes). The steady-state method was performed by establishing a
vertical downward steady-state flow in the sample at approximately unit hydraulic gradient for a series of increasing gas phase pressures. The criterion for steady-state equilibrium was a steady-state water content inside the sample. Times needed to reach steady-state after increasing the gas phase pressure ranged between 300 and 600 minutes. As can be seen from Figure 2.23, the results obtained from the steady-state experiments do not seem to vary significantly from the results obtained from the static experiment.

For the unsteady-state flow experiments, the sample was resaturated after which it was drained again by inducing an outflow of water by increasing the gas phase pressure in steps of 1 to 2 cm of water at frequent time intervals. During the unsteady-state flow, the water content and pressure head were measured at frequent intervals. The results in Figure 2.24 clearly show that the water content-capillary pressure head curves obtained for the unsteady-state flow are significantly different from the curves obtained for static and steady-state conditions. The capillary pressure at the same water content is higher for transient drainage processes than for static equilibrium and steady flow conditions. In addition, the faster the unsteady-state experiment is performed, the higher the water content is for a certain pressure head.

Topp et al. (1967) could not give an explanation for their observations, but they suggested that perhaps the formation of pendular rings could explain the observations.

Another set of experiments that are related to the dynamic effect were performed by Stauffer (1978), who also investigated the non-uniqueness of the \( k_r - S_w \) relationship. Stauffer performed one-dimensional vertical drainage processes in homogeneous and isotropic porous media. He considered an air-water system, where water is displaced by air. The experiments were carried out in vertical columns of quartz sand which were built up in a plexiglas tube. Three different columns with heights of 53.8, 63.8 and 16.9 cm were used. On these columns, both quasi-steady and dynamic experiments were carried out. More information on the experimental setup and procedure can be found in Stauffer (1978).

In Figure 2.24, the capillary pressure head – saturation curve obtained for both transient and steady-state conditions for the column of 63.8 cm is shown. The results show that the \( P_c - S_w \) curve obtained for the dynamic drainage experiment is different from the curve obtained for the quasi-steady experiment. Especially at high water saturations, the \( P_c - S_w \) curve obtained under dynamic conditions shows significantly higher capillary pressures for a given water saturation. Stauffer (1978) expressed the dynamic effect as the difference in capillary pressure \( \Delta P_c \) between the capillary pressure at transient (\( P_{ct} \)) and quasi-steady (\( P_{qst} \)) flow conditions at the same saturation. The dynamic behaviour of the transient drainage process is represented by the derivatives \( \partial S_w / \partial t \) and \( \partial P_w / \partial t \). Figure 2.25 shows the dependence of \( \Delta P_c / \rho_w g \) on the two corresponding derivatives.

As can be seen from Figure 2.25, there seems to be a linear relationship between \( \Delta P_c / \rho_w g \) and \( (\partial S_w / \partial t) \). The slope of the curve, \( \alpha \), was fitted at 700 cm s. The relationship between \( \Delta P_c / \rho_w g \) and \( (\partial P_w / \partial t) \) however is less simple, and shows a nonlinear behaviour. Based on Figure 2.26, Stauffer (1978) derived the following empirical relation to express \( \Delta P_c \):

\[
P_{cp} - P_{cstat} = \Delta P_c = -\alpha \rho_w g \phi_e \frac{\partial S_w}{\partial t} \tag{2.37}
\]
In order to investigate the influence of the flow dynamics on the relative permeability-saturation relation, Stauffer (1978) used a special method. He used the fact that in the drainage experiment, the gradients in water pressure were approximately constant in the beginning drainage phase. Stauffer then stated the function \( k_w \) in the form:

\[
k_w = k_s S_e^\varepsilon
\]

(2.38)

where \( \varepsilon \) is regarded as unknown. Stauffer found that for transient conditions, \( \varepsilon_{tr} \) is 2.4 while for quasi-steady conditions \( \varepsilon_{qst} \) is 3.35. This means that the relative permeability during drainage is higher under transient conditions than under steady-state conditions. Thus, the exponent \( \varepsilon \) is not a constant, but dependent on the flow conditions. Therefore, the permeability-saturation relationship is also non-unique, and subject to dynamic effects.

Stauffer derived an empirical relationship for the slope \( \alpha \) of the line that is obtained when \( (\Delta P_c/\rho_w g) \) is plotted versus \( (\varphi_e \delta S_e/\delta t) \). He found that the slope \( \alpha \) can be given by:

\[
\alpha = \frac{\tau P_b^2}{\rho_w^2 g^2 k_s \lambda}
\]

(2.39)
here $\tau$ is a parameter, $P_b$ is the entry pressure as introduced in the model of Brooks and Corey, $\rho_w$ is the wetting phase density, $g$ is the gravitational acceleration, $k_s$ is the saturated intrinsic permeability, and $\lambda$ is the Brooks-Corey pore size distribution index. When $\tau$ is assumed to be constant, Stauffer suggested that the dynamic effect is important when either $P_b$ is large and/or when $k_s$ and $\lambda$ are small. On the other hand, the dynamic effect should be small when $P_b$ is small and/or $k_s$ and $\lambda$ are large. Based on this consideration, Stauffer suggested that dynamic effects should be large in case of fine sands with a wide grain size distribution. Dynamic effects should be small for coarse sands with a restricted grain size distribution.

The above discussion of observations of dynamic effects in the constitutive relationships is far from complete. There are various other papers that investigate the effect of dynamic flow conditions on the capillary pressure-saturation relationship, and in a lesser extend the relative permeability-saturation relationship. Interested readers are referred for instance to Smiles et al. (1971), or Vachaud et al. (1972). In addition, Hassani Zadeh et al. (2002) provide a literature review of the laboratory work done on the dynamic effect in unsaturated flow. Most of these papers show that in case of drainage, the capillary pressure is higher under dynamic conditions compared to static conditions for the same water content. For imbibition, the opposite is observed, though the effect sometimes is not as clear as it is for drainage experiments. Further, it is commonly observed that the magnitude of the dynamic effects is dependent on flow rates, or the time rate of change of the applied boundary pressures.

### 2.4.2 Origin of dynamic effects

Even though ‘dynamic effects’ manifest themselves in experimentally derived capillary pressure-saturation relationships as well as relative permeability-saturation relationships, what is causing these effects is still a matter of discussion. Hassanizadeh et al. (2002) provide the following overview of suggestions that try to explain dynamic effects:

- **Water entrapment.** When a column is drained at high flow rates, the larger pores will be drained very fast so that the water in the smaller pores can become discontinuous. This water thus stays behind in the column, giving rise to larger wetting phase saturations under dynamic conditions. This would suggest that the relative permeability will be lower under dynamic flow conditions, because the mobile part of the water is reduced. However, larger relative permeabilities are found under dynamic conditions at high saturations, and therefore water entrapment might not be the cause of dynamic effects.

- **Pore water blockage near the outflow boundary.** When a soil sample is drained by suddenly applying a large pressure gradient, the pores near the outflow boundary will be drained very quickly. These pores then are filled with air, which causes blockage for water higher in the column to flow out. Again, water will stay behind in the column, resulting in higher water saturations. In this case, the relative permeability under dynamic conditions should decrease. However, the opposite actually is observed. In addition, this effect need not be present under field conditions, and will only occur if the experimental setup is open to air.

- **Air entrapment.** Air entrapment could occur during a drainage experiment when the wetting phase saturation still is high. The wetting phase can only be drained from the column if the nonwetting phase (in this case the air phase) can get into the column. However, at high wetting phase saturations, the nonwetting phase is not yet continuous, and as a result has a difficulty entering. Again, this will lead to higher wetting phase saturations under dynamic conditions. This effect probably does not occur under field conditions.
• **Dynamic contact angle effect.** This effect was already described before in Section 2.2.3 on hysteresis. As was shown in this section, during drainage, the contact angle of the interface decreases, while during imbibition the contact angle increases compared to the static contact angle. As a result, during drainage a higher capillary pressure can be reached under dynamic conditions. During imbibition, a lower capillary pressure is reached under dynamic conditions. This effect only will be significant for drainage if the static contact angle is rather large (for instance in oil-water systems) and for imbibition if the static contact angle is rather small (for instance in air-water systems).

The first three effects that are described above only can explain dynamic effects under drainage conditions, but dynamic effects also have been observed for imbibition. The only mechanism that can explain dynamic effects in case of imbibition is the dynamic contact angle effect. However, these mechanisms all occur at the pore scale. Hassanizadeh et al. (2002) suggest that even if equilibrium is reached at the pore scale, the upscaling of complex pore scale processes will always introduce non-equilibrium effects. In addition to pore-scale complexities, the presence of micro-heterogeneities also can result in non-equilibrium effects in observations made at the sample scale (Hassanizadeh et al., 2002).

2.5 New theory of two-phase flow

In the previous sections, several phenomena are described that cannot be explained with the traditional theory of two-phase flow. The shortcomings of the traditional theory can be summarized as follows:

- The extended Darcy equation used in the traditional theory for two-phase flow is simply based on the original equation that was derived for a very simple system of slow, single phase flow in a homogeneous isotropic porous medium.
- In the traditional theory, interfaces are not explicitly included in the equations as an independent variable, while they play a very important role in many processes and effects, such as capillarity, dissolution, adsorption of surfactants, transport of microorganisms in the unsaturated zone, evaporation, and drying processes. However, in the current theories of multiphase flow, interfacial area is completely absent.
- The traditional theory of two phase flow cannot explain hysteresis observed in the capillary pressure-saturation relationship.
- The traditional theory of two-phase flow is often used to describe dynamic flow processes. However, as was discussed in Section 2.5, then capillary pressure is no longer a function of saturation only, as is assumed in the traditional theory.

The last couple of years therefore, several researchers have suggested new theories for two-phase flow, that include the effects of interfaces and dynamic effects (e.g. Hassanizadeh and Gray, 1993a, 1993b). Researchers agree that in order to obtain a physically well-founded theory that can explain all the observed phenomena, the thermodynamics and the geometry of the interfaces between the phases need to be considered. Especially the interfaces between the fluid phases are of importance and should be taken into account. Basic principles of mass, momentum and energy conservation can be used to obtain equations that account for all parts of a two-phase system, including bulk phases, interfaces and contact lines. In the new theories for two-phase flow, the extended Darcy’s equation for two-phase flow (Equation (2.12)) is truly extended to the following new form:
\[ q_\alpha = - \frac{k_{ta} K}{\mu_\alpha} (\nabla P_\alpha - \rho_\alpha g - \lambda_1^\alpha \nabla S_\alpha - \lambda_2^\alpha \nabla a_{wn}) \]  

(2.40)

where \( \lambda_1^\alpha \) and \( \lambda_2^\alpha \) are new material coefficients, and \( a_{wn} \) is the specific interfacial area, which is the area of the fluid-fluid interface per unit volume of porous medium (Hassanizadeh and Gray, 1993b). In addition, an area balance equation for fluid-fluid interfaces is needed:

\[ \frac{\partial a_{wn}}{\partial t} + \nabla \cdot (a_{wn} w_{wn}) = r_{wn} (a_{wn}, S_w) \]  

(2.41)

In order to find a new expression for the capillary pressure taking into account the interfaces, Hassanizadeh and Gray (1993a) propose a theory in which the Helmholtz free energy functions for the phases and interfaces depend on state variables such as mass density \( (\rho) \), temperature \( (T) \), saturation \( (S_w) \), porosity \( (n) \), interfacial area density \( (a) \), the solid strain tensor \( (E_s) \), and the excess mass of the \( \alpha \beta \)-interface per unit area \( (\Gamma_{\alpha \beta}) \):

\[
\begin{align*}
A^n &= A^n(\rho_n, T, a_{wn}, a_{ns}, S_w, n) \\
A^w &= A^w(\rho_w, T, a_{wn}, a_{ws}, S_w, n) \\
A^s &= A^s(\rho_s, T, a_{ns}, a_{ws}, E_s, n) \\
A^{\alpha \beta} &= A^{\alpha \beta}(\Gamma_{\alpha \beta}, T, n, a_{\alpha \beta}, S_w)
\end{align*}
\]

(2.42)

Based on these constitutive equations, and by applying the Coleman and Noll method of exploitation of the entropy inequality, Hassanizadeh and Gray (1993a) derive the following equation for the entropy inequality:

\[
- \frac{\partial S_w}{\partial t} \left[ n(P_n - P_w) + \left( nS_w \rho_n \frac{\partial A_w}{\partial S_w} + nS_w \rho_n \frac{\partial A_n}{\partial S_w} + \sum_{\alpha \beta} a_{\alpha \beta} \Gamma_{\alpha \beta} \frac{\partial A_{\alpha \beta}}{\partial S_w} \right) \right] \geq 0
\]  

(2.43)

where \( \partial S/\partial t \) is the material time derivative of the wetting phase saturation, \( P^n \) is the macroscopic pressure of the nonwetting phase, and \( P^w \) is the macroscopic pressure of the wetting phase. At equilibrium, the capillary forces will balance \( P_n - P_w \). Therefore, the macroscopic capillary pressure can be defined thermodynamically by:

\[
P_c = -S_w \rho_w \frac{\partial A_w}{\partial S_w} - S^n \rho^n \frac{\partial A_n}{\partial S_w} - \sum_{\alpha \beta} a_{\alpha \beta} \Gamma_{\alpha \beta} \frac{\partial A_{\alpha \beta}}{n \partial S_w}
\]  

(2.44)

when this is substitutes back into Equation (2.43), then one gets:

\[
- \frac{\partial S_w}{\partial t} [(P_n - P_w) - P_c] \geq 0
\]  

(2.45)
this means that if \( P_n - P_w \) is larger than \( P_c \), for the residual entropy inequality to hold, \( \partial S_w / \partial t \) should be negative. This means the system will undergo drainage. If \( P_n - P_w \) is smaller than \( P_c \), \( \partial S_w / \partial t \) should be positive, and the system will undergo imbibition. Only at equilibrium, thus when \( \partial S_w / \partial t = 0 \), \( P_n - P_w \) will be equal to \( P_c \). Only then the capillary forces will balance \( P_n - P_w \).

For simplification, \( \partial S_w / \partial t \) can be described by an approximate constitutive equation. When a linear approximation is used, the following approximation can be written:

\[
\frac{\partial S_w}{\partial t} = -\frac{1}{\tau} \left[ (P_n - P_w) - P_c \right]
\]  

(2.46)

where \( \tau \) is a nonnegative material coefficient. This coefficient can be considered as a measure of the speed at which the change in saturation takes place. Note that \( \tau \) can still be a function of saturation (Hassanizadeh and Gray, 1993a). \( \tau \) is also known as the damping coefficient, because it actually damps the approach to equilibrium. If \( \tau \) is very small, the change in saturation will be fast. This means that \( P_n - P_w \) and \( P_c \) will become equal to each other almost instantaneously after equilibrium is disturbed. This means that the common definition of capillary pressure,

\[
P_c = P_n - P_w
\]

(2.47)

will give relatively good results as long as equilibrium is reached very fast. However, if this equation is also used for a system that is not at equilibrium, one indirectly assumes that saturation changes are fast and that equilibrium is re-established instantaneously. This means that it is assumed that

\[
\frac{1}{\tau} \gg 1
\]

(2.48)

in case of a linear approximation of the constitutive relationship. This assumption probably only is valid when considering porous media with high permeability.

Equations (2.42) and (2.44) show that the capillary pressure is not only a function of saturation, but actually of 11 independent variables (Hassanizadeh and Gray, 1993a):

\[
P_c = F(\rho_n, \rho_w, T, \Gamma_w, \Gamma_n, a_{wn}, a_{nw}, a_{ws}, \varepsilon, S_w)
\]

(2.49)

This dependency can be simplified if it is assumed that phase densities, interfacial mass densities, temperature, and porosity are constants. In that case, the above equation simplifies to:

\[
P_c = \xi (a_{wn}, a_{nw}, a_{ws}, S_w)
\]

(2.50)
In addition, for most porous media, except at very low wetting phase saturations, it can be assumed that the wetting phase completely coats the solid phase. This means that $a_{ns} = 0$ and $a^{ws} = \text{constant.}$ Thus, Equation (2.50) can be further reduced to:

$$P_c = \zeta(a^{ws}, S_w)$$ (2.51)

Equation (2.51) shows that capillary pressure is not only a function of saturation, but also of the specific interfacial area, $a^{wn}.$ Introduction of specific interfacial area into the theory for two-phase flow makes it possible to model hysteresis in $P_c$-S curves and to account for driving forces specific to two-phase flow. The hysteresis in $P_c$-$S_w$ curves can be explained by considering that the traditional capillary pressure-saturation curves are actually projections of a three dimensional plane in capillary pressure-saturation-interfacial area space onto a 2D plane of capillary pressure versus saturation. This is illustrated in Figure 2.26.

![Figure 2.26: 3-dimensional surface showing the unique relationship between interfacial area, capillary pressure, and saturation. Projections of this surface onto the 2-D $P_c$-$S_w$ plane are causing the observed hysteresis (from Held and Celia, 2001).](image)

Summarizing this section, the new theory of two-phase flow can be described by the following 4 equations:

- Mass balance equation for the fluids

$$\frac{\partial nS_{\alpha} \rho_{\alpha}}{\partial t} + \nabla \cdot (q_\alpha \rho_{\alpha}) = 0 \quad \alpha = w, n$$ (2.52)

This equation still is the same as used in the traditional theory.

- The new expression for Darcy velocity:

$$q_\alpha = -\frac{k_{\alpha}}{\mu_{\alpha}} \nabla P_\alpha - \rho_\alpha g - \lambda_1 \nabla S_{\alpha} - \lambda_2 \nabla a^{wn}$$ (2.53)
• Area balance for the fluid-fluid interfaces:

\[
\frac{\partial a_{wn}}{\partial t} + \nabla \cdot (a_{wn} \mathbf{v}_{wn}) = \mathbf{f}_{wn}(a_{wn}, S_w)
\]  

(2.54)

• A new expression for the capillary pressure, which now includes interfacial area as an independent variable as well as dynamic effects:

\[
P_{c^{\text{dyn}}}(S_w, a_{wn}) = P_n - P_w = P_{c^{\text{stat}}}(S_w, a_{wn}) - \tau \frac{\partial S_w}{\partial t}
\]

(2.55)

At static equilibrium, this equation reduces to:

\[
(P_n - P_w)_{\text{equilibrium}} = P_{c^{\text{stat}}}(S_w, a_{wn})
\]

(2.56)

Note that also Stauffer (1978) and Kalaydjian (1992b) have derived similar expressions for capillary pressure including dynamic effects. Kalaydjian derived his expression for capillary pressure (Equation 2.36) by constructing macroscopic balance equations of mass, momentum, energy, and entropy for two incompressible, immiscible fluids and their interface as well as phenomenological equations on the basis of the theory of irreversible thermodynamic processes (Manthey, 2006). Stauffer (1978) on the other hand derived his expression for capillary pressure empirically (Equation 2.37).

2.6 Thesis perspective

In Section 2.5, the theory of two-phase flow is introduced which includes interfacial area as well as a new expression for capillary pressure. This relatively new and not yet widely accepted theory is derived from thermodynamic considerations, and is able to explain the phenomena of hysteresis and dynamic effects. In this thesis however, the traditional theory of two-phase flow as it is described in Section 2.1.5 will be used. Hysteresis and dynamic effects are left out of this study because the main subject of interest is the effect of factors such as averaging method and boundary conditions, on the obtained sample-scale average $P_c$-$S_w$ curve. Including hysteresis and dynamic effects will only complicate the results, and therefore are not considered.

The simulations that will be performed represent primary drainage experiments. Simulation of imbibition experiments will not be performed. Therefore, hysteresis does not need to be included in the theory. In addition, the simulations are performed using static or steady-state conditions. This means that drainage is performed by increasing the capillary pressure with small increments, each time waiting until equilibrium is reached. Hence dynamic effects can be neglected and the traditional expression for capillary pressure can be used.
Chapter 3

Numerical model

In Chapter 2, the physical-mathematical model of two-phase flow in porous medium is described. However, the mathematical model introduced in Section 2.1.5 gives rise to a non-linear system of partial differential equations. Therefore, the mathematical model can be solved analytically for very simple cases only, such as the Buckley-Leverett problem (Manthey, 2006). For all other cases, the mathematical model needs to be solved numerically, where partial differential equations are discretised in both time and space. Subsequently, this discretised set of equations can be linearized using for instance an algorithm such as the Newton-Raphson method. Finally, the resulting linearized discretised set of equations can be solved using a solver such as Gaussian elimination.

Two numerical models have been used in this thesis, being the model of dr.ir. C. Berentsen from Utrecht University and MUFTE-UG from Universität Stuttgart. In this chapter, the numerical models will be introduced.

3.1 Berentsen Model

This model is developed by dr.ir. C. Berentsen from Utrecht University. The choice for using this model was made because the developer of the program was present at the university, so that any problems could easily be solved through personal correspondence. Below, first the model is described, followed by the discretisation methods and solvers that are used.

3.1.1 Model description

The program of dr. ir. C. Berentsen solves three governing equations, in which it is assumed that there are no changes in density and porosity through both time and space:

- Mass balance for the nonwetting phase:

\[
\frac{\partial S_n}{\partial t} - \frac{1}{n} \nabla \cdot [\alpha_n \kappa \nabla (\Phi_n)] = 0
\]  

(3.1)

- Mass balance for the wetting phase:

\[
\frac{\partial S_w}{\partial t} - \frac{1}{n} \nabla \cdot [\alpha_w \kappa \nabla (\Phi_w)] = - \frac{\partial S_n}{\partial t} - \frac{1}{n} \nabla \cdot [\alpha_n \kappa \nabla (\Phi_n)] = 0
\]  

(3.2)

- Expression for the capillary pressure:
3.1 BERENTSEN MODEL

\[ \Phi_n - \Phi_w - (\rho_n - \rho_w)gz = P_{stat}^c + \tau \frac{\partial S_n}{\partial t} \]  

(3.3)

where \( S_n \) (-) is the saturation of the nonwetting phase, \( S_w \) (-) is the saturation of the wetting phase, \( n \) (-) is the porosity, \( \kappa \) is the intrinsic permeability (L^2), and \( \lambda_n \) and \( \lambda_w \) are the phase mobilities defined as:

\begin{align*}
\lambda_n &= \frac{k_{rn}}{\mu_n} \\
\lambda_w &= \frac{k_{rw}}{\mu_w}
\end{align*}

(3.4)

Here \( k_{rn} \) and \( k_{rw} \) are the relative permeabilities of the nonwetting and wetting phase (-), respectively. \( \mu_n \) and \( \mu_w \) are the viscosities of the nonwetting and wetting phase (ML^{-1}T^{-1}), respectively. \( \Phi_n \) and \( \Phi_w \) are the potentials of the wetting and nonwetting phases, defined as:

\[ \Phi_n = P_n + \rho_n gz \quad \Phi_w = P_w + \rho_w gz \]  

(3.5)

Here \( g \) is the gravitational acceleration and \( z \) is the elevation above a reference plane. \( P_{c,stat} \) is the static capillary pressure, which is the capillary pressure in the column if the changes in saturation through time are not considered or not present. \( \tau \) is the damping factor. In steady-state and static simulations, the damping factor \( \tau \) will be assigned the value zero, so that the traditional equation for capillary pressure is obtained. The extended expression for capillary pressure, which includes dynamic effects as a result of changes in saturation with time, will not be used in the simulations described in this thesis.

In addition to the governing equations, constitutive relations are needed. These are functions that relate the primary variables of the governing equations to the associated secondary variables. The constitutive relations are needed to close the set of governing equations. The three main variables for which the set of governing equations is solved are the nonwetting phase saturation \( (S_n) \), nonwetting phase potential \( (\Phi_n) \), and the wetting phase potential \( (\Phi_w) \). However, the three governing equations contain seven unknowns, being \( \Phi_n, \Phi_w, S_n, S_w, k_{rn}, k_{rw}, \) and \( P_{c,stat} \). Therefore, four constitutive equations are needed that relate the four secondary variables to the three primary variables.

The first constitutive relation is the capillary pressure-saturation relationship, which describes the dependence of the capillary pressure on saturation. There are several formulas that can be used to parameterize this relationship. In this model, the Brooks-Corey formula is used:

\[ P_c(S_e) = P_d \cdot S_e^{\frac{1}{\lambda}} \quad P_c \geq P_d \]  

\[ P_c(S_e) = P_d \quad P_c < P_d \]  

(3.6)

where \( P_d \) is the entry pressure and \( \lambda \) is the Brooks-Corey pore size distribution index. \( S_e \) is the effective saturation, defined as:

\[ S_e = \frac{S_w - S_{we}}{1 - S_{we} - S_{nr}} \]  

(3.7)
where $S_w$ is the wetting phase saturation, $S_{wr}$ is the residual wetting phase saturation, and $S_{nr}$ is the residual nonwetting phase saturation.

The second and third constitutive relations are the relative permeability-saturation relationships. In this model, it is assumed this relationship can be prescribed based on the $P_c$-$S_n$ relationship using the Burdine model in conjunction with the Brooks-Corey model:

$$k_{en}(S_e) = S_e^{2\lambda}$$

$$k_{en}(S_e) = (1 - S_e)^2 \left(1 - S_e^{2\lambda}\right)$$

In addition to these constitutive equations, a consistency relation is used that relates the nonwetting and wetting phase saturations:

$$S_w + S_n = 1$$

### 3.1.2 Temporal and spatial discretisation

As was mentioned before, the set of governing and constitutive equations described in Section 3.1.1 cannot be solved analytically. Therefore, the equations have to be approximated by numerical methods. This requires the temporal and spatial discretisation of the differential equations.

First, the equations are discretised in space. The domain for which the governing equations need to be solved is discretised in a number of cells or control volumes. In the centre of each control volume, a node is placed. The boundaries of the domain are represented by nodes situated at the boundary of the control volumes. An example of such a discretised domain is given in Figure 3.1. In this figure, the boundaries denote the physical boundaries of the
modelling domain. However, depending on boundary condition type, an artificial layer may be needed at the boundary (see Section 4.2.2).

The discretisation that is used in this model is a cell centred finite volume method. The finite volume method is based on the construction of a local mass balance for each control volume. Thus, for each control volume, a mass balance equation such as Equation (3.1) and (3.2) are constructed. These mass balances then can be integrated, so that a volume integral over the derivative of the flux through the control volume is obtained. Subsequently, this volume integral is transformed into a surface integral using the divergence theorem or Gauss’ theorem. This theorem states that a vector field on a surface is related to the behaviour of the vector field inside that surface (Wikipedia Contributors, 2007). The obtained surface integrals represent the fluxes at the boundary of the control volume. These fluxes then are discretised with respect to the primary unknowns (Eymard et al., 2006). The finite volume method thus relates an average value of the variable over the control volume to its fluxes at the boundaries of this control volume. An example of constructing a 1-D discretised equation using the finite volume method is given in Appendix A.

In addition to the spatial discretisation, the governing equations also need to be discretised in time. The temporal discretisation is done using a fully implicit method. This means that the state of the system is found by solving an equation involving both the current state of the system and the later one.

Now, for simplicity we consider a 1-D situation. In that case, the discretised mass-balance equation for the nonwetting phase (equation (3.1)) becomes:

\[
\frac{\phi^i S_n^i}{\Delta t} \frac{S_n^i}{\Delta t} + \frac{1}{\Delta x^2} \left[ \left( K_{n+1} \frac{\lambda_n^{i+1}}{\Delta x} \right) \left( \Phi_n^{i+1} - \Phi_n^i \right) - \left( K_{n-1} \left( \frac{\lambda_n^{i-1}}{\Delta x} \right) \left( \Phi_n^i - \Phi_n^{i-1} \right) \right) \right] = 0
\]

where

\[
\lambda_n^i = \begin{cases} 
\lambda_n^i & \text{if } \Phi_n^i \geq \Phi_n^{i+1} \\
\lambda_n^{i-1} & \text{if } \Phi_n^i < \Phi_n^{i+1}
\end{cases}
\]

\[
\lambda_n^{i+1} = \begin{cases} 
\lambda_n^{i+1} & \text{if } \Phi_n^{i+1} \geq \Phi_n^i \\
\lambda_n^{i+1} & \text{if } \Phi_n^{i+1} < \Phi_n^{i+1}
\end{cases}
\]

and \(k\) and \(i\) refer to a step in time and a step in space, respectively.

This discretisation scheme is a fully implicit scheme in time, and a first order upwind scheme in space. This means that only the values upwind or upstream from the gridcell are used to calculate the value of the parameter inside the gridcell. The fluxes across the interfaces between gridcells are calculated as \(q_n^{i+1/2}\) or \(q_n^{i+1/2}\), respectively. For example, when the potential \(\Phi\) of a phase in cell \(i\) is higher than the potential in cell \(i+1\), the flux will be from \(i\) to \(i+1\), and the phase mobility that is used for the calculation of \(q_n^{i+1/2}\) is the phase mobility of cell \(i\), being the upstream cell. As can be seen from Equation (3.11), the discretisation uses three cells to calculate the value in one cell: it uses cells \(i-1, i\) and \(i+1\). Similar discretisations can be written for the other two governing equations (3.2) and (3.3).

The discretized set of equations now can be linearized using the Newton-Raphson method. This is a root-finding algorithm that uses the first terms of a Taylor series of a function \(f(x)\) in
the vicinity of a suspected root. The method linearizes the set of non-linear discretised equations so that they can be solved with a solver such as Gaussian elimination, or LU decomposition. In Appendix B, a further explanation of the Newton-Raphson method can be found.

3.2 MUFTE-UG

MUFTE-UG is a model that is developed in collaboration between Universität Stuttgart and the University of Heidelberg, both situated in Germany. MUFTE-UG stands for Multiphase Flow Transport and Energy model on Unstructured Grids. It is a numerical simulator that can be used for the simulation of isothermal and non-isothermal multicomponent flow and transport in porous and highly heterogeneous or fractured media. The program consists of two parts: MUFTE and UG. MUFTE consists of spatial discretisation schemes for the multiphase-flow partial differential equations, the constitutive relationships, and the problem description. UG is the toolbox that solves the partial differential equations.

MUFTE-UG is used in this thesis for the modelling of isothermal single-component two-phase flow in homogeneous and heterogeneous porous media. This second model is used in order to get more familiar with different types of models. The major part of the simulations discussed in this thesis however are performed with the Berentsen model.

3.2.1 Model description

MUFTE-UG solves for the same set of governing equations and constitutive equations as was introduced for the Berentsen model, with the minor difference that MUFTE-UG uses pressures in stead of potentials as primary variables. The reader is referred to Section 3.1.1 for governing and constitutive equations.

3.2.2 Temporal and spatial discretisation

The spatial discretisation used in MUFTE-UG is the so-called BOX method. This is a vertex centred finite volume method, using a fully upwind technique. In Figure 3.2, an example of the discretised domain is given. The following explanation of the BOX method is taken directly from Manthey (2006).

The first step in the discretisation of the governing equations is to express the balance equations in their integral form:

\[
\int_{\Omega} n \cdot \frac{\partial S_\alpha}{\partial t} dV - \int_{\Omega} \nabla \cdot \left[ \lambda_\alpha \kappa \nabla (p_\alpha - \rho_\alpha gz) \right] dV = 0
\]  

(3.13)

The integration is performed over the domain \( \Omega \), which can be chosen arbitrarily. Subsequently, the domain is discretised by first constructing a primary grid. This primary grid consists out of a number of elements with corners (Figure 3.2). Note that the BOX method can also be applied to irregular grids. The primary grid is called the Finite Element mesh. Subsequently, a secondary grid can be constructed, by connecting the centre of gravity of an element with the middle of the element’s edges (Figure 3.2). Around each vertex, a control volume can be constructed by connecting the centres of gravity and the middlepoints of the element edges around the vertex. This control volume is called a box. In addition, a subcontrol volume can be defined by the intersection of a control volume with an element.
The boundaries of this subcontrol volume can be subdivided into two sub-control volume faces.

The primary variables $S_\alpha$ and $P_\alpha$ now can be approximated by the ansatz functions $N_j$. In the BOX-method, these are common $C^0$ Lagrangian polynomials. These polynomials are piecewise and continuous, but not continuously differentiable. If the wetting phase pressure is approximated this way, it would give:

$$\tilde{P_w} = \sum_j P_w^j N^j$$  \hspace{1cm} (3. 14)
Thus, the wetting phase pressure inside the sub-control volume can be approximated by the sum of the wetting phase pressures of the neighbouring vertices \( j \) and the vertex \( i \) inside the sub-control volume, multiplied with the ansatz function \( N^j \).

The gradient of the wetting phase pressure can be approximated by:

\[
\nabla \tilde{P}_w = \sum_{j \in \eta^i} (P^j_w - P^i_w) \nabla N^j
\]

(3.15)

where \( \eta^i \) is the set of neighbouring vertices of vertex \( i \). The ansatz function is given by:

\[
N^j(x_i) = \begin{cases} 
1 & \text{for } j = k \\
0 & \text{for } j \neq k 
\end{cases}
\]

(3.16)

As a result, the primary variables are no longer a function of space. However, because the primary variables now are approximated, the balance equations can no longer be solved exactly, so that the terms on the left hand side of Equation (3.13) no longer are equal to zero, but to equal to some residual \( \varepsilon \). This residual can be weighted such that over the domain, on average it becomes zero. The weighting function that is needed for this purpose should be chosen such that

\[
\int_{\Omega} W^i \varepsilon \, dV = 0 \quad \text{for } i = 1,2,K,n_{\text{nodes}}
\]

(3.17)

where \( W_i \) is the weighting function. For the BOX-method, the weighting function is chosen to be piecewise and constant so that

\[
W^i(x) = \begin{cases} 
1 & \text{if } x \in b_i \\
0 & \text{if } x \not\in b_i 
\end{cases}
\]

(3.18)

where \( b_i \) is the control volume around vertex \( i \). In Figure 3.3, examples of the weighting and the ansatz functions are given.

Using the above formulations, Equation (3.13) can be rewritten as:

\[
\int_{\Omega} \frac{\partial}{\partial t} \left(W^i n \sum S_a N^j d\Omega\right) - \int_{\Omega} W^i \nabla \left[ \lambda_a \sum_{j \in \eta^i} (P^j_a - P^i_a) - \rho_a g \sum_{j \in \eta^i} (z^j - z^i) \nabla N^j \right] \, d\Omega = 0
\]

(3.19)

where \( z_i \) is the z-coordinate of vertex \( i \), \( \rho_a \) is the density of phase \( a \), which is assumed to be constant through both time and space.
The first term on the left hand side of Equation (3.19), which is the accumulation term, can be approximated by the mid-point rule, so that:

\[
\int_{\Omega} n \sum \frac{S_a}{\Delta} N^j d\Omega = n S_a |b_i|
\]  

(3.20)

where \( |b_i| \) is the volume of control volume \( b_i \).

The second term in Equation (3.19) is the flux term, to which the product rule can be applied:

\[
\int_{\Omega} W^i \nabla F d\Omega = \int_{\Omega} \nabla \cdot (W^i F) d\Omega - \int_{\Omega} \nabla W^i F d\Omega
\]  

(3.21)

where the flux term is represented by \( F \). The second term on the right hand side of Equation (3.22) however becomes zero due to the chosen weighting functions \( W_i \). Subsequently, the first term on the right hand side of Equation (3.22), which is a volume integral, can be transferred into a surface integral by applying Gauss’s Theorem:

\[
\int_{\Omega} \nabla (W^i F) d\Omega = \oint_{\Gamma} W^i F \cdot n d\Gamma
\]  

(3.22)

where \( n \) is the unit normal vector. Thus, finally, the flux term can be rewritten as:

\[
\int_{\Omega} W^i \nabla \left[ \lambda_a K \left( \Psi^i_a - \Psi^i \right) \nabla N^j \right] d\Omega = \oint_{\Gamma} W^i \lambda_a K \Psi^i_a \nabla N^j \cdot n d\Gamma_b
\]  

(3.23)

where \( \Psi^i_a \) is the total potential:

\[
\Psi^i_a = \sum_{j \neq q} P^j_a - \rho^i_a g \sum_{j \neq q} z^j
\]  

(3.24)

And \( \Psi^i_a \) is the difference in the total potential between the vertices \( i \) and \( j \):

\[
\Psi^i_a = \sum_{j \neq q} \left( P^j_a - P^i_a \right) - \rho^i_a g \sum_{j \neq q} \left( z^j - z^i \right)
\]  

(3.25)
The flux terms are evaluated at the mid-point of a sub-control volume face $\varphi$ at the integration point IP (Figure 3.2), and then weighted on that face. Therefore, the integration over the flux term of one box can be approximated by:

$$
F^i = \sum_{i \in c} \sum_{j \in q} \lambda^i_{\alpha} \Psi^i_{\alpha} \nabla N^j \cdot n \phi^i_{el}
$$

(3.26)

The phase mobility $\lambda^i_{\alpha}$ is defined using a upstream weighting technique:

$$
\lambda^i_{\alpha} = \begin{cases} 
\lambda^i_{\alpha} & \text{if } (\Psi^i_{\alpha} - \Psi^i) \geq 0 \\
\lambda^i_{\alpha} & \text{if } (\Psi^i_{\alpha} - \Psi^i) < 0 
\end{cases}
$$

(3.27)

The same technique is used in the Berentsen model, where the phase mobility is defined according to Equation (3.12). Finally, the spatially discretised form of Equation (3.13) can be written by closing the system with equations (3.6) and (3.10), and solving for the primary variables $P_w$ and $S_n$:

$$
g^i_{\alpha} \left( P^i_w S^i_n \right) = (-1)^{\delta^{\alpha,w}} n \frac{\partial}{\partial t} \left( S^i_{\alpha} \mid b_{i} \right) - \sum_{i \in c} \sum_{j \in q} \lambda^i_{\alpha} K \left( \Psi^i_{\alpha} - \psi^i_{\alpha} \right) \nabla N^j \cdot n \phi^i_{el} - m^i_{\alpha}
$$

(3.28)

where

$$
\Psi^i_{\alpha} = P^i_w + \delta^\alpha P^i_c - \rho^i_{\alpha} g^i
$$

(3.29)

The term $m^i_{\alpha}$ quantifies the flux over the boundary in case $\partial_{b_i} \cap \Gamma_{\alpha,N}$. $\delta^{\alpha,w}$ and $\delta^{\alpha,n}$ are Kronecker delta’s, which are defined as:

$$
\delta^{\alpha,w} = \begin{cases} 
1 & \text{if } \alpha = w \\
0 & \text{if } \alpha \neq w 
\end{cases} \quad \delta^{\alpha,n} = \begin{cases} 
1 & \text{if } \alpha = n \\
0 & \text{if } \alpha \neq n 
\end{cases}
$$

(3.30)

Now that the equation is spatially discretised, it also has to be discretised temporally. Just as in the Berentsen model, the temporal discretisation is performed using a fully implicit Euler method. The fully discretised balance equations then become (Manthey, 1006):

$$
g^l_{\alpha} \left( P^l_w S^l_n \right) = \frac{(-1)^{\delta^{\alpha,w}} n}{\Delta t} \left( S_{\alpha}^{l,\alpha+1} \mid b_{l} - S_{\alpha}^{l,\beta} \mid b_{l} \right) - \sum_{i \in c} \sum_{j \in q} \lambda^{l,\alpha+1}_{\alpha} K \left( \Psi_{\alpha}^{l,\alpha+1} - \psi_{\alpha}^{l,\alpha+1} \right) \nabla N^j \cdot n \phi^{l,\alpha}_{el} - m^{l,\alpha+1}_{\alpha}
$$

(3.31)

Subsequently, the discretised set of governing equations is linearized using the Newton-Raphson method, which is further explained in Appendix B. The linearized, discretised set of equations then is solved through a Gaussian elimination procedure.
Chapter 4

Preliminary simulations

In this chapter, several parameters needed to simulate a static or steady-state primary drainage experiment are investigated. These are:

- Mesh size
- Equilibrium criterion
- Pressure increment magnitude

The values of these parameters will be determined by performing sets of simulations for which either the mesh size, the equilibrium criterion, or the magnitude of the pressure increment is varied. Once the optimal values for these parameters have been determined, static and steady-state drainage experiments can be performed.

In this chapter, the Berentsen model is discussed more rigorously because it is the model that is mostly used for performing the simulations. Therefore, for simulations with MUFTE-UG, the mesh size and magnitude of the pressure increment is simply taken from the Berentsen model. The last section of this chapter contains a comparison between the Berentsen model and MUFTE-UG.

It is important to note that the $P_c$-$S_w$ curves obtained with the Berentsen model in this and following chapters actually display also points that do not represent an equilibrium state. Thus, points are displayed that lay in between the equilibrium $P_c$-$S_w$ points, so that these points actually show the dynamics between the equilibrium points. This is illustrated in Figure 4.1. With MUFTE-UG, only equilibrium points of the $P_c$-$S_w$ curve will be plotted.

![Figure 4.1: The equilibrium $P_c$-$S_w$ curve with and without displaying dynamics between the equilibrium points (based on Gielen, 2007).](image)
Table 4.1 provides an overview of the simulations that will be discussed in this chapter.

Table 4.1: Overview of the simulations referred to in Chapter 4.

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1) Set of steady-state simulations to determine the mesh size</td>
<td>Homogeneous domain, 18.2 cm length, 10 steps of 2000 Pa, equilibrium criterion 10^{-8} m/s, mesh sizes: 8·10^{-2} m, 5·10^{-2} m, 1·10^{-2} m, 5·10^{-3} m, 4·10^{-4} m, 3·10^{-4} m, 1·10^{-4} m</td>
</tr>
<tr>
<td>2) Set of steady-state simulations to determine the equilibrium criterion</td>
<td>Homogeneous domain, 18.2 cm length, 10 steps of 2000 Pa, mesh size 5·10^{-3} m, equilibrium criteria: 10^{-4} m/s, 10^{-5} m/s, 10^{-6} m/s, 10^{-8} m/s, 10^{-10} m/s, 10^{-12} m/s, 10^{-14} m/s</td>
</tr>
<tr>
<td>3) Set of steady-state simulations to determine the pressure increment</td>
<td>Homogeneous domain, 18.2 cm length, mesh size 4·10^{-4} m, equilibrium criterion 10^{-8} m/s, pressure increments of 2000 Pa, 5000 Pa, 3000 Pa, 1000 Pa, 500 Pa, 300 Pa, 200 Pa, 100 Pa, 50 Pa</td>
</tr>
<tr>
<td>4) Set of static simulations performed with MUFTE-UG</td>
<td>Homogeneous domain, 18.2 cm length, mesh size 4·10^{-4} m, pressure increment of 100 Pa, equilibrium criteria (average change in saturation): 2·10^{-6}, 1.9·10^{-6}, 1.8·10^{-6}, 1.6·10^{-6}, 1.3·10^{-6}, 1·10^{-6}, 1·10^{-7}</td>
</tr>
</tbody>
</table>

4.1 Steady-state and static primary drainage experiments

In the determination of capillary pressure-saturation relationships, three types of measurement methods can be distinguished. These methods are based on static equilibrium, steady-state flow, or dynamic/ transient flow. In case of static equilibrium, both the nonwetting and wetting fluid stop flowing when equilibrium is reached. In a drainage experiment, this can be achieved by using a hydrophilic membrane that prevents the nonwetting phase from leaving the sample (see also Chapter 7). In case of steady-state equilibrium during a drainage experiment, the nonwetting phase still flows due to a pressure gradient within the sample but the divergence of the flow field is zero. Thus, the nonwetting phase is allowed to flow out, reaching a steady-state flow velocity when equilibrium is reached. Note that, in case of a drainage experiment, before the nonwetting phase front reaches the outflow of the sample, a static primary drainage experiment will be equal to a steady-state primary drainage experiment. This is because before there will not be a steady-state flow of the nonwetting phase as long as there is no breakthrough. Finally, transient or dynamic flow is time dependent. The boundary capillary pressure for each of these types of flow is illustrated in Figure 4.2.

In this thesis, only the capillary pressure-saturation relationship obtained under steady-state or static conditions for a primary drainage process will be investigated. As was explained in Section 2.3.1, a steady-state or a static capillary pressure-saturation relationship is obtained by increasing the capillary pressure by small increments. After each incremental increase in capillary pressure, the sample is allowed to reach equilibrium. Only when equilibrium is reached, the saturation and capillary pressure in the sample are determined. These measurements then comprise one point on the equilibrium capillary pressure-saturation curve.
method requires the pressure increments to be small because a sufficient amount of points are needed to construct the equilibrium $P_c-S_w$ curve. In contrast, for a dynamic drainage experiment, the capillary pressure is increased only once by a very large amount, after which the saturation and capillary pressure of the sample are monitored as they change. The $P_c-S_w$ relationship obtained using this approach has been shown to be different from the static or steady-state equilibrium $P_c-S_w$ curve by several researchers (e.g. Topp et al., 1967, Stauffer, 1978, Kalaydjian, 1992), and has raised the question whether an equilibrium $P_c-S_w$ curve is appropriate for use in the modelling of dynamic flow processes.

![Figure 4.2: The difference in applied boundary capillary pressure (Pa) (based on Manthey, 2006).](image)

4.2 Procedure

In this section, the numerical domain and the initial and boundary conditions are discussed for the simulations that will be performed in this chapter. For the determination of the optimal mesh size, equilibrium criterion, and pressure increment magnitude, simulations of a steady-state primary drainage experiment are used.

4.2.1 Domain description and medium properties

The domains that will be used in the simulations in this and following chapters have dimensions similar to those used in laboratory experiments. For the simulations in this chapter, the porous medium in the domain is assumed to be homogeneous so that flow occurs only in the vertical direction $z$. The simulation thus can be considered to be 1-D, as there will be no variations in the $x$-direction. The domain used here has a length of 0.182 cm. The numerical grid used in the simulation has a regular spacing of $dz$. The optimal value for $dz$ will be investigated in Section 4.3.

The characteristics of the porous medium and the fluids can be found in Table 4.1. The properties of the wetting phase correspond to those of water, while the properties of the nonwetting phase correspond to those of the DNAPL Perchloroethylene (PCE).

As was mentioned in Chapter 3, the capillary pressure-saturation relationship is parameterised using a Brooks-Corey relationship (Equation 3.6). In Figure 4.3, the obtained relationship for $P_d = 6000$ Pa, $\lambda = 6.11$, and $S_{wr} = 0.104$ is shown. In addition, the figure shows the relative permeability-saturation relationships that are obtained using the Brooks-Corey relationship in combination with the Burdine model (Equations (3.8) and (3.9).

In addition to the domain that represents the actual porous medium, the Berentsen model also requires the use of an artificial layer at the inflow and outflow of the domain. These artificial layers have only a thickness of a single mesh spacing. The layers do not have a physical meaning but they are needed for numerical reasons. This is because in the Berentsen model, the boundary conditions at the top and the bottom of the domain are specified as Dirichlet
conditions for both the nonwetting and wetting phase pressures. Because inside the physical domain, pressures are the unknowns for which we want to solve the governing equations, an extra (artificial) layer is added to the domain to which the boundary pressures can be applied.

Table 4.2: Properties of porous medium and fluids used in the simulations referred to in Chapter 4.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluids</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Density of the wetting phase, (\rho_w)</td>
<td>1000</td>
<td>kg m(^{-3})</td>
</tr>
<tr>
<td>Density of the nonwetting phase, (\rho_n)</td>
<td>1623</td>
<td>kg m(^{-3})</td>
</tr>
<tr>
<td>Viscosity of the wetting phase, (\mu_w)</td>
<td>0.9*10(^{-3})</td>
<td>N m(^{-2}) s</td>
</tr>
<tr>
<td>Viscosity of the nonwetting phase, (\mu_n)</td>
<td>1.0*10(^{-3})</td>
<td>N m(^{-2}) s</td>
</tr>
<tr>
<td>Porous medium</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Intrinsic permeability, (\kappa)</td>
<td>2.21*10(^{-12})</td>
<td>m(^2)</td>
</tr>
<tr>
<td>Porosity, (n)</td>
<td>0.4</td>
<td>-</td>
</tr>
<tr>
<td>Brooks-Corey Entry pressure, (P_d)</td>
<td>6000</td>
<td>Pa</td>
</tr>
<tr>
<td>Residual wetting phase saturation, (S_w)</td>
<td>0.104</td>
<td>-</td>
</tr>
<tr>
<td>Residual nonwetting phase saturation, (S_n)</td>
<td>0</td>
<td>-</td>
</tr>
<tr>
<td>Brooks-Corey coefficient, (\lambda)</td>
<td>6.11</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure 4.3: Capillary-pressure-saturation relationship and relative permeability-saturation relationship as specified for the porous medium. Curves are obtained using a Brooks-Corey formulation in combination with Burdine (red line: \(k_{rw}\); blue line: \(k_{rn}\)).

In Table 4.3, properties of these two artificial layers are presented. As can be seen, the bottom layer has a negative entry pressure. This is a non-physical value, but because the bottom artificial layer is fully saturated by the nonwetting phase throughout a simulation, it actually has no physical meaning. The artificial bottom layer prevents the wetting phase from leaving the domain at this boundary. The artificial layer at the outflow of the domain is assigned a very small positive entry pressure so that the nonwetting phase is allowed to flow out easily. Note that this condition is only used for the simulation of steady-state primary drainage experiments. When simulating a static primary drainage experiment, the top artificial layer will be assigned a high entry pressure, so that the nonwetting phase is prevented from leaving the sample. This mimics the presence of a hydrophilic membrane.

When determining average quantities over the domain, such as saturation and pressure, the artificial layers are excluded from the averaging domain, as they do not represent the porous medium, but are a numerical artefact.
Table 4.3: properties of the artificial top and bottom layer introduced in the Berentsen model

<table>
<thead>
<tr>
<th>Properties of artificial top and bottom layer</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intrinsic permeability top layer</td>
<td>$3 \times 10^{-10}$</td>
<td>m$^2$</td>
</tr>
<tr>
<td>Intrinsic permeability bottom layer</td>
<td>$3 \times 10^{-10}$</td>
<td>m$^2$</td>
</tr>
<tr>
<td>Entry pressure top layer</td>
<td>1</td>
<td>Pa</td>
</tr>
<tr>
<td>Entry pressure bottom layer</td>
<td>-1</td>
<td>Pa</td>
</tr>
<tr>
<td>Residual wetting phase saturation for top layer</td>
<td>0</td>
<td>-</td>
</tr>
<tr>
<td>Residual wetting phase saturation for bottom layer</td>
<td>0</td>
<td>-</td>
</tr>
<tr>
<td>Residual nonwetting phase saturation for top layer</td>
<td>0</td>
<td>-</td>
</tr>
<tr>
<td>Residual nonwetting phase saturation for bottom layer</td>
<td>0</td>
<td>-</td>
</tr>
</tbody>
</table>

4.2.2 Initial and boundary conditions

The initial conditions used in the simulations are given by:

$$\nabla (\lambda_a \nabla \Phi_a) + \nabla (\lambda_n \nabla \Phi_n) = 0 \quad \text{or} \quad \nabla u_f = 0$$  \hspace{1cm} (4.1)

$$S_n = S_n^{\text{init}} = 0$$  \hspace{1cm} (4.2)

These conditions state that, initially, there is no total flow, and the domain is fully wetting phase saturated. In Figure 4.4, the domain and the applied boundary conditions for a steady-state primary drainage experiment are shown. The experiment is constructed such that the nonwetting phase is forced in at the bottom boundary. Flow thus is upward. In laboratory experiments, this approach is used to prevent gravity effects such as fingering.

The east and west boundaries of the domain are no flow boundaries for both the wetting and nonwetting phase:

$$q_n = 0$$  \hspace{1cm} (4.3)

These boundaries are needed because the Berentsen model does not allow for a 1-dimensional domain, but only for 2-dimensional domains. The boundary condition at the top of the column is given by a zero pressure for the wetting phase:

$$p_{nw}^{\text{top}} = 0$$  \hspace{1cm} (4.4)

For numerical reasons, the nonwetting phase pressure cannot be equal to zero too. Therefore, the nonwetting phase top boundary pressure is defined as:

$$p_{nw}^{\text{top}} = p_{nw} + 1$$  \hspace{1cm} (4.5)

This set of boundary conditions allows for the free outflow of the nonwetting and wetting phase from the sample.
At the bottom boundary of the domain, the nonwetting phase is forced to flow into the domain, replacing the wetting phase. This is achieved by increasing the nonwetting phase pressure at the bottom boundary by small increments (see Figure 4.2). The initial bottom boundary nonwetting phase pressure is given by the hydrostatic pressure of the nonwetting phase at the bottom boundary with the addition of one pressure increment:

\[ P_{n,0} = \rho_n g h + \Delta P \]  

(4.6)

where \( \rho_n \) is the density of the nonwetting phase, \( g \) is the gravitational acceleration, \( h \) is the height of the column, and \( \Delta P \) is the incremental pressure increase. Note that this is an arbitrary choice for the initial nonwetting phase pressure at the bottom boundary, which has no effect on the outcome of the simulation. This is because the nonwetting phase will only start infiltrating the porous medium when the entry pressure is reached.

The nonwetting phase pressure at the bottom boundary will be increased by one increment \( \Delta P \) each time steady state is reached. Thus, the sequence of nonwetting phase pressures at the bottom boundary is given by:

\[
P_{n,1}^{\text{bottom}} = P_{n,0}^{\text{bottom}} + \Delta P
\]

\[
P_{n,2}^{\text{bottom}} = P_{n,1}^{\text{bottom}} + \Delta P
\]

\[
P_{n,3}^{\text{bottom}} = P_{n,2}^{\text{bottom}} + \Delta P
\]

\[
P_{n,4}^{\text{bottom}} = P_{n,3}^{\text{bottom}} + \Delta P
\]

\[
\vdots
\]

\[
P_{n,N}^{\text{bottom}} = P_{n,N-1}^{\text{bottom}} + \Delta P
\]

(4.7)
where $N$ is the number of pressure increments that will be applied. The simulation ends at the moment equilibrium is reached after the last nonwetting phase bottom boundary pressure is applied. The optimal magnitude for the pressure increment $\Delta P$ will be investigated in Section 4.5. The wetting phase pressure at the bottom boundary is given by:

$$P_{\text{bottom}}^w = P_{\text{bottom}}^n + 1 \quad (4.8)$$

The boundary condition for the wetting phase pressure results in a negative capillary pressure. However, note again that the boundary conditions are applied at the artificial layers, so that they do not need to have any physical meaning. Actually, the bottom artificial layer is fully saturated with the nonwetting phase at all times, so that the boundary condition for the wetting phase does not have any real meaning. The bottom boundary also acts as a no-flow boundary for the wetting phase, because it is fully saturated with the nonwetting phase at all times, and has a negative entry pressure. As a result, the artificial bottom layer in a way represents a hydrophobic membrane that is used in laboratory experiments to prevent the wetting phase from leaving the sample where the nonwetting phase is forced into the sample. After each incremental pressure increase, the porous medium is allowed to reach an equilibrium distribution of pressures and saturation. However, reaching true equilibrium might take a very long time, because gradients get smaller and smaller as equilibrium is approached. Therefore, a criterion can be used to indicate when equilibrium is approached close enough. This criterion could for instance be based on the maximum saturation change in the domain within a timestep, or the time rate of change of saturation. In the Berentsen model, an equilibrium criterion based on the maximum wetting phase flux is used. This means that it is assumed that equilibrium is approached close enough when the maximum flux of the wetting phase in the domain becomes smaller than a certain predefined value. The choice of a value for the equilibrium criterion is discussed in the Section 4.4.

For the simulation of a static primary drainage experiment, the initial conditions are the same as for a steady-state primary drainage experiment (conditions (4.1) and (4.2)). However, the entry pressure of the artificial top layer now is assigned a high value of 90000 Pa. As a result, this artificial layer now represents a hydrophilic membrane with a very high entry pressure, preventing the nonwetting phase from leaving the column as it cannot enter the top layer. This results in the following set of top boundary conditions:

$$P_{\text{top}}^w = 0 \text{ Pa} \quad (4.9)$$

$$P_{\text{top}}^n = 90000 \text{ Pa} \quad (4.10)$$

The set of bottom boundary conditions is equal to set presented for the steady-state primary drainage experiments. These are the conditions (4.7) and (4.8).

The east and west boundary conditions still are no-flow boundary conditions for the wetting and nonwetting phase as was described in condition (4.3). Figure 4.5 gives an overview of the boundary conditions used for both the simulation of a static and steady-state primary drainage experiment.
BERENTSEN MODEL

Steady-state simulation

<table>
<thead>
<tr>
<th>Boundary Condition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( P_n )</td>
<td>( \rho_w g h + \Delta P )</td>
</tr>
<tr>
<td>( P_w )</td>
<td>( \rho_w g h )</td>
</tr>
</tbody>
</table>

Static simulation

<table>
<thead>
<tr>
<th>Boundary Condition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( P_n )</td>
<td>( \rho_w g h + \Delta P )</td>
</tr>
<tr>
<td>( P_w )</td>
<td>( \rho_w g h )</td>
</tr>
</tbody>
</table>

Figure 4.5: Overview of the boundary conditions used in the Berentsen model for the simulation of a steady-state and static primary drainage experiment, respectively.

Besides the difference in applied boundary conditions between the static and steady-state primary drainage experiment, also the permeability of the artificial layers is adapted. This is because in case of the simulation of a static primary drainage experiment, the artificial layers are used to represent hydrophobic and hydrophilic membranes. However, membranes that are used in laboratory experiments are typically very thin, for example only 1.25 \( \mu m \). In addition, their relative permeability is very low, in the range of \( 10^{-14} \) m\(^2\). The thickness of these membranes thus is smaller than the mesh size that will be used in the simulations. Therefore, the permeability of the artificial layers is scaled to represent the permeability of the membranes, such that the transmissivity (permeability \( K \) times the thickness \( D \)) is kept unchanged:

\[
K_{\text{membrane}} D_{\text{membrane}} = K_{\text{simulated zone}} D_{\text{simulated zone}} \tag{4.11}
\]

Thus, the scaled permeability of the artificial layers can be calculated by:

\[
K_{\text{simulated zone}} = \frac{K_{\text{membrane}} D_{\text{membrane}}}{D_{\text{simulated zone}}} \tag{4.12}
\]

The permeability of the simulated membranes therefore is set to \( 3.17 \times 10^{-17} \) m\(^2\). For simulations performed with MUFTE-UG, different boundary conditions than for the Berentsen model are used. Moreover, an artificial top and bottom layer are not needed. The boundary conditions are simply applied to the boundaries of the domain, directly in contact with the porous medium. In Figure 4.6, an overview of the used boundary conditions in MUFTE-UG is given, for both the simulation of a static and steady-state primary drainage experiment.
For the steady-state primary drainage experiment, the bottom boundary conditions are a Neumann boundary condition for the wetting phase:

\[ q_w^{bottom} = 0 \quad (4.13) \]

and a Dirichlet boundary condition for the nonwetting phase:

\[
\begin{align*}
P_{n,0}^{bottom} &= \rho_n g h + P_d + \Delta P \\
P_{n,1}^{bottom} &= P_{n,0}^{bottom} + \Delta P \\
P_{n,2}^{bottom} &= P_{n,1}^{bottom} + \Delta P \\
P_{n,3}^{bottom} &= P_{n,2}^{bottom} + \Delta P \\
&\vdots \\
P_{n,N}^{bottom} &= P_{n,N-1}^{bottom} + \Delta P 
\end{align*}
\]  

(4.14)

The top boundary conditions are given by a Dirichlet boundary condition for the wetting phase:

\[ P_w^{top} = 100 \text{ Pa} \quad (4.15) \]

and a Dirichlet boundary condition for the nonwetting phase:

\[ P_n^{top} = 101 \text{ Pa} \quad (4.16) \]
For a static primary drainage experiment, the bottom boundary conditions are the same as for the steady-state primary drainage experiment (conditions (4.13) and (4.14)), and the top boundary conditions are given by a Dirichlet boundary condition for the wetting phase, and a Neumann boundary condition for the nonwetting phase:

\[ P_{w}^{\text{top}} = 100 \text{ Pa} \]  
\[ q_{n}^{\text{top}} = 0 \]  

Note that with MUFTE-UG, the end of the simulation is reached when a predefined time is reached. This means that the final applied nonwetting phase boundary pressure and thus the final boundary capillary pressure can vary from simulation to simulation.

### 4.3 Determination of the mesh size

The numerical accuracy of the simulation results can be investigated by performing a number of simulations for which the mesh size is varied. A large mesh size will give poor results, while a very small mesh size might give more accurate results but requires longer computational times. Therefore, some ‘optimal’ mesh size can be found that provides accurate results but requires minimal computation time.

The simulations in this section are for a steady-state primary drainage experiment. Among the simulations, only the mesh size is varied, while all other variables are kept constant. The primary drainage experiment is performed by increasing the nonwetting phase pressure at the bottom boundary in 10 steps of 2000 Pa, each time waiting for equilibrium. For this, the equilibrium criterion for the maximum wetting phase flux is set to \(10^{-8}\) m/s. The simulations are compared by considering the averaged equilibrium \(P_c-S_w\) curve. The averaging is performed using an arithmetic phase volume average for the pressures:

\[
\overline{P}_\alpha = \frac{\sum_{i=1}^{N} P_i^{\alpha} \eta_\alpha}{N_{S_\alpha>0}} \quad \alpha = n, w
\]  

where \(N_{S_\alpha>0}\) is the number of nodes for which the saturation of the \(\alpha\)-phase is larger than zero. \(\eta_\alpha\) represents an indicator function, defined as:

\[
\eta_\alpha = \begin{cases} 
1 & S_\alpha > 0 \\
0 & S_\alpha = 0 
\end{cases}
\]  

and a simple arithmetic average for the saturation:

\[
\overline{S}_\alpha = \frac{\sum_{i=1}^{N} S_i^\alpha}{N} \quad \alpha = w, n
\]
where $N$ is the total number of nodes over which the average is calculated, $P_\alpha$ is the pressure of fluid $\alpha$, and $S_\alpha$ is the saturation of fluid $\alpha$. Note that the average is taken over all nodes in the domain, excluding the boundary nodes and artificial layers. Averaging of the equilibrium $P_c$-$S_w$ curve will be further discussed in Chapter 5. Figure 4.7 shows the obtained averaged equilibrium $P_c$-$S_w$ curves for the different mesh sizes. Note that here attention will be given to the differences between the curves only, and not to the general shape of the curve, which can be shown to be dependent on the averaging method used. Again, this will be discussed in Chapter 5. Figure 4.8 shows the average nonwetting phase saturation as a function of time for different mesh sizes, while Figure 4.9 shows the saturation profiles at an applied nonwetting phase boundary pressure of 8898 Pa. The mesh size should be chosen such that it does not have a (significant) influence on the obtained results. As can be seen from the figures, the large mesh sizes of 8 cm and 5 cm do not give numerically accurate results. This is particularly clear when Figure 4.9 is considered. Mesh sizes of 1 cm and 0.5 cm give better results. However, when the mesh size is set to 0.5 mm and smaller, the results become almost indistinguishable. Thus, for mesh sizes of 0.5 mm and smaller, the results are practically identical, and can be assumed to be numerically accurate. Therefore, the mesh size that will be used for the simulations in this thesis is 0.4 mm.

Figure 4.7: arithmetic phase volume average equilibrium $P_c$-$S_w$ curves for different mesh sizes
Figure 4. 8: average nonwetting phase saturation as a function of time for simulations with different mesh sizes in meter.

Figure 4. 9: nonwetting phase saturation profiles for simulations with varying mesh sizes, at an applied nonwetting phase boundary pressure of 8898 Pa.
4.4 Determination of the equilibrium criterion

In this section, the magnitude of the equilibrium criterion will be determined. In the Berentsen model, the equilibrium criterion is determined by the maximum wetting phase flux in the domain. In MUFTE-UG, the equilibrium criterion is determined by the change in the average saturation between two timesteps. The magnitude of the equilibrium criterion plays an important role in obtaining a static or steady-state \( P_c - S_w \) curve. Ideally, the model would assume that equilibrium is reached when the wetting phase flux or the saturation change becomes zero. However, this could lead to very long computational times as was explained before. Therefore, a value for the equilibrium criterion needs to be found that will result in a (quasi-) equilibrium \( P_c - S_w \) curve, but for which computation times are still reasonable.

4.4.1 Choosing the equilibrium criterion

In order to investigate at which value the equilibrium criterion becomes strict enough so that the obtained \( P_c - S_w \) curve can be assumed to represent an equilibrium \( P_c - S_w \) relationship, simulations are performed for which the equilibrium criterion is varied while all other variables are kept constant.

First, the equilibrium criterion for the Berentsen model is determined. For these simulations, the nonwetting phase pressure at the bottom boundary is increased ten times by 2000 Pa. The mesh size that is used is 0.5 cm. Unfortunately, the mesh size is not 0.4 mm, because the set of simulations with varying equilibrium criterion was performed before the set of simulations with varying mesh size. However, the results presented in this section are assumed to also hold for a mesh size of 0.4 mm.

In Figure 4.10, the applied boundary pressure is plotted as a function of time for the simulations with varying equilibrium criterion. As can be seen, for a loose equilibrium criterion the nonwetting phase pressure at the bottom boundary increases rapidly, as ‘equilibrium’ is reached relatively fast.

![Applied \( P_n \) bottom (\( \times 10^4 \) Pa) as function of time, steady-state simulation](image)

Figure 4. 10: applied nonwetting phase pressure at bottom boundary as a function of time for several values of the equilibrium criterion. Note that the time-axis is on a logarithmic scale.
In addition, the figure shows that a simulated experiment takes longer with increasing strictness of the equilibrium criterion. This is a result of the bottom boundary condition for the nonwetting phase, which uses a predefined number of incremental pressure increases. As a result, the simulations for a stricter equilibrium criterion will reach the end at a later time than the simulations for a looser equilibrium criterion.

Figure 4.11 shows the obtained average equilibrium $P_c$-$S_w$ curves. The pressures and saturations are averaged according to Equations (4.19) and (4.21). As can be seen, an equilibrium criterion for the maximum wetting phase flux of $10^{-4}$ m/s does not represent steady-state conditions. With increasing strictness of the equilibrium criterion however, the averaged equilibrium $P_c$-$S_w$ curves start to converge, especially at high to intermediate average wetting phase saturations. At low wetting phase saturations, a small difference between the averaged equilibrium curves for equilibrium criteria of $10^{-8}$ m/s and stricter can be observed. Therefore, an equilibrium criterion of $10^{-10}$ m/s or even $10^{-12}$ m/s might be more appropriate than an equilibrium criterion of $10^{-8}$ m/s.

Figure 4.11: Arithmetic phase volume averaged equilibrium $P_c$-$S_w$ curves for varying equilibrium criterion

In Figure 4.12, the nonwetting and wetting phase fluxes in the middle of the domain are plotted as a function of time. As can be seen, the nonwetting phase flux increases each time the pressure of the nonwetting phase at the bottom boundary is increased. As equilibrium is approached, the nonwetting phase flux stabilizes and becomes constant. The figure shows that for the more loose equilibrium criteria, the nonwetting phase flux does not completely stabilize when equilibrium is assumed to have been reached. Only the equilibrium criteria of $10^{-12}$ m/s and $10^{-14}$ m/s show a constant nonwetting phase flux at the moment of assumed equilibrium. However, even for these criteria, as the simulation progresses the nonwetting phase flux still is changing when equilibrium is assumed. This is related to the relative permeability of the wetting phase, which approaches becomes very small as the simulation progresses. As a result, the wetting phase will have more difficulty to flow and the
equilibrium criterion of the maximum wetting phase flux is reached already before the pressures and saturations in the domain have reached an equilibrium distribution.

Figure 4.12: nonwetting and wetting phase fluxes in the middle of the domain as a function of time for several values of the equilibrium criterion. Note that the time-axis is on a logarithmic scale.

In Figure 4.12, also the wetting phase flux in the middle of the domain is shown. The wetting phase flux increases when the nonwetting phase pressure at the bottom boundary is increased, because the nonwetting phase then can displace the wetting phase. As equilibrium is approached, the wetting phase flux approaches zero as the pressures and saturations approach a steady-state equilibrium distribution. When the equilibrium criterion is met, the nonwetting phase pressure at the bottom boundary is increased again, and the wetting phase flux increases again in response. Note that for a static primary drainage experiment, both the nonwetting and wetting phase flux will approach zero as static equilibrium is approached.

Although Figure 4.11 and 4.12 indicate that an equilibrium criterion for the maximum wetting phase flux of $10^{-12}$ m/s or $10^{-14}$ m/s would be better than $10^{-8}$ m/s or $10^{-10}$ m/s, we cannot use such strict criteria because computational and experimental times need to be considered. The very strict equilibrium criteria require long times for equilibrium to be reached and demand more computation. This results in a long computational time as well as a long experimental time if the experiment would be performed in the laboratory. For instance, if we consider experimental times, the same ten pressure increments of 2000 Pa would take approximately 5.8 days when an equilibrium criterion of $10^{-8}$ m/s is used, while it would take 92.6 days when a criterion of $10^{-10}$ m/s is used, and 1157.4 days when a criterion of $10^{-12}$ m/s is used. Thus, in real physical laboratory experiments, these stricter criteria will never be used.

Based on the results, it can be concluded that an equilibrium criterion for the maximum wetting phase flux of $10^{-12}$ m/s or even $10^{-14}$ m/s is preferable for use in the simulations over a criterion of $10^{-8}$ m/s. However, considering the long computational and experimental times needed to reach equilibrium for such strict criteria, a criterion of $10^{-8}$ m/s is chosen for the simulation of steady-state and static primary drainage experiments. Thus, in this case a compromise has been made between the accuracy of the results representing equilibrium conditions, and the computation time. In Section 4.4.2, the effect of the equilibrium criterion on the averaged equilibrium Pc-Sw curve will be discussed in more detail.

In Table 4.4, the equilibrium criteria for the maximum wetting phase fluxes are used to calculate the flux that would leave a sample with a diameter of 9.8 cm and a length of 18.2 cm at the moment the equilibrium criterion is met. As can be seen, an equilibrium criterion of $10^{-8}$ m/s would result in a flux of a few of millilitres a day, while an equilibrium criterion of $10^{-10}$ m/s would result in less than a millilitre a day.
Table 4.4: Fluxes leaving a sample of 18.2 length and a diameter of 9.8 cm if the equilibrium criterion is met

<table>
<thead>
<tr>
<th>Equilibrium criterion</th>
<th>Flux leaving the sample at the moment the equilibrium criterion is met</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-8}$ m/s</td>
<td>6.52 ml/day</td>
</tr>
<tr>
<td>$10^{-10}$ m/s</td>
<td>0.065 ml/day</td>
</tr>
<tr>
<td>Amount of wetting phase present initially</td>
<td>549 ml</td>
</tr>
</tbody>
</table>

The equilibrium criterion used in MUFTE-UG is different from the one used in the Berentsen model. In MUFTE-UG, a criterion for the change in average saturation between two successive timesteps is used. The saturation is averaged only over those nodes for which the nonwetting phase is present:

$$\bar{S}_\alpha = \frac{\sum_{i=1}^{N} S_n^i \left(S_n^i > 0\right)}{\sum_{i=1}^{N} n^i \left(S_n^i > 0\right)} \quad \alpha = n, w$$ (4.22)

The equilibrium criterion is stated as:

$$\Delta S_n < A$$ (4.23)

where $\Delta S_n$ is the average saturation change between the current and the previous timestep, and $A$ is some prespecified value. Figure 4.13 shows the arithmetic phase volume averaged equilibrium $P_e-S_w$ curves obtained for different equilibrium criteria with MUFTE-UG. Note that these simulations are for a static primary drainage experiment in stead of a steady-state primary drainage experiment. Moreover, pressure increments with a magnitude of 100 Pa are used in stead of 2000 Pa. As can be seen, the obtained curves have a similar shape, but the main difference is the residual wetting phase saturation that is attained in each of the simulations. The stricter the equilibrium criterion in MUFTE-UG becomes, the higher the average wetting phase saturation at the end of the simulation is. This is actually opposite to what can be observed for the Berentsen model (see Figure 4.11), and can be explained as follows. In MUFTE-UG, the simulation is ended when a specified time is reached. In this case, the simulations are ended after $2 \times 10^6$ seconds. As the equilibrium criterion becomes stricter, a longer time is needed to reach equilibrium after each incremental increase in the nonwetting phase boundary pressure. As a result, in the same amount of time a lesser number of pressure increments can be added to the boundary pressure. Therefore, the final applied nonwetting phase pressure at the bottom boundary is different for each simulation shown in Figure 4.13, so that the resulting average residual wetting phase saturation and capillary pressure are different too. In order to reach the same final applied boundary pressure in MUFTE-UG, with increasing strictness of the equilibrium criterion, the end time of the simulation needs to be increased. In the Berentsen model, the end of a simulation is reached when a specified number of pressure increments have been performed. Therefore, the simulations for which the average curves are shown in Figure 4.11 all end at the same applied nonwetting phase boundary pressure. The times at which the simulations end however now are variable.
Figure 4.13: Arithmetic phase volume averaged $P_c-S_w$ curves for different equilibrium criteria, simulations are of a static primary drainage experiment, performed with MUFTE-UG.

Figure 4.14: Cumulative mass outflow in kg as a function of time for the simulations with different equilibrium criteria, static primary drainage experiment, pressure increments of 100 Pa, MUFTE-UG.

In Figure 4.14, the mass outflow as a function of time is shown for the different simulations performed with MUFTE-UG. As can be seen, initially all curves show a stabilising mass outflow when the equilibrium criterion is met. However, for the less strict equilibrium criteria, as the simulation progresses the mass outflow is still changing when equilibrium is assumed to have been reached. Just as with the Berentse model, this has to do with the relative
permeability of the wetting phase, which becomes very low as the drainage process progresses. This restrains flow of the wetting phase, and as a result the change in average saturation reaches the equilibrium criterion even though the pressure and saturation have not yet reached equilibrium distributions. The stricter equilibrium criteria of $10^{-5}$ and $10^{-7}$ do result in a mass outflow that stabilises when the criterion is met, but these criteria require a long computation time. Moreover, only a few pressure increments can be performed in $2 \cdot 10^6$ seconds (23 days).

The choice for the value of the equilibrium criterion in MUFTE-UG will be made such that the results are in agreement with the simulation results obtained with the Berentsen model using an equilibrium criterion for the maximum wetting phase flux of $10^{-8}$ m/s. In Figure 4.15, the average wetting phase saturation is shown as a function of time, for simulations of a static primary drainage experiment performed with MUFTE-UG and the Berentsen model. In these simulations, the magnitude of the pressure increments is 100 Pa. Note that for the curves obtained with MUFTE-UG, only saturations are displayed for which equilibrium is reached.

When considering the evolution of the wetting phase saturation, the MUFTE-UG simulation where an equilibrium criterion of $2 \cdot 10^{-6}$ is used approaches the evolution of the average saturation obtained with the Berentsen model best. As can be seen, an equilibrium criterion somewhere between $4 \cdot 10^{-5}$ and $2 \cdot 10^{-6}$ could result in comparable evolutions of the average wetting phase saturation between the Berentsen model and MUFTE-UG.

![Figure 4.15: average wetting phase saturation as a function of time. For each simulation, also the final applied nonwetting phase boundary pressure is shown.](image)

In Table 4.5, an overview is given for the different simulations performed with MUFTE-UG compared to the Berentsen model. As can be seen, when an equilibrium criterion is used of $2 \cdot 10^{-6}$, the final applied nonwetting phase bottom boundary pressure obtained with MUFTE-UG is much higher as the pressure achieved in the Berentsen model. Choosing an equilibrium criterion that is even looser would result in even higher final applied nonwetting phase boundary pressures. However, this is found to be caused by the time the simulation is allowed to run, which is $2 \cdot 10^6$ s. In comparison, the simulation of a static drainage experiment performed with the Berentsen model, using an equilibrium criterion for the maximum wetting phase flux of $10^{-8}$ m/s, ends at $1.6 \cdot 10^6$ s. If the simulation in MUFTE-UG using an equilibrium
criterion for the average saturation change of $2 \times 10^{-6}$ is performed again, but where now the end of the simulation now is reached at $1.6 \times 10^{-6}$ s, the results show that the final applied nonwetting phase pressure at the bottom boundary is actually lower than the attained pressure in the simulation performed with the Berentsen. Therefore, it must be possible to choose an equilibrium criterion with a value between $4 \times 10^{-5}$ and $2 \times 10^{-6}$, such that the evolution of saturation and pressures is approximately equal to the evolution of saturation and pressure in the simulation performed with the Berentsen model.

In the simulations performed with MUFTE-UG in the following chapters, it was decided to use an equilibrium criterion for the average change in saturation of $2 \times 10^{-6}$, even though a somewhat looser criterion would approximate the simulations performed with the Berentsen model better. The reason for this is the time constraint to perform more simulations with equilibrium criteria between $4 \times 10^{-5}$ and $2 \times 10^{-6}$ so that the criterion which matches the criterion used in the Berentsen model best can be found by trial and error. While a 1D simulation of a primary drainage experiment in a 1D homogeneous domain with the Berentsen model only takes three hours, the same simulation takes more than a day with MUFTE-UG (the two models are run on different computers).

### Table 4.5: Comparison of the simulation data obtained with simulations of a static primary drainage experiment in the Berentsen model, and MUFTE-UG, for which the equilibrium criterion is varied

<table>
<thead>
<tr>
<th>Simulation of static primary drainage experiment</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Equilibrium criterion</td>
<td>Time</td>
<td>Final applied nonwetting phase pressure at bottom boundary</td>
<td>Attained average wetting phase saturation</td>
</tr>
<tr>
<td><strong>Berentsen Model</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Maximum $q_w = 10^{-8}$ m/s</td>
<td>$1.6 \times 10^{6}$ s</td>
<td>32898 Pa</td>
<td>0.172</td>
</tr>
<tr>
<td><strong>MUFTE-UG</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Delta &lt;S_w&gt; = 2 \times 10^{-6}$</td>
<td>$2 \times 10^{5}$ s</td>
<td>584000 Pa</td>
<td>0.159</td>
</tr>
<tr>
<td>$\Delta &lt;S_w&gt; = 2 \times 10^{-6}$</td>
<td>$1.6 \times 10^{5}$ s</td>
<td>11198 Pa</td>
<td>0.204</td>
</tr>
<tr>
<td>$\Delta &lt;S_w&gt; = 1.9 \times 10^{-6}$</td>
<td>$2 \times 10^{5}$ s</td>
<td>279700 Pa</td>
<td>0.161</td>
</tr>
<tr>
<td>$\Delta &lt;S_w&gt; = 1.8 \times 10^{-6}$</td>
<td>$2 \times 10^{5}$ s</td>
<td>14908 Pa</td>
<td>0.166</td>
</tr>
<tr>
<td>$\Delta &lt;S_w&gt; = 1.6 \times 10^{-6}$</td>
<td>$2 \times 10^{5}$ s</td>
<td>11898 Pa</td>
<td>0.178</td>
</tr>
<tr>
<td>$\Delta &lt;S_w&gt; = 1.3 \times 10^{-6}$</td>
<td>$2 \times 10^{5}$ s</td>
<td>11198 Pa</td>
<td>0.200</td>
</tr>
<tr>
<td>$\Delta &lt;S_w&gt; = 1 \times 10^{-6}$</td>
<td>$2 \times 10^{5}$ s</td>
<td>10698 Pa</td>
<td>0.232</td>
</tr>
<tr>
<td>$\Delta &lt;S_w&gt; = 1 \times 10^{-7}$</td>
<td>$2 \times 10^{5}$ s</td>
<td>8398 Pa</td>
<td>0.757</td>
</tr>
</tbody>
</table>

4.4.2 The effect of the equilibrium criterion on the average equilibrium $P_c-S_w$ curve

The strictness of the equilibrium criterion can have an effect on the residual average wetting phase saturation and capillary pressure that can be reached in a simulation. For the purpose of showing this, two simulations performed with the Berentsen model are considered. One simulation uses an equilibrium criterion for the maximum wetting phase flux of $10^{-8}$ m/s, while the other uses the much stricter criterion of $10^{-14}$ m/s. Figure 4.16 shows the obtained arithmetic phase volume averaged $P_c-S_w$ curves for the two simulations. Note that the pressure of the nonwetting phase at the bottom boundary is increased in 300 steps with increments of 100 Pa, and that the simulations represent static primary drainage experiments.
Figure 4.16: $P_c$-$S_w$ curves obtained using a relatively loose and a more strict equilibrium criterion for the maximum wetting phase flux, Berentsen model, simulation of a static primary drainage experiment.

For the same final applied nonwetting phase boundary pressure of 32898 Pa, the two curves reach very different average residual wetting phase saturations and capillary pressures. For the averaged equilibrium $P_c$-$S_w$ curve obtained with an equilibrium criterion of $10^{-8}$ m/s, an average residual saturation of 0.172 and an average capillary pressure of 9187 Pa are attained. However, with an equilibrium criterion of $10^{-14}$ m/s, an average residual saturation as low as 0.105 and an average capillary pressure of 18386 Pa is reached. Note that this residual saturation is very close to the intrinsic residual saturation of the porous medium, which is 0.104.

Thus, using a stricter equilibrium criterion results in an average $P_c$-$S_w$ curve which goes to lower wetting phase saturations and higher capillary pressures. This is also illustrated in Figure 4.17.

Figure 4.17: a) average wetting phase saturation as a function of the applied nonwetting phase boundary pressure for two simulations where a different value for the equilibrium criterion for the maximum wetting phase flux was used (magenta line: eq. criterion $10^{-8}$ m/s blue line: eq. criterion $10^{-14}$ m/s) ; b) average capillary pressure as a function of the applied nonwetting phase bottom boundary pressure for the same set of simulations.
In this figure, the average wetting phase saturation and capillary pressure are plotted as a function of the applied nonwetting phase bottom boundary pressure. As can be seen, at some moment in the simulations the average wetting phase saturation does not decrease any further even though the nonwetting phase pressure at the bottom boundary is increased. However, for a simulation with a stricter equilibrium criterion, the average wetting phase saturation at which this occurs is much lower.

**Figure 4.18:** pressure profiles for different moments in the drainage process after equilibrium is assumed to have been reached, a) equilibrium criterion is $10^{-8}$ m/s, b) equilibrium criterion is $10^{-14}$ m/s.

A similar observation can be made for the average capillary pressure. The dependency of the residual average wetting phase saturation and capillary pressure on the magnitude of the equilibrium criterion is caused by the decreasing relative permeability of the wetting phase
during the drainage process. As the relative permeability of the wetting phase decreases, it becomes more difficult for this phase to flow, and as a result the equilibrium criterion is already reached before the pressure and saturation distributions have equilibrated to the new applied nonwetting phase boundary pressure. Therefore, while a certain magnitude of the equilibrium criterion at high an intermediate wetting phase saturations does result in equilibrium distributions of pressure and saturation when the criterion is met, at lower wetting phase saturations this criterion is no longer sufficient. This is illustrated in Figure 4.18, which shows the pressure distributions in the domain at several moments during the simulations after equilibrium criteria have been met.

When a static equilibrium is reached, pressure distributions will be linear. In case of the wetting phase, it will be equal to the hydrostatic pressure, while in case of the nonwetting phase, it will be equal to the oligostatic pressure (at least after the nonwetting phase reaches the outflow). If the pressure distribution is non-linear, it means that the fluids inside the domain did not have enough time to equilibrate to the new nonwetting phase boundary pressure. As can be seen, when an equilibrium criterion of $10^{-8}$ m/s is used, the wetting phase pressure distribution is non-linear and not equal to the hydrostatic pressure for the applied nonwetting phase boundary pressures of 15051 Pa and 27755 Pa. With an equilibrium criterion of $10^{-14}$ m/s however, only the wetting phase pressure distribution is non-linear and deviating from the hydrostatic pressure for the applied nonwetting phase boundary pressure of 27755 Pa. This shows that the stricter the equilibrium criterion, the longer it takes before equilibrium is reached even when the wetting phase relative permeability decreases. Note that only the wetting phase pressure distribution becomes nonlinear as the simulation progresses, while the nonwetting phase pressure distribution stays linear and attains equilibrium. This is because while the relative permeability of the wetting phase decreases during drainage, the relative permeability of the nonwetting phase increases. Therefore, the nonwetting phase can flow easily and equilibrates to the new boundary pressure well within the time needed for the equilibrium criterion to be met.

A solution for the problem with the equilibrium criterion could be to start using a stricter equilibrium when the relative permeability of the wetting phase or the wetting phase saturation reaches a certain value. In that case, the saturation and pressure distributions are allowed to reach equilibrium even for lower wetting phase relative permeabilities. However, this will increase computation times.

The above discussion shows that care should be taken when discussing and comparing average residual wetting phase saturations obtained from numerical experiments, as these are dependent on the equilibrium criterion used. Consequently, they are not necessarily an intrinsic property of the simulated porous medium.

### 4.5 Determination of the pressure increment

In this section, we investigate the magnitude of the incremental pressure increase which will be added to the nonwetting phase bottom boundary pressure each time after equilibrium in the domain is reached. The pressure increment should have such a value that the equilibrium $P_c - S_w$ curve is resolved in enough detail. However, just as for the mesh size and the equilibrium criterion, computation time (as well as experimental time) increases with decreasing magnitude of the pressure increment.

In order to investigate the appropriate magnitude of the pressure increment, simulations are performed with the Berentsen model for which the magnitude of the pressure increment is varied while all the other variables are kept constant. The mesh size is set to 0.4 mm, while the equilibrium criterion for the maximum of the wetting phase flux is set to $10^{-8}$ m/s. Figure 4.19 shows the resulting average equilibrium capillary pressure-saturation relationships. The
pressures are averaged using the arithmetic phase volume average as defined by Equation (4.19). The average saturation is calculated using Equation (4.21). One of the simulations shown in Figure 4.19 represents a ‘dynamic’ experiment, meaning that the nonwetting phase bottom boundary pressure is increased only once by the large value of 20000 Pa. The points thus plotted in Figure 4.19 for this simulation all are representing dynamic conditions. Note that the differences between the curves for different pressure increments are only related to the dynamic points. The points for which equilibrium is reached all lay on the same curve, which is the averaged equilibrium $P_c$-$S_w$ curve. If the pressure increment is chosen too large, details of the averaged equilibrium $P_c$-$S_w$ curve for high average wetting phase saturations will not be captured. Therefore, a sufficiently small magnitude for the pressure increment has to be chosen, such that the equilibrium $P_c$-$S_w$ curve is resolved. Note that the curves shown in Figure 4.19 all were obtained for simulations using different amounts of pressure increments and magnitude. Therefore, the final applied nonwetting phase boundary pressures are not the same for each simulation. The different average residual saturations for the different simulations that can be observed in the figure merely are a reflection of that.

**Figure 4.19:** averaged equilibrium $P_c$-$S_w$ curves for simulations with different magnitudes of the pressure increments with which the nonwetting phase bottom boundary pressure is increased. Simulations are for a steady-state drainage experiment, performed with the Berentsen model.

Based on Figure 4.19, it is decided to use a pressure increment of the magnitude of 100 Pa for the simulations representing static and steady-state primary drainage experiments. With this magnitude, the equilibrium capillary pressure-saturation relationship is resolved accurately, while computation times are still reasonable.

### 4.6 Comparison between the Berentsen model and MUFTE-UG

In the sections above, several differences between the Berentsen model and MUFTE-UG were discussed. First of all, the two models use different discretisation schemes. The Berentsen model uses a cell-centred finite volume method, while in MUFTE-UG, the BOX-method is
used. A second difference is the equilibrium criterion that the models use. The Berentsen model uses a criterion for the maximum wetting phase flux, while MUFTE-UG uses a criterion for the average change in saturation. In addition, for the Berentsen model, the end of a simulation is reached when the nonwetting phase bottom boundary pressure has been increased by a predefined number of increments. But with MUFTE-UG, the end of a simulation is reached when a predefined time is reached. Finally, the two models use different types of boundary conditions. The Berentsen model uses Dirichlet boundary conditions for the nonwetting phase and the wetting phase at both the top and the bottom of the domain. MUFTE-UG however uses a Neumann boundary condition for the wetting phase in combination with a Dirichlet boundary condition for the nonwetting phase at the bottom of the domain. The boundary conditions at the top of the domain are dependent on the type of simulation performed. For a simulation of a steady state primary drainage experiment, the boundary conditions at the top of the domain are a Dirichlet boundary condition for both the wetting phase and nonwetting phase. In case of the simulation of a static primary drainage experiment, the top boundary conditions are defined by a Dirichlet boundary condition for the wetting phase together with a Neumann boundary condition for the nonwetting phase. Despite the differences between the two models, they do result in comparable average equilibrium $P_c - S_w$ curves. This is shown in Figure 4.20 for the arithmetic phase volume averaged equilibrium $P_c - S_w$ relationships obtained from the simulation of a static primary drainage experiment. The mesh size in these simulations is set to 0.4 mm, while the bottom boundary nonwetting phase pressure is increased with increments of 100 Pa each time equilibrium is reached. For the simulation performed with the Berentsen model, an equilibrium criterion for the maximum wetting phase flux is used of $10^{-8}$ m/s, while for MUFTE-UG an equilibrium criterion for the average change in saturation of $2 \cdot 10^{-6}$ is used. The averaging is performed according to Equation (4.19) and Equation (4.21).

As can be seen, the global shape of the curves is similar.
4.7 Summary and conclusions

In this chapter, preliminary simulations are discussed that have been performed to determine the values of three parameters that are needed to perform simulations of steady-state and static primary drainage experiments. These parameters are the mesh size, the equilibrium criterion, and the magnitude of the pressure increments. The following is concluded:

- A mesh size of 0.4 mm will give numerically accurate results.
- An equilibrium criterion for the maximum wetting phase flux of $10^{-8}$ m/s is chosen to simulate a static or steady-state drainage experiment. For simulations with MUFTE-UG, an equilibrium criterion for the change in average saturation of $2 \cdot 10^{-6}$ is chosen.
- Pressure increments of 100 Pa can be used to simulate a static or steady-state drainage experiment.

In the simulations in the following chapters, these values will be used unless stated otherwise.

The Berentsen model and MUFTE-UG both result in average equilibrium $P_e-S_w$ curves that are more or less the same. In the remainder of this thesis, simulations will predominantly be performed with the Berentsen model. Event though MUFTE-UG is more sophisticated than the Berentsen model, the Berentsen model was used first and for the longest period of time. Therefore, most of the simulations referred to in the coming chapters were already performed with the Berentsen model and due to time limitations they could not be repeated with MUFTE-UG. MUFTE-UG however has been useful in showing that the results obtained with the Berentsen model can also be obtained with a second model. This proves the independence of the results on the numerical model used.
Chapter 5

The average equilibrium $P_c-S_w$ curve for a homogeneous domain

In this chapter, the average equilibrium capillary pressure-saturation relationship for a homogeneous domain will be investigated. In the numerical model described in Chapter 3, a capillary pressure-saturation relationship is needed to close the set of governing equations. Thus, for the simulated porous medium, already a $P_c-S_w$ relationship is specified before the simulation is performed. This $P_c-S_w$ relationship in a way is the ‘true’ or intrinsic capillary pressure-saturation relationship of the porous medium. In this and following chapters, the $P_c-S_w$ relationship specified for the porous medium will be referred to as the ‘input curve’, or the ‘reference curve’. During a simulation, each node inside the numerical domain will have a saturation and capillary pressure that is derived from the input curve. When we want to obtain an average $P_c-S_w$ relationship representing the whole sample, we need to average the capillary pressures and saturations for each node over the whole sample domain. It would be expected that the average equilibrium $P_c-S_w$ curve is equal to the input curve, as the simulations represent a static primary drainage experiment in a homogeneous domain. However, averaging of pressures and saturations can be done in various ways, and this might have an influence on the obtained average equilibrium $P_c-S_w$ relationship. Therefore, in this chapter the following points will be addressed:

- Derivation of an average equilibrium $P_c-S_w$ relationship for a homogeneous domain under static conditions.
- Investigation of different averaging methods.
- Identification and explanation of possible deviations of the average curve from the input curve.

Appendix C provides an overview of the different averaging methods that will be discussed. Table 5.1 provides an overview of the simulations that will be referred to in this chapter.

Table 5.1: overview of simulations referred to in this chapter

| Simulation | 1) static simulation, Berentsen model  
| 300 steps of 100 Pa |
| 2) static simulation, Berentsen model  
| xx steps of 100 Pa  
| No gravity |
| 3) static simulation, MUFTE-UG  
| xx steps of 100 Pa (end of simulation reached at predefined time of $2*10^6$ s)  
| Linear reference curve |
| 4) static simulation, Berentsen model  
| 300 steps of 100 Pa  
| Including gravity  
| Flow of nonwetting phase from top to bottom |
5.1 The concept of averaging

As was discussed in Section 2.1.3, it is desirable to describe processes such as two-phase flow in porous media on the macroscale rather than the microscale. This is because a porous medium, even at the laboratory sample scale, already contains a large number of pores. When such a system is to be solved using microscale relations, these relations need to be solved for every single pore and pore body connecting the pores. For the amount of pores and pore bodies present in a laboratory sample this is not possible, and macroscale equations are needed. These macroscale equations can be derived from the microscale equations by averaging the microscale equations over a Representative Elementary Volume (REV). However, even larger scales than the macroscale exist, and average variables for these scales can be obtained by averaging the macroscale variables. The different scales are illustrated in Figure 5.1 (see also Figure 2.7). For instance, small scale heterogeneities on the order of centimetres can be present at the macroscale, and in order to obtain average variables for a larger scale, the macroscale variables can be averaged over the microscale heterogeneities. Note that in this thesis, upscaling of macroscale variables is performed, as the numerical model itself already is based on macroscale equations. In this case, averaging from the local scale (the nodes inside the sample domain) to the sample scale will be performed. The local scale values for pressure and saturation will be averaged to obtain average values at the sample scale. In Chapter 6, micro-heterogeneities will be introduced at the sample scale, after which the effect of these micro-heterogeneities on the sample-scale average $P_c$-$S_w$ curve can be investigated.

Figure 5.1: The different spatial scales (taken from Manthey, 2006).

5.2 Procedure

The simulations referred to in this chapter are obtained with the Berentsen model, unless stated otherwise. Note that only simulations of static primary drainage experiments are considered. Thus, the nonwetting phase is prevented from leaving the sample at the outflow by the simulation of a hydrophilic membrane.
5.2.1 Domain description and medium properties
The domain and medium properties used for the simulations in this chapter are identical to the domain and medium properties described in Section 4.2.1.

5.2.2 Boundary and initial conditions
The boundary and initial conditions applied in the simulations referred to in this chapter are identical to the conditions introduced in Section 4.2.2 for a static primary drainage experiment.

5.3 Arithmetic volume average and weighted phase volume average
As was mentioned in the introduction, there are several methods to obtain an average capillary pressure for the equilibrium $P_c$-$S_w$ relationship. In this section, the arithmetic volume average pressure and weighted phase volume average pressure will be considered.

The average saturation of a sample domain follows directly from its definition (Equation (2.10)), and is a simple arithmetic mean:

$$\bar{S}_\alpha = \frac{\int n S_\alpha dV}{\int n dV} \quad \alpha = w, n \quad (5.1)$$

In case of a numerical domain with discrete nodes, constant porosity and a uniform mesh, Equation (5.1) can be expressed in terms of a sum over the nodes in the domain, giving:

$$\bar{S}_\alpha = \frac{\sum_{i=1}^{N} S_\alpha^i}{N} \quad \alpha = w, n \quad (5.2)$$

Where $S_\alpha^i$ is the saturation of phase $\alpha$ at node $i$, and $N$ is the total number of nodes in the domain. However, pressures can be averaged in several ways. Two of the possibilities are the arithmetic phase volume and phase volume averages. The arithmetic phase volume average is given by:

$$\bar{P}_\alpha = \frac{\int P_\alpha \eta_\alpha dV}{\int \eta_\alpha dV} \quad \alpha = w, n \quad (5.3)$$

where $\eta_\alpha$ represents an indicator function, defined as:

$$\eta_\alpha = \begin{cases} 
1 & S_\alpha > 0 \\
0 & S_\alpha = 0 
\end{cases}$$

The weighted phase volume average is defined as:
5.3 ARITHMETIC VOLUME AVERAGE AND WEIGHTED PHASE VOLUME AVERAGE

\[ \langle P_\alpha \rangle = \frac{\int n S_\alpha P_\alpha dV}{\int n S_\alpha dV} = \frac{\int n S_\alpha P_\alpha dV}{n S_\alpha V} = \frac{\int n S_\alpha P_\alpha dV}{V_\alpha} \quad \alpha = w, n \] (5.4)

When considering discrete nodes, constant porosity and a uniform mesh, Equations (5.3) can be rewritten as:

\[ \overline{P_\alpha} = \frac{\sum_{i=1}^{N} P_\alpha^i n_\alpha^i}{N_{S_\alpha > 0}} \quad \alpha = w, n \] (5.5)

where \( N_{S_\alpha > 0} \) represents the number of nodes for which the saturation of the \( \alpha \)-phase is larger than zero. Likewise, Equation (5.4) can be rewritten as:

\[ \langle P_\alpha \rangle = \frac{\sum_{i=1}^{N} S_\alpha^i P_\alpha^i}{\sum_{i=1}^{N} S_\alpha^i} \quad \alpha = w, n \] (5.6)

Where \( P_\alpha^i \) is the pressure of phase \( \alpha \) at node \( i \), \( S_\alpha^i \) is the saturation of phase \( \alpha \) at node \( i \), and \( n^i \) represents node \( i \). When the average nonwetting and wetting phase pressures are determined, the average capillary pressure follows from:

\[ \overline{P_c} = \overline{P_\alpha} - \overline{P_w} \] (5.7a)

\[ \langle P_c \rangle = \langle P_\alpha \rangle - \langle P_w \rangle \] (5.7b)

5.3.1 The arithmetic phase volume and phase volume averaged equilibrium capillary pressure-saturation relationship

The averages as defined in Equations (5.2), (5.5), and (5.6) can be used to construct average equilibrium \( P_c-S_w \) curves for the performed simulations. Figure 5.2 shows the resulting curves. As can be seen, both the averaged \( P_c-S_w \) curves show a deviation from the specified reference curve. The arithmetic phase volume averaged curve shows a strong non-monotonic behaviour at high wetting phase saturations. At an average wetting phase saturation of approximately 0.63, the arithmetic phase volume average becomes equal to the reference curve. It can be shown that this average wetting phase saturation is reached when the nonwetting phase reaches the outflow of the sample. For the weighted phase volume average, the non-monotonic behaviour is less strong, but on the whole the weighted phase volume averaged relationship deviates more from the reference curve. The weighted phase volume averaged curve seems to approach the reference curve only at low wetting phase saturations. Thus, the average equilibrium \( P_c-S_w \) curves using an weighted phase volume average or an arithmetic phase volume average to determine the average pressure both deviate from the reference or input curve.
However, there are several reasons why the results of Figure 5.2 seem to be incorrect. First of all, as was mentioned before, it would have been suspected that the averaging would have resulted in exactly the same \( P_c-S_w \) relationship as was put into the model, because the curves are equilibrium curves. As after every time equilibrium is reached, the pressure profiles are linear, and no flow occurs anymore. Therefore the averaging should result in an average capillary pressure that is equal to the reference curve.

In addition, both averaging methods introduce non-monotonic behaviour into the averaged equilibrium \( P_c-S_w \) curve. This non-monotonic behaviour of the average curve cannot be explained in any physical way, as it actually indicates non-physical behaviour of the infiltration front. This can be illustrated by considering the fractional flow formulation of the two-phase flow equation (Equation (2.15), now including sources and sinks), which expresses the two-phase flow equation in terms of saturation (Helmig, 1997):

\[
-\nabla \cdot \left[ \lambda \frac{dP_c}{dS_w} \nabla S_w \right] - \left[ \nu_t \frac{df_w}{dS_w} + (\rho_w g - \rho_n g) \frac{d\lambda}{dS_w} \right] \nabla S_w - n \frac{\partial S_w}{\partial t} - q_w + f_w g = 0
\]

\( \lambda_a \) is the phase mobility,

\[
\lambda_a = \frac{k_{ra}}{\mu_a}
\]

\( \nu_t \) is the total flow velocity,
\( \mathbf{v}_t = \mathbf{v}_w + \mathbf{v}_n \)

\( f_\alpha \) is the fractional flow constant, defined as

\[
f_w = \frac{\lambda_w}{\lambda_w + \lambda_n}, \quad f_n = \frac{\lambda_n}{\lambda_w + \lambda_n}
\]

Finally, \( \lambda^- \) is defined as

\[
\lambda^- = \frac{\lambda_w \lambda_n}{\lambda_w + \lambda_n}
\]

As can be seen, this formulation has identical terms to the transport equation, as it has an advection-diffusion form. The first term in the equation can be considered as a dispersion term, as it contains the divergence of the gradient of the saturation. This also indicates that when \( \frac{dP_c}{dS_w} \) is negative, the saturation front is as is shown in Figure 5.3. The front has a ‘regular’ shape as would be expected as a result of dispersion. However, when \( \frac{dP_c}{dS_w} \) is positive, as would be the case when the \( P_c-S_w \) curve shows non-monotonic behaviour, the saturation front becomes the reverse, which is physically incorrect.

---

**Advection only**

\[ S_n \]

\[ x \]

---

\( \frac{dP_c}{dS_w} < 0 \)

\[ S_n \]

\[ x \]

---

\( \frac{dP_c}{dS_w} > 0 \)

\[ S_n \]

\[ x \]

---

**Figure 5.3**: movement of the front for a) flow when there is only advection; b) flow where there is an advection term and a diffusion term, with \( \frac{dP_c}{dS_w} > 0 \); c) flow where there is an advection term and a diffusion term, with \( \frac{dP_c}{dS_w} < 0 \)
Finally, the obtained averaged $P_c$-$S_w$ curves show a much higher apparent entry pressure than is inherent from the reference curve. If the averaging was correct, then at least the curves should start at an entry pressure close to 6000 Pa, as was put into the model. This is because only slowly the domain will be infiltrated by nonwetting phase, so that node after node will obtain a nonwetting phase saturation larger than zero. When averaging is done, initially all the nodes will have a capillary pressure equal to the entry pressure of the input curve. Then slowly as more and more nodes are infiltrated by the nonwetting phase, the average capillary pressure slowly increases accordingly. However, this is not observed from the arithmetic phase volume averaged and weighted phase volume averaged curves, as they immediately start from a capillary pressure as high as 7000 Pa. Even when the pressure increment size is decreased from 100 Pa to 10 Pa or 1 Pa, such that infiltration is slower and really node after node is infiltrated by the nonwetting phase, the averaged curves are not observed to approach the entry pressure of 6000 Pa, as is shown in Figure 5.4.

The question now is why the arithmetic phase volume and weighted phase volume averaged equilibrium capillary pressure-saturation relationships do not result in an average $P_c$-$S_w$ curve that is equal to the input curve, and why they display non-monotonic behaviour. As a first step, an identical simulation is performed, with the only difference that now the effect of gravity is excluded. This is done by setting the gravimetric acceleration $g$ equal to zero in the simulation. The arithmetic phase volume and phase volume averages are calculated again from equations (5.5) and (5.6). Figure 5.5 shows the resulting averaged $P_c$-$S_w$ curves. As can be seen, for the simulation without gravity, both averaged equilibrium $P_c$-$S_w$ curves become equal to the reference curve. Note that the etwsmall deviations at high water saturations are only points on the average $P_c$-$S_w$ curve that lay in between the equilibrium points (see Figure 4.1). Thus, this simulation shows that the deviation in the average equilibrium $P_c$-$S_w$ curves using arithmetic phase volume and weighted phase volume average is dependent on the presence of gravitational forces.

As a second step, the dependency of the averaged equilibrium $P_c$-$S_w$ curve on the non-linearity of the reference $P_c$-$S_w$ curve is examined. This is done by performing a simulation including gravity, but with a linear capillary pressure-saturation relationship as reference curve. The entry pressure of this reference $P_c$-$S_w$ curve is set to zero Pa, with a slope of 4000 Pa. Note that this simulation was performed with MUFTE-UG.
Figure 5.5: average equilibrium capillary pressure saturation relationships obtained for simulations without gravity \((g = 0)\). Note that the simulations were performed with less than 300 pressure increments of 100 Pa, because the behaviour of the average \(P_c\)-\(S_w\) curve at high wetting phase saturations only is of interest. This is why the obtained \(P_c\)-\(S_w\) curves end already at relatively high average wetting phase saturation (compared to for instance Figure 5.2).

The results of the simulation are shown in Figure 5.6. If the deviation of the averaged equilibrium \(P_c\)-\(S_w\) relationship is due to the non-linearity of the reference \(P_c\)-\(S_w\) curve, using a linear reference curve would result in averaged equilibrium \(P_c\)-\(S_w\) curves that are equal to the reference curve. However, as Figure 5.6 shows, the averaged capillary pressure-saturation relationships for a simulation with a linear reference curve still show a deviation from the reference curve.

Figure 5.6: average equilibrium \(P_c\)-\(S_w\) relationships obtained for a simulation of a static primary drainage experiment including gravity, with a linear input curve. a) using an arithmetic phase volume average to obtain average pressures. Red line: arithmetic phase volume average \(P_c\)-\(S_w\) curve, black line: reference curve; b) using an weighted phase volume average to obtain average pressures. Blue line: weighted phase volume average \(P_c\)-\(S_w\) curve; black line: reference curve.
While the arithmetic phase volume averaged $P_c$-$S_w$ curve only shows a deviation from the linear reference curve before the nonwetting phase reaches the outflow of the sample (which occurs around an average wetting phase saturation of 0.88), the weighted phase volume averaged curve shows a deviation throughout the saturation range, though it is strongest at high wetting phase saturations.

The observation that for the arithmetic phase volume average $P_c$-$S_w$ curve the deviation from the reference curve only occurs before the nonwetting phase reaches the outflow, suggests that the deviation has something to do with the presence of an infiltration front. This is further investigated by plotting the nonwetting and wetting phase pressures as a function of saturation for each node in the domain at a certain moment in the drainage process. Figure 5.7 shows the obtained plots. In Figure 5.7a, the nonwetting and wetting phase pressures and saturations for the nodes are plotted for the simulation using a linear reference curve. The points are plotted after equilibrium is reached at an applied nonwetting phase bottom boundary pressure of 9398 Pa. In Figure 5.7b, the nonwetting phase pressures and saturations for the nodes are plotted for the simulation using the non-linear Brooks-Corey $P_c$-$S_w$ relationship as reference curve. The values for the nodes are plotted after equilibrium is reached at an applied nonwetting phase bottom boundary pressure of 8098 Pa.

In addition, the arithmetic phase volume averaged nonwetting and wetting phase pressures, as well as the capillary pressure obtained from these are plotted. These averages thus are obtained by applying equation (5.2) and (5.5) to the values for the pressures of the nodes as shown in Figure 5.7.

As can be seen, in both Figure 5.7a and 5.7b, there are still some nodes that are not infiltrated by the nonwetting phase, as they have a wetting phase saturation of one. However, these nodes do show a varying nonwetting and wetting phase pressure, because before a node is infiltrated by the nonwetting phase, the pressures in that node are specified as:

$$P_n^j = P_d + \rho_w g (h - z^j)$$  \hspace{1cm} (5.9a)

$$P_w^j = \rho_w g (h - z^j)$$  \hspace{1cm} (5.9b)
Where $z_i$ is the height of node $i$, and $h$ is the total domain height.

When we look at the averaged pressures, it can be noted that the arithmetic phase volume averaged wetting phase pressure is positioned in the middle of the range of wetting phase pressures covered by the nodes, as would be expected when taking the arithmetic average. However, for the nonwetting phase, the arithmetic phase volume averaged phase pressure lies well above the center of the range of nonwetting phase pressures covered by the nodes. As a result, the capillary pressure derived by subtracting the average wetting phase pressure from the average nonwetting phase pressure, is overestimated. This is also shown in Figure 5.7.

The reason for the overestimation of the arithmetic phase volume average nonwetting phase pressure is very simple. It is due to the way the arithmetic phase volume average is defined:

$$\bar{P}_\alpha = \frac{\sum_{\alpha=1}^{N} p_{\alpha}^n \eta_{\alpha}}{N_{S_n>0}}$$

(5.10)

Defined this way, the average pressures for wetting and nonwetting phase are calculated over different parts of the domain. The arithmetic phase volume average nonwetting phase pressure is calculated by only including nodes for which the nonwetting phase saturation is larger than zero. Before the nonwetting phase reaches the outflow of the sample, there is only a part of the column for which the nonwetting phase saturation is larger than zero, as the infiltration front has not yet reached the outflow of the column. However, the arithmetic phase volume average wetting phase pressure is calculated including nodes for which the wetting phase saturation is larger than zero. As the column is initially fully saturated with the wetting phase, all the nodes are always included when the wetting phase average pressure is calculated. In addition, the wetting phase saturation also is calculated including all the nodes in the domain. This difference in averaging window is illustrated in Figure 5.8b.

![Figure 5.8](image-url)

**Figure 5.8**: Arithmetic phase volume average pressures before the nonwetting phase has reached the domain outflow. Thus, not all nodes have been invaded yet by the nonwetting phase, and still have a wetting phase saturation of 1. a) the pressure distribution inside the sample after equilibrium is reached when the nonwetting phase infiltration front is moving through the sample. b) the averaging windows for $P_n$, $P_w$, $S_n$, and $S_w$. 
As Figure 5.8 shows, the average nonwetting phase pressure is determined by taking only those nodes into account for which nonwetting phase is actually present. For all the other averages however, calculations are done including all the nodes of the domain. Figure 5.8a shows the pressure distribution inside the sample after equilibrium is reached when the nonwetting phase infiltration front is moving through the sample. In this case, the pressure distribution is assumed to be linear. For the wetting phase, the pressure will obtain a hydrostatic distribution after static equilibrium is reached. For the nonwetting phase, the pressure distribution is oligostatic in addition to the pressure that is applied at the inflow boundary in case of a drainage experiment. For the parts of the column where no nonwetting phase is present, the nonwetting phase pressure is equal to the hydrostatic pressure plus the entry pressure of the porous medium. Note that this is artificial as in reality, when there is no nonwetting phase, the nonwetting phase pressure is undefined. Thus, the pressure distributions are given by:

\[
\begin{align*}
P_n(z) &= P_n^{\text{bottom}} - \rho_n g z_{\text{front}} \\
\text{if } S_n > 0 \\
\end{align*}
\]

\[
\begin{align*}
P_w(z) &= \rho_w g (h - z_{\text{front}}) \\
\end{align*}
\]

\[
\begin{align*}
P_s(z) &= P_d + \rho_w g (h - z') \\
\text{if } S_n = 0 \\
\end{align*}
\]

\[
\begin{align*}
P_{\alpha}(z) &= \rho_w g (h - z') \\
\end{align*}
\]

The arithmetic phase volume average wetting phase pressure is determined by averaging over all the nodes, giving rise to \( \overline{P_w} \) in Figure 5.8. On the other hand, the arithmetic phase volume nonwetting phase pressure is determined by averaging over the nodes for which \( S_n > 0 \), giving rise to \( \overline{P_n} \) Figure 5.8. As can be seen, the capillary pressure determined based on these average pressures will be larger than the capillary pressure derived from averages over identical averaging windows. The same is true for the weighted phase volume averaged pressures. Summarizing, the reason for the deviation of the arithmetic phase volume and weighted phase volume average \( P_c-S_w \) curve from the reference curve is the difference in averaging window when averaging the pressures and saturations according to Equation (5.2), (5.5) and (5.6). This is due to the presence of an infiltration front. Below this front, a two-phase system is present, while above it a single-phase system is present. Note that this deviation will be strongest in a vertical column, and only occurs if gravity forces are taken into account. Based on the above observations, new averages can be proposed that only average over that part of the column which is already infiltrated by the nonwetting phase (i.e. which is a two-phase system). In this case, the arithmetic phase volume average pressures become:

\[
\overline{P_{\alpha}}_{\text{new}} = \frac{\sum_{i=1}^{N} P_{\alpha}(S_n^i > 0)}{N_{S_n>0}} \tag{5.12}
\]

The weighted phase volume average pressures become:
5.3 ARITHMETIC VOLUME AVERAGE AND WEIGHTED PHASE VOLUME AVERAGE

\[
\langle P_\alpha \rangle_{\text{new}} = \frac{\sum_{i=1}^{N} S'^i_\alpha P'^i_\alpha (S'_n > 0)}{\sum_{i=1}^{N} S'_n (S'_n > 0)} \tag{5.13}
\]

Finally, the saturation also needs to be averaged only over that part of the domain for which
the nonwetting phase is present:

\[
\overline{S'_\alpha}_{\text{new}} = \frac{\sum_{i=1}^{N} S'^i_\alpha (S'_n > 0)}{N_{S'_n > 0}} \tag{5.14}
\]

The new averaging windows and capillary pressure are illustrated in Figure 5.9. As can be
seen, now the arithmetic phase volume averaged wetting phase pressure is determined only
over that part of the column for which the nonwetting phase is present. The same is true for
the saturations. As a result, the new average capillary pressure is smaller than the capillary
pressure as it was determined before.

Figure 5.9: a) now the wetting phase pressure is also determined by averaging only over the nodes for
which \(S'_n > 0\). This gives rise to the new arithmetic phase volume average \(\langle P_\alpha \rangle_{\text{new}}\). As can be seen, the
capillary pressure derived from using these averaged pressures is smaller than the ‘old’ capillary
pressure. b) the averaging window for \(P_n, P_w, S_n, \) and \(S_w\) now is equal in size for each variable.

Figure 5.10 shows the resulting averaged equilibrium capillary pressure-saturation
relationships for the linear reference curve, while Figure 5.11 shows the new averaged
equilibrium \(P_c - S_w\) relationships for the non-linear Brooks-Corey reference curve.
Figure 5.10: Average equilibrium capillary pressure-saturation relationships obtained for a simulation using a linear reference curve; a) new arithmetic phase volume average $P_c$-$S_w$ relationship; b) new weighted phase volume average $P_c$-$S_w$ relationship.

Figure 5.11: Average equilibrium capillary pressure-saturation relationships obtained for a simulation using the non-linear Brooks-Corey reference curve; a) new arithmetic phase volume average $P_c$-$S_w$ relationship; b) new weighted phase volume average $P_c$-$S_w$ relationship.

Note that as the nonwetting phase front is moving through the sample, the averaging window changes. Only after the nonwetting phase reaches the outflow boundary of the sample, everywhere in the domain the nonwetting phase saturation has become larger than zero, and averaging will be performed over the whole domain length. This is illustrated in Figure 5.12 for the arithmetic phase volume average over the two-phase domain.

As can be seen from Figure 5.10 and 5.11, the ‘new’ arithmetic phase volume average results in an average equilibrium capillary pressure-saturation relationship which is almost identical to the reference curve. However, the ‘new’ weighted phase volume average still gives rise to a deviation in the average equilibrium $P_c$-$S_w$ relationship from the reference curve. This can be explained by the fact that in order to obtain the weighted phase volume average pressure, the pressure is weighted by saturation.
Figure 5.12: the arithmetic phase volume average over that part of the domain for which $S_n>0$. This causes the averaging window to change according to the movement of the nonwetting phase infiltration front. This is illustrated by the numbers in the Figure, which indicate the number of nodes over which the averaging is performed. Only after the nonwetting phase reaches the outflow, averaging occurs over the whole domain (i.e. over 455 nodes).

Figure 5.13: a) pressure distribution in the sample at an applied nonwetting phase bottom boundary pressure of 8450 Pa; b) saturation distribution in the sample at an applied nonwetting phase bottom boundary pressure of 8450 Pa; c) distribution of pressure weighted by saturation ($S_n P_n$) at an applied nonwetting phase bottom boundary pressure of 8450 Pa.
In Figure 5.13, the terms $S_w P_w$ and $S_n P_n$ are plotted against the column height for a moment in the drainage process when the nonwetting phase front has reached approximately halfway of the column, and the fluids have reached an equilibrium distribution. As can be seen, both the nonwetting and wetting phase pressure have attained a linear distribution. However, the saturation distribution is non-linear, so that when the pressures are weighted with the saturations, a non-linear profile results. This non-linearity causes the weighted phase volume average capillary pressure to deviation from the reference curve. In addition, it explains why the intrinsic phase averaged $P_c-S_w$ curve does not become equal to the reference curve even after the nonwetting phase reaches the outflow, as the saturation profile remains non-linear.

Note that when gravity is absent, as is the case in Figure 5.5, the weighted phase volume average does result in an average $P_c-S_w$ curve that is close to the reference curve. This is because without gravity, the saturation will be the same throughout the column when equilibrium is reached.

In Section 5.5, a new averaging method is discussed, proposed by Nordbotten et al (2007). This averaging method calculates a new macroscale average pressure from the traditional weighted phase volume average pressure.

### 5.3.2 Scale dependency of average equilibrium $P_c-S_w$ relationship

As was shown in Section 5.3.1, the traditional arithmetic phase volume and weighted phase volume averages result in deviations of the average equilibrium $P_c-S_w$ relationship from the reference curve. These deviations are related to gravity forces, and can be shown to be scale dependent. When obtaining an average equilibrium $P_c-S_w$ curve for different averaging length scales, it becomes clear that with increasing averaging length scale, the deviation of the averaged $P_c-S_w$ curve becomes stronger. This is illustrated in Figure 5.15, for the traditional arithmetic phase volume and weighted phase volume averages. Figure 5.14 shows the different averaging length scales referred to in Figure 5.15 and 5.16.

![Figure 5.14: Different averaging windows referred to in Figure 5.15 and 5.16](image)

Figure 5.16 shows the average $P_c-S_w$ curves obtained using the new arithmetic phase volume and phase volume averages (Equations (5.12), (5.13), and (5.14)) for varying averaging length scale. The new arithmetic phase volume averaged equilibrium $P_c-S_w$ curve is independent of
the averaging window used. On the other hand, the new weighted phase volume averaged equilibrium \( P_c-S_w \) curve still changes according to the averaging window.

Thus, for the traditional arithmetic phase volume and weighted phase volume averages, with increasing averaging length scale the deviation from the reference curve becomes stronger. This is due to the increasing influence of the gravity forces on these averaging methods. A quantification of the deviation related to these gravity forces will be given in the next section.

![Figure 5.15: Average \( P_c-S_w \) relationships obtained for a simulation of a static primary drainage experiment, using different averaging windows; a) arithmetic phase volume average \( P_c-S_w \) curves; b) weighted phase volume average \( P_c-S_w \) curves](image)

![Figure 5.16: Average \( P_c-S_w \) relationships obtained for a simulation of a static primary drainage experiment using different averaging windows; a) ‘new’ arithmetic phase volume average \( P_c-S_w \) curves; b) ‘new’ weighted phase volume average \( P_c-S_w \) curves](image)

### 5.3.3 Influence of gravity forces

In this section, the influence of gravity forces will be investigated. As was already shown in Section 5.3.2, the deviation of the arithmetic phase volume and weighted phase volume averaged equilibrium \( P_c-S_w \) relationship is dependent on the averaging length scale. This
directly has to do with the dependency on gravity forces. With increasing averaging length scale, the gravity forces become more important and the deviation becomes larger.

In this section a correction term is proposed for the arithmetic phase volume and weighted phase volume averaging methods as described in Equation (5.5) and (5.6). This correction term gives an indication of the order of error that is caused by using these averaging methods. The influence of the gravity forces can be derived in several ways, each giving rise to the same result:

- When considering Figure 5.9, we can say that the difference between the average capillary pressure determined through arithmetic phase volume or weighted phase volume averaging and the average capillary pressure determined with the new arithmetic phase volume and weighted phase volume averages is equal to:

  $$\Delta P_c = \langle P_c \rangle_{\text{old}} - \langle P_c \rangle_{\text{new}}$$  \hspace{1cm} (5.15)

  The figure shows that this difference is equal to the ‘new’ average wetting phase pressure minus the traditionally averaged wetting phase pressure:

  $$\Delta P_c = \langle P_w \rangle_{\text{new}} - \langle P_w \rangle_{\text{old}}$$  \hspace{1cm} (5.16)

  The wetting phase pressure distribution is assumed to be linear and hydrostatic when equilibrium in the sample is reached, so that the average wetting phase pressures can be derived directly from the linear wetting phase distribution:

  $$\langle P_w \rangle_{\text{new}} = \rho_w \frac{g}{2} \left( h - \frac{1}{2} z_{\text{front}} \right)$$  \hspace{1cm} (5.17)

  $$\langle P_w \rangle_{\text{old}} = \frac{1}{2} \rho_w gh$$  \hspace{1cm} (5.18)

  where $\rho_w$ is the density of the wetting phase, $h$ is the height of the domain, and $z_{\text{front}}$ is the height of the nonwetting phase front.

  Thus, the deviation of the arithmetic phase volume averaged equilibrium capillary pressure can be described by:

  $$\Delta P_c = \rho_w g \left( h - \frac{1}{2} z_{\text{front}} \right) - \frac{1}{2} \rho_w gh = \frac{1}{2} \rho_w g \left( h - z_{\text{front}} \right)$$  \hspace{1cm} (5.19)

  Another way of determining the influence of gravity forces is to look at the definitions of the traditional arithmetic phase volume averaged capillary pressure and the new arithmetic phase volume averaged capillary pressure:
\[
\bar{P}_c = \frac{\sum_{i=1}^{N} P_{n}^i (S_{n}^i > 0)}{\sum_{i=1}^{N} n^i (S_{n}^i > 0)} - \frac{\sum_{i=1}^{N} P_{w}^i (S_{w}^i > 0)}{\sum_{i=1}^{N} n^i (S_{w}^i > 0)} \tag{5.20}
\]

\[
\bar{P}_{c\text{new}} = \frac{\sum_{i=1}^{N} P_{n}^i (S_{n}^i > 0)}{\sum_{i=1}^{N} n^i (S_{n}^i > 0)} - \frac{\sum_{i=1}^{N} P_{w}^i (S_{w}^i > 0)}{\sum_{i=1}^{N} n^i (S_{w}^i > 0)} \tag{5.21}
\]

which gives

\[
\Delta \bar{P}_c = \bar{P}_c - \bar{P}_{c\text{new}} = \frac{\sum_{i=1}^{N} P_{n}^i (S_{n}^i > 0)}{\sum_{i=1}^{N} n^i (S_{n}^i > 0)} - \frac{\sum_{i=1}^{N} P_{w}^i (S_{w}^i > 0)}{\sum_{i=1}^{N} n^i (S_{w}^i > 0)} \tag{5.22}
\]

The wetting phase pressure is assumed to be linear and hydrostatic after each time equilibrium is reached, such that it can be expressed in terms of hydrostatic pressure. This gives for $\Delta \bar{P}_c$ the following expression:

\[
\Delta \bar{P}_c = \frac{\sum_{i=1}^{N} \rho \left(h - z^i\right) (S_{n}^i > 0)}{\sum_{i=1}^{N} n^i (S_{n}^i > 0)} - \frac{\sum_{i=1}^{N} \rho \left(h - z^i\right) (S_{w}^i > 0)}{\sum_{i=1}^{N} n^i (S_{w}^i > 0)} \tag{5.23}
\]

Following a similar approach for the weighted phase volume average, the correction becomes:

\[
\Delta \langle \bar{P}_c \rangle = \frac{\sum_{i=1}^{N} \rho \left(h - z^i\right) S_{n}^i (S_{n}^i > 0)}{\sum_{i=1}^{N} S_{n}^i (S_{n}^i > 0)} - \frac{\sum_{i=1}^{N} \rho \left(h - z^i\right) S_{w}^i (S_{w}^i > 0)}{\sum_{i=1}^{N} S_{w}^i (S_{w}^i > 0)} \tag{5.24}
\]

Both expressions for $\Delta \bar{P}_c$ result in the same correction of the traditional arithmetic and weighted phase volume averages. Now we can check this correction by subtracting $\Delta \bar{P}_c$ from the arithmetic and weighted phase volume averaged equilibrium $P_c-S_w$ curves. Note that in order to get good results, we should plot the corrected pressures as a function of the average saturation over the two-phase domain only, which can be calculated from Equation (5.14). The result is shown in Figure 5.17. As can be seen, the correction term completely accounts for the deviation of the arithmetic phase volume average equilibrium $P_c-S_w$ relationship. For the weighted phase volume average equilibrium $P_c-S_w$ curve, the correction term reduced the deviation to the part that is not due to gravity forces. Applying the correction term results in
the same averaged curve that is obtained by averaging over the part of the domain that is a two-phase system.

\[ P_{c-S_w} \text{ curve, static simulation, arithmetic phase volume average} \]

\[ P_{c-S_w} \text{ curve, static simulation, weighted phase volume average} \]

Figure 5.17: Average \( P_{c-S_w} \) curves obtained for the simulation of a static primary drainage experiment, a) the arithmetic phase volume average \( P_{c-S_w} \) curve and the curve obtained when subtracting \( \Delta P_c \) from this curve; b) the weighted phase volume average \( P_{c-S_w} \) curve and the curve obtained when subtracting \( \Delta P_c \) from this curve.

The correction term \( \Delta P_c \) determined above shows that the deviation is linearly related to gravity forces, due to the occurrence of the gravitational acceleration. Moreover, as was already shown in Section 5.3.2, the deviation is length scale dependent. Note that \( h \) refers to the length over which the averaging is performed.

5.3.4 The averaged \( P_{c-S_w} \) curve for a dynamic simulations

The results discussed above where all obtained for a simulation that used pressure increments of 100 Pa, and as a result the obtained capillary pressure-saturation relationship can be assumed to represent the equilibrium \( P_{c-S_w} \) relationship. The different kind of averages however can also be applied to obtain average capillary pressure-saturation relationships that are not equilibrium curves. Figure 5.18 shows the obtained averaged capillary pressure-saturation curves for pressure increments of 100, 5000, 10000, and 20000 Pa.

Note that the larger the pressure increment, the further from equilibrium the system will be. As can be seen, for the traditional arithmetic phase volume and weighted phase volume averaged capillary pressure-saturation relationships, the larger the pressure increment, the larger the deviation is from the reference curve. However, the new arithmetic phase volume average again results for all cases in an average \( P_{c-S_w} \) curve that is equal to the reference curve.

The deviation from the reference curve obtained by using arithmetic phase volume and weighted phase volume averaging was quantified in Section 5.3.3 by assuming a hydrostatic wetting phase pressure distribution. However, this does not hold for the simulations performed under dynamic conditions (i.e. a large pressure increase of 10-20 kPa at once) because then the wetting phase pressure distribution is non-linear and not hydrostatic. This is illustrated in Figure 5.19, which shows the averaged wetting phase pressure as a function of time for the different simulations.
Figure 5.18: Average $P_c - S_w$ relationships obtained for the simulations of ‘dynamic’ experiments, using pressure increments of 20000 Pa, 10000 Pa, 5000 Pa, and 100 Pa. a) arithmetic phase volume average; b) weighted phase volume average; c) ‘new’ arithmetic phase volume average; d) new weighted phase volume average.

Figure 5.19: Wetting phase pressure in the middle of the column as a function of time, for the simulations using different pressure increments of 2000 Pa, 10000 Pa, 5000 Pa, 2000 Pa.
As can be seen from Figure 5.19, the wetting phase pressure at the middle of the column is no longer equal to the hydrostatic pressure for simulations that use pressure increments of 2000 Pa and larger. Therefore, the deviation of the averaged $P_c$-$S_w$ curve from the reference curve is not equal to the correction terms suggested in Equation (5.23) and (5.24), which assumes a hydrostatic pressure distribution of the wetting phase.

### 5.4 The centroid phase average

In Section 5.3.2, it was shown that even when the weighted phase volume average is used only on that part of the domain that is a two-phase system, the weighted phase volume average $P_c$-$S_w$ curve does not become equal to the reference curve (see Figure 5.11b). Thus, part of the deviation observed when using weighted phase volume averaging must be due to something other than gravity forces. In order to investigate this further, in this section the centroid phase average is used to determine an average equilibrium $P_c$-$S_w$ relationship. The same simulation is used as in Section 5.3.

The centroid phase average pressure was introduced by Nordbotten et al. in 2007. They noted that in the two-phase expression of Darcy’s law, it is not clear what exactly the macroscale pressure is. Traditional deviations of the macroscale Darcy’s law from the microscale Stokes equation always use volume averaging methods. By doing this, it is assumed that the macroscale pressure is represented by an intrinsic phase average pressure. However, in these deviations, several assumptions are made which create restrictions on the use of Darcy’s law. For instance, Nordbotten et al. (2007) showed that in case of gradients in fluid distribution and pressure, the weighted phase volume average can lead to untraditional gravitational forces in Darcy’s law. They showed that the gravitational forces became spatially dependent. Therefore, Nordbotten et al. perform an analysis, which shows that the macroscale pressure does not equal the weighted phase volume average pressure unless sub-scale heterogeneities, either in material properties or fluid distribution, are absent. They derive a family of macroscale pressures $[P_\alpha]_n$, where $n$ refers to the order of the approximation to a smooth macroscale function $[P_\alpha]$. The approximations take the form:

\[
[P_\alpha]_0 = \langle P_\alpha \rangle \\
[P_\alpha]_1 = \langle P_\alpha \rangle + \frac{1}{V\langle z_\alpha \rangle} (z - \langle z_\alpha \rangle) \cdot \nabla \langle P_\alpha \rangle \\
[P_\alpha]_N = \langle P_\alpha \rangle + \sum_{k=1}^{N} C^{(k)}_{k,N} \frac{\partial}{\partial z} \langle P_\alpha \rangle
\]

where $C^{(k)}_{k,n}$ is a tensor of coefficients. $<z_\alpha>$, the average coordinate $z$, is the centroid of the phase. As can be seen, the zeroth order approximation to the macroscale pressure results in the weighted phase volume averaged pressure $<P_\alpha>$. The first order approximation is equal to the weighted phase volume averaged pressure, corrected for the distance between the centroid of the phase and the centroid of the averaging volume. Note that the centroid of the phase, $z$, is in this case equal to the middle of the domain, thus $z = 0.091$ m.

In this section, we will determine the first order approximation of the macroscale pressure. In addition to the weighted phase volume averaged pressure, this requires the determination of
the phase volume average coordinate \( z_\alpha \), and the derivatives of the weighted phase volume average pressure and average coordinate \( z \).

The average coordinate \( z \) can be calculated the same way as the weighted phase volume average pressure is calculated:

\[
\langle z_\alpha \rangle = \frac{\sum_{i=1}^{N} z_i \left( S_i^\alpha > 0 \right) S_i^\alpha}{\sum_{i=1}^{N} S_i^\alpha}
\]

\( \alpha = w, n \) (5.28)

Thus, the weighted phase volume averaged coordinate \( z \) is dependent on the phase for which we want to determine the macroscale pressure.

The derivatives of the weighted phase volume averaged pressure and coordinate can be determined as follows (Nordbotten, personal communication):

\[
\nabla \langle \omega \rangle = \frac{\langle S_\alpha \omega \rangle}{\langle S_\alpha \rangle}
\]

\[
= -\frac{\nabla S_\alpha}{S_\alpha^2} \langle S_\alpha \omega \rangle + \frac{1}{S_\alpha} \nabla \langle S_\alpha \omega \rangle
\]

\[
= -\frac{\nabla S_\alpha}{S_\alpha} \langle \omega \rangle + \frac{1}{S_\alpha} \int_{\bar{V}} \mathbf{n} \cdot \langle S_\alpha \omega \rangle dA
\]

\[
= \frac{1}{S_\alpha V} \left[ -\langle \omega \rangle \int_{\bar{V}} \mathbf{n} \cdot S_\alpha dA + \int_{\bar{V}} \mathbf{n} \cdot (S_\alpha \omega) dA \right]
\]

For this particular situation of a 1-D homogeneous vertical domain, this can be written as:

\[
\nabla \langle \omega \rangle = \frac{1}{S_\alpha V} \left[ -\langle \omega \rangle (S_{\alpha \text{top}} - S_{\alpha \text{bottom}}) + (S_{\alpha \text{top}} \omega_{\text{top}} - S_{\alpha \text{bottom}} \omega_{\text{bottom}}) \right]
\]

(5.30)

where \( \omega \) represents the variable for which we need the derivative, \( \langle \omega \rangle \) is the weighted phase volume average of \( \omega \), and \( S_\alpha \) is the saturation of the phase under consideration. The superscripts top and bottom refer to the value of the variable at the top and the bottom of the domain, respectively. Furthermore, \( V \) is the volume of the domain, which in this case is equal to the length of the averaging domain, as we are considering a 1-D situation.

Now, the centroid phase averaged pressures can be calculated from Equation (5.26). When these are plotted against the average wetting phase saturation as defined in Equation (5.2), the centroid phase averaged equilibrium capillary pressure-saturation relationship is obtained. Figure 5.20 shows the resulting curve. As can be seen, the centroid phase average capillary pressure-saturation curve lies close to the reference curve for wetting phase saturations below 0.9. For wetting phase saturations between 0.9 and 1.0 however, the curve shows smaller capillary pressure, which even becomes negative when a wetting phase saturation of 1.0 is approached. On closer examination, the average curve starts at a capillary pressure of approximately 5000 Pa, after which it drops to \(-3000\) Pa.
The average equilibrium PC-Sw curve for a homogeneous domain

Figure 5.20: the centroid phase averaged capillary pressure-saturation relationship. The complete relationship showing the deviation of the centroid phase average curve from the reference curve at high wetting phase saturations (i.e. early in drainage process).

Figure 5.21: centroid phase averaged nonwetting and wetting phase pressures as a function of average wetting phase saturation.

Figure 5.21 shows the centroid phase averaged nonwetting and wetting phase pressures as a function of the average wetting phase saturation. As can be seen, the reason for the sudden decrease in the averaged capillary pressure curve of Figure 5.20 is due to the centroid phase...
averaged nonwetting phase pressure. At a wetting phase saturation just below one, this pressure initially is 6000 Pa, but drops suddenly to –2500 Pa when the wetting phase saturation decreases a little but further.

This can be explained as follows. As the nonwetting phase infiltrates the domain, the weighted phase volume average coordinate $z$ for the nonwetting phase increases starting from zero (Figure 5.22a). Moreover, the derivative of the weighted phase volume average coordinate for the nonwetting phase (Figure 5.22b) also starts increasing from zero. However, the initially very small values for this derivative result in a very large correction term for the weighted phase volume average nonwetting phase pressure, due to the term $(\nabla \langle z_\alpha \rangle)^{-1}$ in Equation (5.26). This correction term is negative due to the negative derivative of the weighted phase volume average nonwetting phase pressure (Figure 5.22c). Thus, this very large negative correction to the traditional weighted phase volume average at averaging wetting phase saturations just below one leads to a low centroid phase average nonwetting phase pressure, which even becomes negative.

Concluding, the centroid phase average corrects the deviation from the reference curve that was observed when using the weighted phase volume averaging method. Results are best for an average wetting phase saturation below 0.9.

Figure 5.22: a) $\langle z \rangle_\alpha$ as a function of average wetting phase saturation, b) $\nabla \langle z \rangle$ as a function of average wetting phase saturation, static simulation, c) $\nabla \langle P \rangle_\alpha$ as a function of average wetting phase saturation, static simulation.
5.5 Simple arithmetic average

The different averages introduced for capillary pressure and saturation in the sections above are not the simplest average over the domain that can be determined, as they include averaging of pressures and/or saturations over part of the domain. The most simple average however would be to average both pressures and saturations over the whole domain, regardless whether a phase is present or not. This simple arithmetic average can be defined as:

\[
\langle P^i \rangle_{\text{whole domain}} = \frac{\sum_{i=1}^{N} P^i}{N}
\]

(5.31)

\[
\langle S^i \rangle_{\text{whole domain}} = S = \frac{\sum_{i=1}^{N} S^i}{N}
\]

(5.32)

The resulting average \( P_c-S_w \) curve is shown in Figure 5.23. As can be seen, the obtained curve is situated close to the reference curve. Thus, a simple arithmetic average over the whole domain returns good results.

With the simple arithmetic average (Equation (5.31) and (5.32)), the pressures are averaged over the whole domain, including the part that has not yet been infiltrated by the nonwetting phase before the nonwetting phase reaches the outflow of the sample. In this part, the nonwetting phase pressure actually is non-existent as there is no nonwetting phase. However, in the numerical simulations, the nonwetting phase pressure in the part of the domain that is
not yet infiltrated by the nonwetting phase is set equal to the wetting phase pressure plus the entry pressure:

\[ P_n(S_n = 0) = P_d + P_w \]  \hspace{1cm} (5.33)

This is an artefact from the used Brooks-Corey parameterisation, which prescribes that the capillary pressure is equal to the entry pressure of the porous medium if the wetting phase saturation is equal to one, which occurs when the capillary pressure is smaller than the entry pressure:

\[ P_c^i = P_n^i - P_w^i = P_d \quad \text{if} \quad P_c^i < P_d \]  \hspace{1cm} (5.34)

In reality however, the capillary pressure is not defined when the non-wetting phase is not present. Therefore, another average is investigated in which the capillary pressure at a node is set equal to zero if the nonwetting phase is not present. Thus:

\[ P_c^i = 0 \quad \text{if} \quad P_c^i < P_d \]  \hspace{1cm} (5.35)

which gives

\[
P_n^i = \begin{cases} 
P_w^i & \text{if } S_n = 0 \\ 
P_n^{i,\text{simulation}} & \text{if } S_n > 0 
\end{cases} \]  \hspace{1cm} (5.36)

\[ P_w^i = P_w^{i,\text{simulation}} = \rho_w g z^i \]

The two different types of averaging are illustrated in Figure 5.24. The resulting equilibrium capillary pressure-saturation curve is shown in Figure 5.25.

Figure 5.24: Two different methods to perform a simple arithmetic average over the whole domain. a) for the part of the column that is a single phase domain, use the nonwetting phase pressure based on the simulations results; b) for the part of the column that is a single phase domain, set \( P_n = P_w = \rho_w g z \)
The average equilibrium PC-Sw curve for a homogeneous domain

Figure 5.25: Average capillary pressure-saturation relationship obtained for the simulation of a static primary drainage experiment, using a simple arithmetic average, assuming $P_c = 0$ for the nodes that have not yet been infiltrated by the nonwetting phase.

As can be seen, before the nonwetting phase reaches the outflow, which happens around an average wetting phase saturation of approximately 0.63, the equilibrium capillary pressure-saturation relationship lies below the reference curve, going towards zero Pa at a wetting phase saturation of one. This is also to be expected as in a single phase system, both the nonwetting phase and wetting phase have a hydrostatic pressure distribution, so that the capillary pressure is zero. Thus, this averaging method also results in a deviation from the reference curve, although now it is a negative deviation. Again, the deviation is dependent on the length scale of averaging, as is shown in Figure 5.26, where the averaging window is chosen according to Figure 5.14.

Figure 5.26: Average capillary pressure-saturation relationship obtained for the simulation of a static primary drainage experiment, using a simple arithmetic average that assumes $P_c = 0$ when $S_w = 0$. Average $P_c$-$S_w$ curves are plotted for different averaging windows.
5.6 Global average

In the laboratory determination of $P_c$-$S_w$ curves, as was described in Section 2.3.4, usually the capillary pressure is determined by measuring the wetting phase and/or nonwetting phase pressure with pore pressure transducers situated in the fluid reservoirs connected to the sample. In this section, it will be shown that this method can result in an overestimation of the residual wetting phase saturation, even though for high and intermediate average wetting phase saturations good results are obtained.

The global average pressure can be defined as:

$$\langle P_c \rangle^{\text{global}} = P_n^{\text{reservoir}} - P_w^{\text{reservoir}}$$

which for this particular situation becomes:

$$\langle P_c \rangle^{\text{global}} = P_n^{\text{bottom}} - P_w^{\text{top}}$$

However, this can lead to erroneous results in case of a vertical column of considerable length, as is illustrated in Figure 5.27.

Figure 5.27: pressure distribution inside the domain after equilibrium is reached. Note that the pressure distribution shown here is the one that is assumed by the numerical model, which assumes that when the nonwetting phase is not present, still there is a nonwetting phase pressure that is equal to: $P_n(S_n = 0) = P_d + \rho_w g z$. 
This is because usually, the reservoirs are at different levels. In that case, the obtained global average capillary pressure should be corrected for gravitational forces. This can be done by calculating the average capillary pressure over the part of the column being a two-phase system \((z < z_{\text{front}})\) from the top and bottom pressures and assuming linear pressure distributions inside the sample. The corrected global average capillary pressure then follows from:

\[
P_{c_{\text{front}}} = P_{n_{\text{front}}} - P_{w_{\text{front}}}
\]

\[
P_{n_{\text{front}}} = P_{n_{\text{bottom}}} - \rho_n g z_{\text{front}}
\]

\[
P_{w_{\text{front}}} = \rho_w g (h - z_{\text{front}})
\]

\[
P_{c_{\text{bottom}}} = P_{n_{\text{bottom}}} - P_{w_{\text{bottom}}}
\]

\[
P_{n_{\text{bottom}}} = P_{n_{\text{bottom}}}
\]

\[
P_{w_{\text{bottom}}} = \rho_w gh
\]

\[
\langle P_c \rangle_{\text{global \ corrected}} = \frac{P_{c_{\text{front}}} + P_{c_{\text{bottom}}}}{2}
\]

\[
= \frac{P_{n_{\text{bottom}}} - \rho_n g z_{\text{front}} - \rho_w g (h - z_{\text{front}}) + P_{n_{\text{bottom}}} - \rho_w gh}{2}
\]

\[
= P_{n_{\text{bottom}}} + \frac{1}{2} (\rho_w - \rho_n) g z_{\text{front}} - \rho_w gh
\]

Once the nonwetting phase reaches the outflow boundary, Equation (5.41) reduces to:

\[
\langle P_c \rangle_{\text{global \ corrected}} = P_{n_{\text{bottom}}} - \frac{1}{2} (\rho_w + \rho_n) gh
\]

The global averaged equilibrium capillary pressure-saturation curve is shown in Figure 5.28, corrected and not corrected for gravity forces. Note that the average wetting phase saturation is obtained from Equation (5.2) in case the global average is not corrected for gravity effects, and from Equation (5.14) if the global average is corrected for gravity effects.

Figure 5.28 shows that the global average equilibrium capillary pressure-saturation relationship corrected for gravity (Equation (5.41)) closely resembles the reference curve, except at low wetting phase saturations. At low wetting phase saturations, the global averaged curve shows a strong increase in capillary pressure already at a wetting phase saturation of 0.17, while the reference curve continues to lower wetting phase saturations. Note that the reference curve asymptotically goes to the specified residual wetting phase saturation of 0.104. The global average equilibrium capillary pressure-saturation curve that is not corrected for gravity effects (Equation (5.38)) shows an overestimation in capillary pressure compared to the reference curve. This overestimation will increase with increasing column length. Therefore, if the uncorrected global average is used to determine capillary pressure for a
longer column (for instance longer than 3 cm), significant overestimation of the entry pressure of the porous medium can occur. Normally however, this method is used for samples in the range of 3 cm, and then the overestimation is not that large.

Figure 5.28: global average equilibrium $P_c$-$S_w$ relationship obtained for a simulation of a static primary drainage experiment, a) global average corrected for gravity effects (Equation (5.41)); b) global average not corrected for gravity effects (Equation (5.38)).

In Figure 5.29, the global averaged capillary pressure-saturation relationship is compared to the arithmetic phase volume average capillary pressure-saturation curve as determined from Equation (5.12) and (5.14). As can be seen, the most significant difference occurs at low wetting phase saturations, where the global average increases to a very high capillary pressure. As indicated by Equation (5.42), the global average capillary pressure after the nonwetting phase has reached the outflow of the domain is simply equal to the nonwetting phase bottom boundary pressure with some hydrostatic correction. The fast increase in the global average capillary pressure at low wetting phase saturations is the result of the fast increase of the nonwetting phase bottom boundary pressure. This is due to the relative permeability of the wetting phase, which approaches zero as the wetting phase saturation decreases. As a result, the equilibrium criterion is reached faster and faster, so that the nonwetting phase bottom boundary pressure is increased by a lot of small increments in a short amount of time while the saturation inside the domain does not significantly changes anymore. This will be further explained below.

In Figure 5.30, the arithmetic phase volume average as well as the global average capillary pressure are plotted as a function of the applied nonwetting phase bottom boundary pressure. As can be seen, the global average capillary pressure keeps on increasing with increasing applied nonwetting phase boundary pressure, while the arithmetic phase volume average capillary pressure becomes constant as the applied nonwetting phase boundary pressure increases.

Figure 5.29 also indicates that both the global averaged and the arithmetic phase volume averaged $P_c$-$S_w$ curves end at the same wetting phase saturation. Thus, one could say they give rise to the same residual wetting phase saturation. However, usually the laboratory measurements of $P_c$-$S_w$ curves are parameterised using a fitting procedure in order to obtain van Genuchten or Brooks-Corey parameters that can be used in a numerical model.
Figure 5.29: Global average capillary pressure-saturation relationship corrected for gravity and the ‘new’ arithmetic phase volume average capillary pressure relationship, obtained for a simulation of a static primary drainage experiment including gravity.

Figure 5.30: Average capillary pressure as determined from either arithmetic phase volume average over nodes in the domain, or from the global average, as a function of the applied nonwetting phase bottom boundary pressure.
If we parameterise the average \( P_c-S_w \) curves plotted in Figure 5.29, using a Brooks-Corey parameterisation, a larger residual wetting phase saturation will be found for the global averaged \( P_c-S_w \) curve due to the strong increase in capillary pressure at low wetting phase saturations. This is illustrated in Figure 5.31, which shows a fitted curve through the global averaged capillary pressure-saturation curve and the arithmetic phase volume average capillary pressure-saturation relationship. Table 5.2 contains the fitted Brooks-Corey parameters.

The fitted curves and the derived parameters of Table 5.2 show that for the global average equilibrium \( P_c-S_w \) curve, a higher residual saturation is obtained than the reference curve, or the arithmetic phase volume average over the 2-phase domain.

In 2003, Oung and Bezuijen observed the same type of behaviour for a laboratory experiment. They measured \( P_c-S_w \) curves for water and a DNAPL using two different measurement methods: inside the sample with selective pore pressure transducers, and outside the sample with pressure gauges installed in the fluid reservoirs. Their resulting capillary pressure-saturation curves are shown in Figure 5.32.

### Table 5.2: fitted Brooks-Corey parameters for the corrected global average and arithmetic phase volume average. In addition, the \( R^2 \) and Root Mean Squared Error values are shown.

<table>
<thead>
<tr>
<th>( P_c-S_w ) curve</th>
<th>Fitted Brooks–Corey parameters</th>
<th>Goodness of fit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference curve (Brooks Corey parameterisation)</td>
<td>( \lambda ), ( P_d ) (Pa)</td>
<td>( S_{wr} )</td>
</tr>
<tr>
<td>Global averaged ( P_c-S_w ) curve corrected for gravitational forces Static simulation</td>
<td>6.98, 6093</td>
<td>0.165</td>
</tr>
<tr>
<td>Arithmetic phase volume average over two-phase domain Static simulation</td>
<td>6.09, 6023</td>
<td>0.103</td>
</tr>
</tbody>
</table>
Figure 5.32: Comparison between capillary pressures $P_c$ (in fluids), measured by PPTs placed in the fluid reservoirs, and $P_c$ (in sand) measured by selective pore pressure transducers in contact with sand. Note that both the primary drainage and main imbibition curves are shown (figure taken from Oung and Bezuijen, 2003)

As can be seen, at low wetting phase saturations, the capillary pressure measured inside the sample (in the sand) for the drainage curve is higher than the capillary pressure obtained from the fluid reservoirs. Oung and Bezuijen explained their observation by stating that at low wetting phase saturations, the capillary pressure as measured by the selective pore pressure transducers inside the sample stayed constant with decreasing saturation. This is because the water inside the sample becomes discontinuous, so that it is no longer connected to the water reservoir outside the sample. As a result, when the DNAPL pressure is increased, the water pressure inside the sample will increase according to the DNAPL pressure. Thus, the water pressure measured inside the sample will be larger than is measured in the water reservoir outside the sample. When at low wetting phase saturations now the DNAPL pressure of the reservoir is further increased, both the DNAPL and water pressure inside the sample will increase accordingly, so that the capillary pressure inside the sample stays more or less constant. The capillary pressure determined from the fluid reservoirs however will continue to increase as the pressure in the DNAPL reservoir is increased, and the water pressure in the water reservoir stays constant.

The simulations performed here are for a 1-D homogeneous domain, so that the wetting phase actually cannot become discontinuous. However, still the relative permeability of the wetting phase approaches zero as the capillary pressure increases and water is drained from the domain. Because of this low relative permeability, within the column the wetting phase pressure will increase along with the nonwetting phase pressure, so that the capillary pressure inside the domain does not change anymore. Note that this is the result of the equilibrium criterion becoming insufficient because it is already reached before the wetting phase pressure has had enough time to adapt to the newly imposed nonwetting phase bottom boundary pressure. The capillary pressure at the boundaries of the domain will keep increasing as the nonwetting phase pressure at the inflow boundary keeps to be increased.

Concluding, the global average returns good results (i.e. an average equilibrium curve that is close to the reference curve) as long as the relative permeability of the wetting phase is not
too low. As the relative permeability approaches zero, the capillary pressure as determined from the global average no longer represents the average capillary pressure inside the domain. This can have consequences for the residual wetting phase saturation that is determined through a fitting procedure of a Brooks-Corey or van Genuchten parameterisation.

5.7 Importance of averaging on sensor scale

As was shown in Section 5.3.2, the influence the averaging method has on the averaged equilibrium \( P_c-S_w \) curve is related to the averaging window, or length scale over which the averaging is performed. As the length scale decreases, the effect of the used averaging method decreases too, and the averaged equilibrium \( P_c-S_w \) relationship approaches the reference curve. This is to be expected as the smallest ‘averaging’ length scale would be a single node, and for a single node the reference curve always is retrieved. In this section we consider the length scale of sensors such as pore pressure transducers (PPT) and time domain reflectometers (TDR) in order to determine whether the different averaging methods that were discussed in the sections before have a significant influence on the averaged equilibrium \( P_c-S_w \) relationship.

Sensors such as TDRs and PPTs will measure an average variable representative for the volume they are measuring, as was explained in Section 2.3.4. Thus, sensor measurements are not local measurements but averages over the volume they sample. Depending on the size of a sensor, the measured variable will become more and more an average, and less and less a local value. Though it is not clear what kind of average a sensor actually measure, we can make a comparison of all the averages suggested above for typical sensor sizes. In Figure 5.33, the averaged equilibrium \( P_c-S_w \) curves are shown for different averaging methods, for a sensor with a size of 1 cm and one with a size of 2 cm. As can be seen, the differences between the obtained curves are negligible. Only the simple arithmetic average as was suggested in Section 5.5 (Equation (5.31) and (5.36)) shows a significant deviation at high wetting phase saturations. This is due to the fact that with this average, the capillary pressure at a wetting phase saturation always will be zero, as the nonwetting and wetting phase pressures then both are equal to the hydrostatic pressure.

![Figure 5.33: \( P_c-S_w \) curves obtained using different averaging methods for a 1 cm sensor in the middle of the domain of 18.2 cm](image)

![Figure 5.33: \( P_c-S_w \) curves obtained using different averaging methods for a 2 cm sensor in the middle of the domain of 18.2 cm](image)
Thus, we can conclude that normally a sensor like a TDR or a PPT is so small that the obtained $P_c$-$S_w$ curve from these sensors represents the reference curve. Thus, it can be assumed that the sensor measures an actual local curve, characteristic of the porous medium, which is independent of the way the sensor averages the variable it is measuring. Note that when sensors inside the sample are used to determine capillary pressure, the capillary pressure does not go to infinity at low wetting phase saturations, as is the case when the capillary pressure is determined from pressures outside the sample.

5.8 Different orientations of the domain

In this section different orientations of the domain are investigated. The different set-ups are shown in Figure 5.34. Some of the averaging methods discussed above are influenced by gravity forces. Therefore, we investigate here different orientations with respect to the direction of gravity, and the resulting averaged equilibrium capillary pressure-saturation relationships.

![Figure 5.34](image_url)

**Figure 5.34:** various experimental set-ups for the numerical simulations. Set-up I has been used in the previous sections.

Set-up I is the set-up that was used in the simulations discussed in the preceding sections. In this set-up, the nonwetting phase is forced into the sample from below, so that the flow of nonwetting phase is opposite to the direction of the gravitational forces. At the top of the column, the wetting phase is allowed to flow out, but the nonwetting phase is prevented from leaving the sample by a hydrophilic membrane. The upward flow of nonwetting phase during a drainage process however is not that common in for instance field situations or even laboratory experiments. Therefore, in this section we consider set-up II, where the nonwetting phase is forced in from above, and is prevented to flow out at the bottom boundary. Boundary and initial conditions are the same as were described in Section 4.2.2 for a static primary drainage experiment. Only the nonwetting phase boundary pressure at the inflow now is set to

$$P_{n,\text{low}}^{\text{inf}} = \Delta P$$

instead of

$$P_{n,\text{low}}^{\text{inf}} = \rho_n g h + \Delta P$$

(5.44)

Note that now the flow of nonwetting phase is in the same direction as the direction of the gravity forces. Therefore, it may be expected that the averaged equilibrium $P_c$-$S_w$ curves
obtained using this set-up are different from the ones obtained using set-up I. Note that in the simulation, not the flow is inverted, but the gravitational acceleration is. Thus:

Set-up I: \( g = 9.81 \text{ m/s} \)

Set-up II: \( g = -9.81 \text{ m/s} \)  \hspace{1cm} (5.45)

Figure 5.35 shows the pressure and saturation distribution at several moments in the drainage process. There are significant differences between the profiles obtained for set-up I and those obtained for set-up II (see also Figure 5.13). This is because in the first case, gravity counteracts the flow of the nonwetting phase, while in the latter it assists the flow. Thus, for set-up II, a fast descent of the nonwetting phase through the sample can be observed, after which it starts accumulating above the hydrophilic membrane. Figure 5.35 shows a fast descent of the nonwetting phase through the domain. The nonwetting phase reaches the outflow boundary of the column already within the first pressure increment after the nonwetting phase starts infiltrating the sample. Note that infiltration of the nonwetting phase starts at a boundary capillary pressure of 4300 Pa, which is lower than the entry pressure of 6000 Pa. However, now the outflow of the column is at the bottom, so that the wetting phase pressure there is equal to zero.

As a result of the hydrostatic pressure distribution inside the sample, the wetting phase pressure at the top of the column becomes equal to the negative of the hydrostatic pressure. Therefore, the nonwetting phase pressure that has to be applied to overcome the entry pressure of the porous medium is only:

\[
P_n^b = 6000 - 1000 \cdot 9.81 \cdot 0.182 = 4215 \text{ Pa}
\]  \hspace{1cm} (5.46)

From Figure 5.35, it can further be observed that the nonwetting phase reaches the outflow very fast, while the nonwetting phase saturation is still relatively small.

Because a hydrophilic membrane is simulated at the outflow, the nonwetting phase cannot leave the domain, and as a result it starts accumulating above the outflow boundary. This causes a reversed saturation profile (see Figure 5.35b), with low nonwetting phase saturations at the inflow because the applied boundary pressure is not that high yet, and high nonwetting phase saturations at the outflow because the nonwetting phase accumulates fast there. Figure 5.36 shows the obtained average equilibrium \( P_c-S_w \) curves using set-up II, applying the traditional and ‘new’ arithmetic phase volume and weighted phase volume averages discussed in the previous sections. As can be seen, the deviation of the average arithmetic phase volume and weighted phase volume equilibrium \( P_c-S_w \) curves before the nonwetting phase reaches the outflow of the sample is negative. Thus, the capillary pressure is underestimated when the traditional arithmetic phase volume or weighted phase volume averaging methods are used to average the domain before the nonwetting phase reaches the outflow. This results in the underestimation of the entry pressure by approximately 900 Pa.

Note also that the average wetting phase saturation at which the nonwetting phase reaches the outflow occurs is much higher than was the case for the curves obtained for set-up I (see Figure 5.2). This is because for set-up II, gravity works in the advantage of the nonwetting phase, and it can move much faster through the column, while the saturation of the nonwetting phase stays relatively low (see Figure 5.34). As a result, the nonwetting phase...
reaches the outflow at a much lower average wetting phase saturation than was the case for set-up I.

Figure 5.35: pressure and saturation profiles for a simulation performed using set-up II, note that now $z=0$ at the top of the column, and $z=0.182$ at the bottom of the column, a) $S^w$ and $P^w$ profiles for an applied nonwetting phase top boundary pressure of 4300 Pa, b) $S^w$ and $P^w$ profiles for an applied nonwetting phase top boundary pressure of 4400 Pa, c) $S^w$ and $P^w$ profiles for an applied nonwetting phase top boundary pressure of 28400 Pa.
5.8 Different Orientations of the Domain

Figure 5.36: Averaged equilibrium \( P_c-S_w \) curves obtained using set-up II, a) traditional arithmetic and phase volume averaged equilibrium \( P_c-S_w \) curves, b) arithmetic and weighted phase volume averaged equilibrium \( P_c-S_w \) curves over 2-phase system.

Figure 5.37: Average capillary pressure-saturation relationships for different averaging methods, for a static simulation with flow parallel to gravity forces.

Further, when the ‘new’ arithmetic phase volume average \( P_c-S_w \) curve is determined, the reference curve is retrieved just as was shown in Section 5.3.1. Again, the ‘new’ weighted phase volume averaged equilibrium \( P_c-S_w \) curve does not result in a curve equal to the reference curve.

Finally, with set-up II, a much higher residual saturation of the average equilibrium capillary pressure-saturation relationship is obtained than in case of set-up I, as the nonwetting phase sinks through the column and starts accumulating at the bottom very early in the drainage process. As a result, the relative permeability of the wetting phase in this region becomes very
low at the outflow, and the flow of water out of the sample domain is inhibited by the accumulated nonwetting phase. This effect is much less for set-up I, where the nonwetting phase saturation increases gradually and it takes a longer time for the nonwetting phase to reach the outflow of the sample, as gravity forces oppose flow. Figure 5.35 indicates that the average wetting phase saturation reached performing 300 incremental pressure steps of 100 Pa for set-up I is 0.17, while the same amount of pressure increments results in an average wetting phase saturation of 0.23. The effect of a hydrophilic membrane on the residual saturation of a sample is further investigated in Chapter 7.

Figure 5.37 shows several other average equilibrium $P_c$-$S_w$ curves obtained for set-up II, using the averaging methods that were discussed in this chapter. As can be seen, the centroid phase average pressure results in an average equilibrium curve that follows the reference curve closely. The simple arithmetic average $P_c$-$S_w$ curve again shows an underestimation of the capillary pressure at high average wetting phase saturation.

Unfortunately, set-up III is difficult to model with the Berentsen model, and therefore is not considered.

### 5.9 Summary and conclusions

In this chapter, a vertical 1-D homogeneous domain of 18.2 cm was used to perform a numerical drainage experiment under static conditions, where a DNAPL replaces water. At the outflow of the domain, a hydrophilic membrane was simulated in order to prevent the nonwetting phase from leaving the domain. This is a common approach used in laboratory experiments. After the simulations, average equilibrium capillary pressure-saturation relationship were obtained, using several averaging methods. Appendix C gives an overview of the different averaging approaches used in this chapter.

The following can be concluded:

- The averaging method used to obtain an average equilibrium $P_c$-$S_w$ curve can lead to an average curve that is not equal to the $P_c$-$S_w$ curve characteristic of the porous medium (the reference curve) when gravity is included.
- The arithmetic phase volume average over that part of the domain that is a 2-phase system will return the reference curve. However, before the nonwetting phase reaches the outflow of the sample, this averaging approach results in a changing averaging length scale.
- The weighted phase volume average always results in a curve deviating from the input curve, due to non-linearity of the saturation distribution. The centroid phase average introduces a correction to the weighted phase volume average, giving good results except for the highest average wetting phase saturations.
- The global average equilibrium $P_c$-$S_w$ curve gives good results, but care should be taken when lower wetting phase saturations are reached. When the relative wetting phase permeability becomes low, the global average equilibrium $P_c$-$S_w$ curve shows a fast increase in capillary pressure, while inside the domain the capillary pressure stays more or less constant. This can have significant effects on the average residual wetting phase saturation that is obtained from the average $P_c$-$S_w$ curve.

The overall conclusion in this chapter is that care should be taken when averaging pressures and saturations in the presence of gravity forces. Several commonly used averaging methods in that case do not result in an equilibrium $P_c$-$S_w$ curve that is only characteristic of the porous medium.
Finally, it has to be noted here that the above results were obtained for a DNAPL-water system. The use of other systems could give different results. Another system for instance would be an air-water system. In this case, usually it is assumed that the air phase reaches equilibrium instantly, and that it is equal to the atmospheric pressure in the whole of the domain throughout the drainage process. Thus, the average nonwetting phase pressure would be equal to the atmospheric pressure at all times.

Note also that the results discussed above were obtained for a particular set of boundary and initial conditions. Other sets of boundary and initial conditions could also lead to different results.
Chapter 6

The average equilibrium $P_c-S_w$ curve for a heterogeneous domain

In Chapter 5, the average equilibrium capillary pressure-saturation relationship was discussed for a homogeneous porous medium. However, even though laboratory samples are usually assumed to be homogeneous, often they contain micro-heterogeneities. These are small heterogeneities with a size of millimetres to tens of centimetres, occurring at the macroscale (e.g. on the sample-scale). If, for example, a soil or rock sample is taken in the field and experiments are performed on the intact sample, micro-heterogeneities can be the result of layers, fractures, or small lenses that are present in the field. If an experimental column is packed with a loose porous medium, micro-heterogeneities can be formed due to non-homogeneous packing of the porous medium. Actually, it is impossible to pack a sand column perfectly homogeneous, and some type of heterogeneity will always be introduced.

Even though micro-heterogeneities are relatively small, they can have a significant effect on the distribution and location of fluids during two-phase flow in a porous medium. Consequently, the measured sample-scale two-phase flow relationships, such as the capillary pressure-saturation relationship, may be influenced by micro-heterogeneities inside the laboratory sample as well.

Several authors have investigated the effect of micro-heterogeneities on soil characteristic curves, like the capillary pressure-saturation relationship and the relative permeability-saturation relationships. For instance, Ataie-Ashtiani et al. (2002) investigated the effect of micro-heterogeneities on the equilibrium $P_c-S_w-k_r$ relationships on the laboratory sample scale for a DNAPL-water system. They did this by performing simulations that represented the experimental procedures that are commonly used to determine capillary pressure-saturation-relative permeability relationships. Ataie-Ashtiani et al. (2002) used two relatively simple patterns, consisting of 2 or 3 blocks of fine sand imbedded into a coarse sand matrix to represent micro-heterogeneities. The two patterns used were a straight pattern, consisting of two heterogeneities on a line, and a staggered pattern, consisting of one heterogeneity in the middle of the top half of the sample, and two half heterogeneities at the edges of the lower half of the sample. With their simulations, Ataie-Ashtiani et al. (2002) showed that the presence of micro-heterogeneities influences the obtained constitutive relationships from a laboratory size sample. They found that the irreducible water saturation is a function of capillary number, so that with decreasing capillary number the irreducible water saturation increases. Moreover, heterogeneities were shown to enhance the effect of boundary conditions on the obtained constitutive relationships, both for drainage and imbibition.

In 2004, Das et al. performed numerical simulations in order to investigate how variations in nature, amount, and distribution of micro-heterogeneities affect the $P_c-S_w-k_r$ relationships for a DNAPL-water system. They used 14 different binary heterogeneity patterns in combination with different sand types (coarse/fine or fine/coarse). The simulations performed by Das et al. (2004) represent flow-through experiments that are commonly used in laboratory measurements. It was found that for the used heterogeneity patterns in a domain representative of laboratory samples, the upscaled equilibrium capillary pressure-saturation...
curve follows mainly the corresponding background sand $P_c-S_w$ curve. However, the residual wetting phase saturation is influenced by the presence and intensity of the heterogeneities. Both Ataie-Ashtiani et al. (2002) and Das et al. (2004) assume the imposed capillary pressure represents the average capillary pressure for the sample. This is comparable to the global average described in this thesis in Section 5.6. The resulting upscaled $P_c-S_w$ relationships they obtain therefore show fast increasing capillary pressures at low wetting phase saturations. However, inside the sample domain most probably the upscaled capillary pressure did not increase to such an extent. As was explained in Section 5.6, this difference is the result of the decoupling of the imposed capillary pressure and the capillary pressure inside the sample, due to the decreasing relative wetting phase permeability in combination with the strictness of the used equilibrium criterion.

In this chapter, the effect of heterogeneities on the average equilibrium capillary pressure-saturation relationship will be investigated. A two-dimensional domain will be used, that is divided into 36 blocks with different permeabilities and entry pressures, randomly chosen from a lognormal distribution. The following points will be discussed in this chapter:

- Determination of an analytical average equilibrium capillary pressure-saturation relationship that can be used as a reference curve.
- Determination of an average equilibrium capillary pressure-saturation relationship.
- The effects of micro-heterogeneities on the sample-scale average equilibrium capillary pressure-saturation relationship.

Table 6.1 provides an overview of the simulations that will be discussed in this chapter.

<table>
<thead>
<tr>
<th>Simulation</th>
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</thead>
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<tr>
<td>1) Static simulation, 2D heterogeneous domain 3 cm × 6 cm, no gravity</td>
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<td>• 300 steps of 100 Pa</td>
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<tr>
<td>• Low intensity heterogeneities</td>
</tr>
<tr>
<td>2) Static simulation, 2D heterogeneous domain, 3 cm × 6 cm, gravity</td>
</tr>
<tr>
<td>• 300 steps of 100 Pa</td>
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<tr>
<td>• Low intensity heterogeneities</td>
</tr>
<tr>
<td>3) Static simulation, 2D heterogeneous domain, 3 cm × 6 cm, gravity</td>
</tr>
<tr>
<td>• 300 steps of 100 Pa</td>
</tr>
<tr>
<td>• High intensity heterogeneities</td>
</tr>
<tr>
<td>4) Static simulation, 2D homogeneous domain, 3 cm × 6 cm, no gravity</td>
</tr>
<tr>
<td>5) Static simulation, 2D homogeneous domain, 3 cm × 6 cm, gravity</td>
</tr>
</tbody>
</table>

### 6.1 Procedure

The simulations discussed in this chapter are representing static primary drainage experiments. Thus, the nonwetting phase is prevented from leaving the sample at the outflow.

### 6.1.1 Domain description and medium properties

Just as for the homogeneous domain discussed in Chapter 5, for the heterogeneous domain in this chapter dimensions are chosen that are similar to those used in laboratory experiments. The heterogeneities are created in a 2-dimensional domain with a width of 6 cm, and a height of 3 cm. The characteristics of the fluids are the same as for the homogeneous domain, and can be found in Table 4.1. The heterogeneities in the domain are represented by zones having
different permeability and entry pressure. However, the porosity, residual wetting phase saturation, and Brooks-Corey coefficient $\lambda$ are assumed to be constant for each heterogeneity and equal to the values presented in Table 6.2. The heterogeneities are created by dividing the 6 cm × 3 cm domain into 6 × 6 blocks. Table 6.2 shows the specifications of the domain and porous medium.

Table 6.2: Properties of the 2-dimensional heterogeneous domain used in Chapter 6.

<table>
<thead>
<tr>
<th>Properties of the 2D heterogeneous domain</th>
<th>value</th>
<th>unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width</td>
<td>0.06</td>
<td>m</td>
</tr>
<tr>
<td>Height</td>
<td>0.03</td>
<td>m</td>
</tr>
<tr>
<td>Blocks in x direction</td>
<td>6</td>
<td></td>
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<tr>
<td>Number of nodes in x direction (single block)</td>
<td>25</td>
<td></td>
</tr>
<tr>
<td>NBZ</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td>Blocks in z direction</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Number of nodes in z direction (single block)</td>
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<td></td>
</tr>
<tr>
<td>Mesh size in x-direction</td>
<td>$4 \cdot 10^{-4}$ m</td>
<td></td>
</tr>
<tr>
<td>Mesh size in z direction</td>
<td>$3.75 \cdot 10^{-4}$ m</td>
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<tr>
<td>Intrinsic permeability</td>
<td>Assigned to each heterogeneity block based on lognormal distribution</td>
<td></td>
</tr>
<tr>
<td>Entry pressure</td>
<td>Related to permeability through Leverett $J$-function</td>
<td></td>
</tr>
<tr>
<td>Porosity</td>
<td>0.4</td>
<td></td>
</tr>
<tr>
<td>Brooks Corey parameter $\lambda$</td>
<td>6.11</td>
<td></td>
</tr>
<tr>
<td>Residual wetting phase saturation</td>
<td>0.104</td>
<td></td>
</tr>
</tbody>
</table>

The permeabilities for each individual heterogeneity are drawn from a lognormal distribution. A normal distribution cannot be used because it can result in negative values for the permeability when the mean of the distribution is close to zero or the standard deviation of the distribution is large. The lognormal distribution has the following probability density function:

$$f(K | \mu, \sigma) = \frac{1}{K \sigma \sqrt{2\pi}} e^{-\frac{(\ln K - \mu)^2}{2\sigma^2}}$$  \hspace{1cm} (6.1)$$

where $f$ is the probability density, $K$ is the intrinsic permeability, and $\mu$ and $\sigma$ are the mean and standard deviation of the logarithm of the permeability $K$. Note that a log-normal distribution of a variable is the probability distribution of a variable whose logarithm is normally distributed.

In Figure 6.1, the used lognormal distribution for the intrinsic permeability is shown. This distribution has the following mean and standard deviation:

$$\mu = 2.24 \cdot 10^{-12} \text{ m}^2$$  \hspace{1cm} (6.2)$$

$$\sigma = 4.53 \cdot 10^{-13} \text{ m}^2$$  \hspace{1cm} (6.3)$$

These values are chosen such that the obtained variation in the intrinsic permeability and related entry pressure can be considered representative for small-scale heterogeneities in a laboratory sample.
The permeability for each heterogeneity is randomly drawn from the lognormal distribution described above, using the normal random number generator in MATLAB (function `lognrnd`). The generator is seeded so that for every simulation that is performed, the same set of permeabilities is drawn ‘randomly’ from the distribution.

After each heterogeneity has been assigned an intrinsic permeability, the entry pressure can be calculated accordingly using the Leverett J-function, which was introduced in Section 2.3.3. The Leverett J-function is given by:

\[ J(S_w) = \frac{P_c}{\sigma \cos \theta \sqrt{\frac{n}{K}}} \]  \hspace{1cm} (6.4)

Thus, using Equation (6.4), the entry pressure of a heterogeneity can be related to the entry pressure of a reference porous medium for which both the intrinsic permeability and entry pressure are known:

\[ J(S_w)^{\text{reference}} = J(S_w)^{\text{heterogeneity}} \]  \hspace{1cm} (6.5)

so that:

\[ \frac{P_c^{\text{reference}}}{\sigma \cos \theta \sqrt{\frac{n}{K^{\text{reference}}}}} = \frac{P_c^{\text{heterogeneity}}}{\sigma \cos \theta \sqrt{\frac{n}{K^{\text{heterogeneity}}}}} \]  \hspace{1cm} (6.6)
In Equation (6.6) it is assumed that the same two-phase flow system is considered, in which case the surface tension $\sigma$ and the contact angle $\theta$ are the same in both porous media under consideration. Moreover, it is assumed that the porosity of the heterogeneities is constant. Equation (6.6) can be rewritten such that the entry pressure of the heterogeneity can be calculated from the intrinsic permeability and entry pressure of the reference medium:

$$
P_{d, \text{heterogeneity}} = P_{d, \text{reference}} \left( \frac{K_{\text{reference}}}{K_{\text{heterogeneity}}} \right)
$$

(6.7)

In this case, the reference values are taken from the porous medium properties that were used in the homogeneous case.
6.1 Procedure

\[ P_{\text{reference}} = 6000 \text{ Pa} \]  

\[ K_{\text{reference}} = 2.2 \cdot 10^{-12} \text{ m}^2 \]

As all the terms on the right hand side of Equation (6.7) are known, the associated entry pressure of each heterogeneity can be calculated. In Figure 6.2, the resulting heterogeneous domain is shown. As can be seen, the permeability varies between $1.44 \cdot 10^{-12} \text{ m}^2$ and $2.62 \cdot 10^{-12} \text{ m}^2$, with the entry pressure varying between 5498 Pa and 7414 Pa.

6.1.2 Boundary and initial conditions

The boundary and initial conditions for the simulations performed in this chapter are the same as were described in Section 4.2.2 for a static primary drainage experiment.

6.2 Determining an analytical equilibrium \( P_c-S_w \) curve for a heterogeneous domain

When considering homogeneous domains, the analytical equilibrium capillary pressure-saturation relationship is simply equal to the relationship specified for the porous medium comprising the domain. In Chapter 5, this curve was referred to as the 'reference curve'. However, for heterogeneous domains, porous medium properties inside the domain vary and the analytical average equilibrium capillary pressure-saturation relationship for the domain needs to be determined differently. It is needed to combine the \( P_c-S_w \) curves for all the heterogeneities in the domain to one upscaled macroscale relationship. One way to do this is by applying the assumption of capillary equilibrium to the distribution of local \( P_c-S_w \) relationships, so that the saturation distribution can be found for a given capillary pressure. Subsequently, the weighted arithmetic mean of this saturation distribution gives one point on the upscaled equilibrium \( P_c-S_w \) curve (Braun et al., 2005). The procedure will be explained in more detail below.

As was discussed in Section 6.1.1, each heterogeneity in the domain has been assigned its own intrinsic permeability and related entry pressure. The different entry pressure for each heterogeneity results in a different local capillary pressure-saturation relationship for these heterogeneities. The analytical sample-scale equilibrium \( P_c-S_w \) curve thus has to be obtained in some way from the collection of local capillary pressure-saturation relationships that is specified for the heterogeneities. Simply adding up the relationships and dividing them by the number of heterogeneities would give such an average curve. However, this average curve does not really represent the sample-scale equilibrium \( P_c-S_w \) curve for a sample containing heterogeneities, because the entry pressures and accessibility are not taken into account. Therefore, another approach is used. This approach is based on the assumption of capillary equilibrium, which assumes that for a certain capillary pressure, the sample has reached a true equilibrium distribution of saturation, so that the saturation for each heterogeneity can be determined from the local capillary pressure-saturation relationship specified for each heterogeneity (Braun et al., 2005). Note that in this approach, gravity is not considered, so that for each capillary pressure a uniform saturation can be assumed inside each
The average equilibrium PC-Sw curve for a heterogeneous domain. This saturation can be derived from the local capillary pressure-saturation relationship. The followed procedure is illustrated in Figure 6.3.

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<td>Pd = 5500 Pa</td>
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</tr>
</tbody>
</table>

Determination of $\langle S_{w}\rangle$

If $P_d^{i} > P_c$

OR

If heterogeneity is not connected to NW reservoir:

$S_{w}^{i} = 1$

If $P_d^{i} \leq P_c$

AND

If heterogeneity is connected to NW reservoir:

$S_{w}^{i} = (P_d/P_c)^k (1-S_{w}) + S_{wr}$

$\langle S_{w}\rangle = \sum S_{w}^{i} V^{i} / \sum V^{i}$

Figure 6.3: The procedure followed in obtained the analytical sample-scale equilibrium $P_c$-$S_w$ relationship for a heterogeneous domain. The numbers correspond to several applied capillary pressures for which the equilibrium distribution of saturations is determined based on Brooks-Corey relationship for each heterogeneity. Subsequently, a point on the analytical $P_c$-$S_w$ curve can be found for each applied capillary pressure.
Naturally, a heterogeneity can only be infiltrated by the nonwetting phase if its entry pressure is below the applied capillary pressure, thus if:

\[ P_d^i \leq P_c \quad i = 1,2,\ldots,N \]

where \( N \) represents the number of heterogeneities present in the sample, which in this case equals 36.

In addition, the concept of accessibility is applied. This means that the nonwetting phase can only infiltrate a heterogeneity if that heterogeneity is connected to the nonwetting phase reservoir, either directly or through other heterogeneities that are already infiltrated by the nonwetting phase. Thus, if a heterogeneity has an entry pressure that is larger than the applied entry pressure, or if that heterogeneity has an entry pressure that is lower than the applied entry pressure but it is not directly or indirectly connected to the nonwetting phase reservoir, its wetting phase saturation will be one:

\[ S_w^i = 1 \quad i = 1,2,\ldots,N \]

However, if a heterogeneity has an entry pressure that is lower than the applied capillary pressure and it is connected directly or indirectly to the nonwetting phase reservoir, its wetting phase saturation can be determined from the local capillary pressure-saturation relationship specified for that particular heterogeneity:

\[ S_w^i = \left( \frac{P_d^i}{P_c} \right)^\lambda \]

\[ S_w^i = \left( \frac{P_d^i}{P_c} \right)^\lambda (1 - S_{wr}) + S_{wr} \quad i = 1,2,\ldots,H \]

Where \( H \) is the number of heterogeneities in the domain.

After the wetting phase saturation is determined for each heterogeneity for a certain capillary pressure, the average wetting phase saturation of the sample can be determined by taking the arithmetic mean of the saturations of the heterogeneities, weighted by the volume of each heterogeneity:

\[ \langle S_w \rangle = \frac{\sum_{i=1}^{H} S_w^i V^i}{\sum_{i=1}^{H} V^i} \quad i = 1,2,\ldots,H \]

In this case, there are 36 heterogeneities of equal size, so that the average saturation can be determined by simply adding the saturations for each heterogeneity and dividing this sum by 36.

If the sample-scale analytical wetting phase saturation is determined for a certain capillary pressure, one point on the sample-scale analytical \( P_c-S_w \) curve is obtained, and the capillary
pressure can be increased in order to determine the next point on the $P_c$-$S_w$ curve (see Figure 6.3).

Figure 6.4 shows the obtained sample-scale analytical capillary pressure-saturation relationship for the heterogeneous sample that was introduced in Section 6.1.1 (Figure 6.2).

![Figure 6.4: The obtained sample-scale analytical equilibrium capillary pressure-saturation relationship](image)

Note that in obtaining the analytical sample-scale equilibrium $P_c$-$S_w$ curve shown in Figure 6.4, it is assumed that a heterogeneity is connected to the nonwetting phase reservoir indirectly if it is in contact with an already infiltrated heterogeneity either at its sides or at its corners (Figure 6.5). Alternatively, it could also be assumed that a heterogeneity is only connected to the nonwetting phase reservoir indirectly through contact only at its sides. This would lead to the slightly different analytical $P_c$-$S_w$ curve as is shown in Figure 6.6. This difference will be further discussed in Section 6.3.

![Figure 6.5: Different assumptions for accessibility; a) Assuming that a heterogeneity is indirectly connected to the nonwetting phase reservoir if it is in contact through its sides or corners with a neighbouring heterogeneity already infiltrated by the nonwetting phase, b) Assuming that a heterogeneity is indirectly connected to the nonwetting phase reservoir if it is in contact only through its sides with a neighbouring heterogeneity already infiltrated by the nonwetting phase.](image)
6.2 Determining an Analytical Equilibrium P\(_c\)-S\(_w\) Curve for a Heterogeneous Domain

In order to investigate the effect of heterogeneities on the sample-scale average equilibrium P\(_c\)-S\(_w\) curve, also a set of homogeneous simulations of a static primary drainage experiment will be performed. The domain properties, boundary and initial conditions correspond to those introduced in Section 4.2, with the only difference that now the domain length is 3 cm, and gravity is neglected. The input curve for these homogeneous simulations is obtained by fitting a Brooks-Corey relationship through the sample-scale analytical equilibrium P\(_c\)-S\(_w\) curve obtained for the heterogeneous domain. Results are shown in Figure 6.7.

The best overall fit is obtained when the analytical heterogeneous capillary pressure-saturation data for high wetting phase saturations (0.8 < S\(_w\) < 1.0) is excluded. However, this
causes the entry pressure of the fitted curve to be higher than the entry pressure of the heterogeneous analytical curve. Including the data for high wetting phase saturations results in a bad fit at intermediate and low wetting phase saturations, as is shown in Figure 6.7b. The obtained parameters are given in Table 6.3. In the following sections, the fit obtained by excluding the analytical heterogeneous Pc-Sw data for high wetting phase saturations will be used as the input curve for the homogeneous simulations because this fit approaches the analytical equilibrium Pc-Sw curve for the heterogeneous domain better at low and intermediate wetting phase saturations.

Table 6.3: obtained Brooks-Corey parameters for the homogeneous local curve from the 2D heterogeneous sample-scale analytical equilibrium Pc-Sw relationship.

<table>
<thead>
<tr>
<th>Pc-Sw curve</th>
<th>Fitted Brooks-Corey parameters</th>
<th>Goodness of fit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Local homogeneous curve (excluding data 0.8 &lt;Sw&lt;1)</td>
<td>λ, 6168, 0.102, 0.9969, 0.0067</td>
<td></td>
</tr>
<tr>
<td>Local homogeneous curve (including all data)</td>
<td>4.09, 5821, 0.094, 0.983, 0.0234</td>
<td></td>
</tr>
</tbody>
</table>

### 6.3 The average equilibrium Pc-Sw relationship for a heterogeneous domain

Now that the analytical sample-scale Pc-Sw relationship for the 2D heterogeneous domain is determined, it can be used to investigate the heterogeneous average Pc-Sw curve that can be obtained from the different averaging methods that were discussed in Chapter 5. For simplicity, we start with a simulation of a static primary drainage experiment for a 2D heterogeneous domain that neglects gravity. Note that the sample-scale analytical equilibrium Pc-Sw curve derived in Section 6.2 also is obtained by neglecting gravity. First, the traditional arithmetic phase volume and weighted phase volume averages are considered, as determined from Equations (5.2), (5.5), and (5.6). Naturally, it would be expected that the traditional arithmetic phase volume and weighted phase volume averages result in curves equal to the analytical curve as gravitational forces do not play a role (see also Figure 5.5). The arithmetic phase volume and weighted phase volume average equilibrium Pc-Sw curves for the heterogeneous domain are shown in Figure 6.8.

![Figure 6.8: a) Traditional arithmetic phase volume averaged equilibrium Pc-Sw relationship, b) traditional weighted phase volume averaged equilibrium Pc-Sw relationship.](image-url)
As can be seen, the curves correspond relatively well to the analytical curve. At high average wetting phase saturations there is a slight deviation of the average equilibrium \( P_c - S_w \) curves from the analytical \( P_c - S_w \) curve. Contrary to the observations made in Chapter 5, in this case this deviation is due to the way the analytical curve is determined, and not to the averaging method used to obtain the average equilibrium \( P_c - S_w \) relationship from the simulation data. The observed deviation is related to the assumptions made about the connectivity of the heterogeneities to the nonwetting phase reservoir when applying the assumption of capillary equilibrium. As is discussed in Section 6.2, it is assumed that a heterogeneity is in indirect contact with the nonwetting phase reservoir if one of the neighbouring heterogeneities at either its sides or its corners is already infiltrated by the nonwetting phase. In that case, the heterogeneity can also be infiltrated if its entry pressure is below the applied capillary pressure. When comparing the saturation distributions obtained from simulation data to the distributions obtained using the assumption of capillary equilibrium, a difference in their evolution can be observed (Figure 6.9). The evolution of the saturation distribution obtained from simulation data indicates that the heterogeneities are only infiltrated by the nonwetting phase if they are connected to already infiltrated heterogeneities by their sides and not by their corners (compare Figure 6.9a and 6.9b). A difference in the saturation distributions is particularly observed at the beginning of the drainage process \( (P_c < 6700 \text{ Pa}) \), and at the end of the drainage process \( (P_c = 30000 \text{ Pa}) \).

Thus, actually it should be assumed that a heterogeneity is only in indirect contact with the nonwetting phase reservoir when it is in contact with an already infiltrated heterogeneity at its sides only. If this assumption is used to obtain a sample-scale analytical capillary pressure saturation relationship, the resulting curve matches the averaged \( P_c - S_w \) curve obtained from the simulation data to a larger extent (Figure 6.10). Note that the observed ‘wiggles’ in the average \( P_c - S_w \) curve obtained from the simulation of a static primary drainage experiment are caused by the evolution of the infiltration of the nonwetting phase in the sample. At times when suddenly several heterogeneities with a relatively low entry pressure are infiltrated with nonwetting phase, the average capillary pressure inside the sample will increase suddenly. This is because before infiltration of the nonwetting phase into these heterogeneities, the capillary pressure of these heterogeneities is equal to their corresponding entry pressure. However, after infiltration, the capillary pressure in these heterogeneities can be much higher, especially if the applied nonwetting phase bottom boundary is significantly higher than the entry pressure of the heterogeneity. This can occur because for a heterogeneity to be infiltrated with nonwetting phase, it has to be connected to the nonwetting phase reservoir either directly or indirectly, which makes it possible for heterogeneities with relatively low entry pressures to be infiltrated with nonwetting phase at an applied nonwetting phase boundary pressure significantly higher than the entry pressures.

The corresponding evolution of the saturation distribution is shown in Figure 6.9c. As can be seen, this evolution shows a better resemblance to the evolution of the saturation that occurs in the simulation. However, still some differences are present, especially at low applied capillary pressures \( (P_c < 6300 \text{ Pa}) \). This is also observed in Figure 6.10, where at high wetting phase saturations the obtained \( P_c - S_w \) curve deviates slightly from the analytical curve. In the simulation, the nonwetting phase infiltrates the sample at a lower rate than is observed when applying the assumption of capillary equilibrium. Therefore, it can be concluded that early in the drainage process, this assumption does not hold. Capillary equilibrium in the heterogeneous domain is not reached at this stage. This can be explained as follows. If a heterogeneity is connected to the nonwetting phase reservoir through other heterogeneities with entry pressures that are close to the applied capillary pressure, flow of nonwetting phase to this heterogeneity will be slow. This is because the saturation in these neighbouring heterogeneities is small. Therefore, for these heterogeneities a long time is needed to reach an
equilibrium saturation, as the nonwetting phase first has to flow through the heterogeneities with high entry pressures and low wetting phase saturations.

![Image of saturation distribution](image1)

![Image of saturation distribution](image2)

![Image of saturation distribution](image3)

Figure 6. 9: saturation distribution at capillary pressures of (l.t.r.) 6000 Pa, 6300 Pa, 6700 Pa, 7300 Pa, 8200 Pa, 9200 Pa, and 30000 Pa; a) saturation distributions for the simulation of a static primary drainage experiment in a 2D heterogeneous domain; b) saturation distributions assuming capillary equilibrium, indirect connection to the nw phase reservoir through both sides and corners of a heterogeneity; c) saturation distributions assuming capillary equilibrium, indirect connection to the nw phase reservoir through the sides of a heterogeneity only.
However, the equilibrium criterion used in the simulation is already met before this equilibrium saturation is realised. This is especially true for the difficult accessible heterogeneities that are connected to the nonwetting reservoir only through heterogeneities with entry pressures close to the applied capillary pressure. In the assumption of capillary equilibrium this effect is not taken into account as it is assumed that capillary equilibrium is reached instantaneously, so that the heterogeneities that can be infiltrated by the nonwetting phase immediately reach the saturation according to the Brooks-Corey relation specified for them. As the drainage process progresses, more and more heterogeneities are infiltrated by the nonwetting phase, so that the nonwetting phase can flow easily and the difference between the saturation distributions obtained from the simulation data and the distributions obtained by applying the assumption of capillary equilibrium becomes negligible.

![Image](image-url)

Figure 6.10: Averaged equilibrium $P_c-S_w$ curves obtained from simulation data compared to the sample-scale analytical equilibrium $P_c-S_w$ relationship, where it is assumed that indirect contact of heterogeneities with the nonwetting phase reservoir only occurs through the sides of the heterogeneity, and not the corners.

As the end of the drainage process is approached, again a difference between the saturation distributions can be observed. This difference is due to the equilibrium criterion used in the numerical simulation. It is not strict enough so that when low wetting phase saturations and low wetting phase relative permeabilities are reached in the domain, the equilibrium criterion is already met even before pressure and saturation had enough time to adapt to the new applied boundary pressure. As a result, the residual wetting phase saturation that can be reached is higher than could be reached with a stricter equilibrium criterion, or when assuming capillary equilibrium. This was also discussed in Section 4.4.2.

Thus, the traditional arithmetic phase volume and weighted phase volume average equilibrium $P_c-S_w$ curves show good results with the analytical curve when gravity is not included, as would be expected. In Figure 6.11, the arithmetic phase volume and weighted phase volume average equilibrium $P_c-S_w$ curves are compared for a simulation with and without gravity.

The difference between the two curves is small, especially when compared to the difference that was observed in Section 5.3.1 for a homogeneous domain. However, it has to be noted that the heterogeneous domain used in the simulations of this chapter only is 3 cm in length, so that the effect of gravity forces is relatively small compared to the effect that was observed in Section 5.3.1 for a homogeneous domain of 18.2 cm. In Figure 6.12, the arithmetic phase volume average equilibrium $P_c-S_w$ curves for a homogeneous domain of 3 cm with and
without gravity are shown. The curves show that the effect of gravity forces is small for a 3 cm homogeneous column, just as for the 3 cm heterogeneous column. Note that the weighted phase volume average is no longer shown as the same results are obtained for this averaging method.

Figure 6.11: Comparison between average equilibrium Pc-Sw curves obtained for simulations with (a) and without gravity (b), for a 2D heterogeneous domain of 3 cm× 6 cm.

In Section 5.3.1., it was shown that the deviation of the arithmetic phase volume and weighted phase volume average equilibrium Pc-Sw curves from the analytical curve for simulations including gravity is caused by the difference in averaging window for the nonwetting phase and wetting phase pressures. This is because the traditional definition of the intrinsic averages considers pressures or saturations for the nodes for which phase \( \alpha \), the phase under consideration, is present. However, the wetting phase is present for every node, while the nonwetting phase initially only is present at the nodes which are already infiltrated by the
nonwetting phase. When gravity is included, this results in an overestimation of the nonwetting phase pressures, or more precisely an underestimation of the wetting phase pressures.

Therefore, adapted arithmetic phase volume and phase volume averages were introduced (Equations (5.12), (5.13) and (5.14)), that average the pressures and saturations for each phase only over those nodes for which both the nonwetting phase and wetting phase are present. These newly defined averages then result in average equilibrium curves that are close to the local or reference curve. Figure 6.13 shows that the same results are obtained for a homogeneous domain of 3 cm length. Moreover, the figure shows that when a simulation without gravity is considered, both the traditional and the ‘new’ arithmetic phase volume averages give rise to an average $P_c$-$S_w$ curve that is equal to the reference curve (apart from the small deviation at wetting phase saturations $S_w > 0.95$, but this is only due to the dynamics between the equilibrium points).

Figure 6.13: Traditional arithmetic phase volume average $P_c$-$S_w$ curve and the ‘new’ arithmetic phase volume average $P_c$-$S_w$ curve obtained by averaging only over that part of the domain that is infiltrated by the nonwetting phase, for a simulation with and without gravity, homogeneous 3 cm domain.

Figure 6.14: Traditional arithmetic phase volume average $P_c$-$S_w$ curves and ‘new’ arithmetic phase volume average $P_c$-$S_w$ curves obtained by averaging over 2-phase domain only, for a 2D heterogeneous domain, and a simulation with (a) and without gravity (b), respectively.
If for the heterogeneous domain the ‘new’ arithmetic phase volume averages as defined by Equations (5.12) and (5.14) are used to obtain an average $P_c$-$S_w$ curve, the results shown in Figure 6.14 are obtained. The figure shows the average $P_c$-$S_w$ curves obtained from simulations performed with and without gravity. From this figure, two observations can be made:

1. The average $P_c$-$S_w$ curves obtained by using the ‘new’ arithmetic phase volume average as defined by Equations (5.12) and (5.14) are significantly different from the analytical equilibrium $P_c$-$S_w$ curve as determined by applying the assumption of capillary equilibrium.
2. The average $P_c$-$S_w$ curve obtained by using the ‘new’ arithmetic phase volume average is significantly different from the analytical equilibrium $P_c$-$S_w$ curve as well as the traditional arithmetic phase volume averaged $P_c$-$S_w$ curve for a simulation without gravity.

These observations do not correspond to the results that are obtained for the homogeneous domain. For the homogeneous domain, the ‘new’ arithmetic phase volume averaged $P_c$-$S_w$ curve is very close to the reference curve, and for a simulation without gravity there is no difference between the reference curve, the traditional arithmetic phase volume averaged $P_c$-$S_w$ curve and the ‘new’ arithmetic phase volume averaged $P_c$-$S_w$ curve (see Figure 6.13).

The first observation can be explained by considering again the method used to obtain the sample-scale analytical equilibrium $P_c$-$S_w$ relationship (Section 6.2). The saturations obtained for the heterogeneities by assuming capillary equilibrium are averaged according to Equation (6.13). As the equation shows, the averaging is performed over all heterogeneities, so that also the heterogeneities which are not yet infiltrated by the nonwetting phase are included. As a result, the ‘analytical’ curve that is obtained represents an average over the whole 2D heterogeneous domain. Alternatively, the averaging could also be performed only over those heterogeneities which are infiltrated by the nonwetting phase. The difference between the two averaging methods is illustrated in Figure 6.15. In that case, the average wetting phase saturation can be obtained through:

$$
\langle S_w \rangle = \frac{\sum_{i=1}^{H} S_w^i (S_w^i < 1) V^i}{\sum_{i=1}^{H} V^i (S_w^i < 1)}
$$

where $N$ represents the number of heterogeneities in the domain.

Figure 6.16 now shows the resulting analytical $P_c$-$S_w$ curve. As can be seen, the newly defined analytical curve corresponds with the ‘new’ arithmetic phase volume averaged $P_c$-$S_w$ curve. This simply is because both are averages over that part of the domain that is infiltrated by the nonwetting phase only, thus over the 2-phase domain.

Note however that the analytical curve obtained by averaging only over the 2-phase domain displays interesting behaviour around an average wetting phase saturation of 0.6. Here the curve suddenly shows an increase in the average wetting phase saturation again, after which the average saturation decreases further. This means that around this saturation, multiple values of the capillary pressure are found. Therefore, the curve cannot be considered a function, which requires that there is a unique output for every input.
Figure 6.15: Different ways of averaging the wetting phase saturations obtained by applying the assumption of capillary equilibrium.

Figure 6.16: Traditional and ‘new’ arithmetic phase volume averaged equilibrium $P_c$-$S_w$ curves and the sample scale analytical equilibrium $P_c$-$S_w$ curves obtained by applying the assumption of capillary equilibrium and averaging the wetting phase saturation over the whole domain or the 2-phase domain only.

The same trend is observed for the ‘new’ arithmetic phase volume averaged $P_c$-$S_w$ curve obtained from the simulation data (obtained using Equations (5.12) and (5.14)). The reason for the increase in average wetting phase saturation at a saturation of approximately 0.6 is related to the infiltration of many new heterogeneities around this point. When an applied boundary pressure of 6400 Pa is reached, suddenly 8 heterogeneities that are directly or indirectly connected to the nonwetting reservoir are infiltrated as their entry pressure is overcome (Figure 6.17). However, these heterogeneities have entry pressures just below the applied capillary pressure, so that their equilibrium nonwetting phase saturations will be low. When now an average over the 2-phase domain is considered, these heterogeneities are taken into account in the average, but their nonwetting phase saturation is relatively low. Therefore, suddenly the average wetting phase saturation will increase again, as the domain over which...
the averaging is performed is extended with 8 heterogeneities with a high wetting phase saturation. This effect does not occur when the traditional phase volume arithmetic average is used (Equations (5.1) and (5.5)), as then averaging is performed over the whole domain at all times.

Thus, the so-called analytical curve derived from the method described in Section 6.2 is itself dependent on averaging, and as a result a different ‘analytical’ curve can be obtained by applying different averaging methods. Although it is clear for a homogeneous domain what the sample-scale analytical curve should be, for a heterogeneous domain it is more complicated.

![Figure 6.17: saturation distribution at an applied boundary pressure of a) 6300 Pa, and b) 6400 Pa; at 6400 Pa, 8 heterogeneities are newly infiltrated by the nonwetting phase, which results in an increase in the average wetting phase saturation when averaging over the 2-phase domain only. Static simulation without gravity, 2D heterogeneous domain.](image)

The second observation that can be made when considering Figure 6.14 is that the traditional and new arithmetic phase volume average $P_c$-$S_w$ curves for a simulation without gravity are significantly different. Actually, the curves are more or less the same as the curves obtained for a simulation with gravity. As was mentioned however, for a homogenous simulation it was found that for a simulation without gravity the $P_c$-$S_w$ curves obtained by applying the traditional arithmetic phase volume average or the ‘new’ arithmetic phase volume average are similar, and equal to the reference curve. The difference for a simulation without gravity for a 2D heterogeneous domain indicates that now, the difference between the two curves is not due to gravity forces, as these are absent, but to some other reason. In Figure 6.18, several $P_c$-$S_w$ curves are plotted that were obtained by using different types of averaging for both saturation and pressure, for a simulation without gravity in a 2D heterogeneous domain.

As can be seen, if the saturation is averaged over the whole domain while the pressures are averaged only over the 2-phase domain, the obtained curve is almost equal to the curve obtained by averaging both saturation and pressures over the whole domain. This indicates that the way the saturation is averaged has a large influence on the obtained average equilibrium $P_c$-$S_w$ curve for the 2D heterogeneous domain.

For a homogeneous simulation without gravity, pressures and saturations will be constant throughout the domain when equilibrium is reached. The traditional phase volume averages will give exactly the same results as the phase volume averages over the 2-phase domain only, as for every node the saturation and pressures will be identical, and there is no infiltration front. This is illustrated in Figure 6.19. Alternatively, for a heterogeneous simulation without gravity, pressures and saturations are different for each heterogeneity, as the heterogeneities have different entry pressures. As a result, there will be a difference between traditional phase
volume averages and phase volume averages only over the 2-phase domain, whether gravity is present or not.

Figure 6.18: Different average equilibrium $P_c$-$S_w$ curves, where either both pressures and saturation are averaged over the whole domain, over the two-phase domain, or for saturation over the whole domain and pressures over the 2-phase domain.

Up till now, the only averages discussed are the traditional and new arithmetic phase volume averages. In Chapter 5 however, several other averages were introduced. Unfortunately, it is difficult to obtain the centroid phase average as it is defined in Section 5.4 for the 2D heterogeneous domain, as the gradients of pressure and coordinate $z$ cannot be derived the same way they were for the homogeneous domain (Equation 5.30).

Figure 6.19: Difference between homogeneous domain and heterogeneous domain when gravity is neglected.
In Figure 6.20, the average $P_c$-$S_w$ curve is plotted that is obtained by performing a simple arithmetic average as defined by Equations (5.31) and (5.32) over the whole domain in case of a heterogeneous domain. As can be seen, using a simple arithmetic average results in a sample-scale average equilibrium $P_c$-$S_w$ curve that overestimates the entry pressure of the sample. This overestimation is due to the assumption made when using a Brooks-Corey formulation of the $P_c$-$S_w$ relationships. As was also explained in Section 5.4, it is assumed that if a heterogeneity is not infiltrated with nonwetting phase, its capillary pressure is equal to its entry pressure. As a result, if averaging of pressures is performed over the whole domain, the average capillary pressure will be overestimated until all the heterogeneities are infiltrated by the nonwetting phase. This overestimation does not occur in the analytical curve because there a capillary pressure is applied to the domain and not derived from averaging pressures. In addition, this overestimation also does not occur when an arithmetic phase volume average is used because then the nodes which are not yet infiltrated by the nonwetting phase are excluded in the average nonwetting phase pressure. Note that in case of a homogeneous domain, the overestimation is absent too, because the entry pressure is constant throughout the domain (see Figure 5.23).

Thus, it can be concluded that a simple arithmetic average does not return the analytical capillary pressure-saturation relationship in case of a heterogeneous domain.

\[ P_c \text{ vs. } S_w \text{ curve, static simulation, simple arithmetic average, no gravity} \]

\[ \text{Simple arithmetic average over whole domain} \]

\[ \text{Reference curve (obtained by applying the assumption of capillary equilibrium)} \]

**Figure 6.20:** Average $P_c$-$S_w$ curve obtained by performing a simple arithmetic average over the whole domain for the simulation of a static primary drainage experiment in a 2D heterogeneous domain, neglecting gravity

When the simple arithmetic averaged $P_c$-$S_w$ curve is calculated by setting the nonwetting phase pressure equal to the wetting phase pressure when the nonwetting phase has not yet infiltrated a node (Equation 5.36), Figure 6.20 results. As can be seen, just as for simulations using a homogeneous domain, this averaged curve starts at a capillary pressure of zero when the wetting phase saturation is equal to 1. Then gradually the capillary pressure approaches the analytical sample-scale $P_c$-$S_w$ curve, until it becomes equal to the analytical curve when all heterogeneities are infiltrated with the nonwetting phase (around an average wetting phase saturation of 0.45).
6.3 The average equilibrium $P_c$-$S_w$ relationship for a heterogeneous domain

Finally, in Figure 6.22, the global average as was described in Section 5.6 is plotted for the heterogeneous domain. Note that now, the global average is simply defined as:

\[
\langle P_c \rangle_{\text{global}} = P_{n_{\text{bottom}}} - P_{w_{\text{top}}}
\]

since the simulation is performed without gravity. Moreover, even if the simulation would include gravity, the correction derived in Equation (5.41) cannot be used as the nonwetting phase pressure distribution is not homogeneous in the x-direction anymore. Just as for the homogeneous domain, good results are obtained at high and intermediate average wetting phase saturations. However, as the lower average wetting phase saturations are approached, the global averaged curve asymptotically approaches a higher residual saturation compared to the analytical sample-scale equilibrium $P_c$-$S_w$ curve. As was already explained in Section 5.6, this difference is due to the fact that at low wetting phase saturations, the pressures outside the domain are no longer related to the pressures inside. When averages are used that determine average pressures inside the domain, the fast increase in capillary pressure at low wetting phase saturations is not observed, and the capillary pressure at some point becomes constant. Note that actually the residual saturation for both inside and external averages is the same. However, if one would fit a Brooks-Corey relationship through both types of curves, very different residual saturations will be found. This was also illustrated for a homogeneous domain (Table 5.2).

Concluding this section, it is clear that the determination of the analytical sample-scale equilibrium $P_c$-$S_w$ curve in case of a heterogeneous domain is somewhat subjective. Where for a homogeneous domain, the reference or analytical curve follows a priori from the curve that is specified for the porous medium, for a heterogeneous domain the determination of the
analytical curve is based on the assumption of capillary equilibrium and requires averaging itself. For a heterogeneous domain, the traditional arithmetic phase volume and phase volume averages result in average $P_c-S_w$ curves that represent the analytical sample-scale equilibrium $P_c-S_w$ relationship obtained by applying the assumption of capillary equilibrium. Using a simple arithmetic average over the whole domain results in an overestimation of the entry pressure compared to the analytical sample scale equilibrium $P_c-S_w$ relationship. Finally, a global average gives good results at high and intermediate wetting phase saturations, but shows a deviation at low wetting phase saturations, just as was observed for a homogeneous domain.

In the next section, the effect of heterogeneities on the residual saturation that can be reached in a sample will be discussed.

![Figure 6.22: Average $P_c-S_w$ curve obtained by using a global average ($P_c = P_{a \text{ reservoir}} - P_{w \text{ reservoir}} \Rightarrow P_c = P_{a \text{ bottom}} - P_{w \text{ top}}$) for the phase pressures.](image)

6.4 The effect of heterogeneities on the average residual wetting phase saturation

In this section, the effect of heterogeneities on the residual wetting phase saturation that can be reached in a sample will be investigated. It would be expected that when a sample contains heterogeneities, the residual wetting phase saturation that can be reached in the sample will be higher compared to a sample that is homogeneous. This is because heterogeneities with a low entry pressure are infiltrated by the nonwetting phase relatively fast, so that heterogeneities with a higher entry pressure can become surrounded by heterogeneities that have already a low wetting phase saturation. As a result, drainage of the higher entry pressure heterogeneities is inhibited, and the average residual wetting phase saturation that is reached will be higher than for a homogeneous case.
In Figure 6.23, the average equilibrium $P_c - S_w$ curve obtained for a homogeneous domain is compared to the average equilibrium $P_c - S_w$ curve obtained for a heterogeneous domain. The results are shown for simulations including gravity, as that would be the case in real laboratory experiments. However, it was also shown in Section 6.3 that the influence of gravity forces on the sample-scale $P_c - S_w$ relationship is negligible due to the short length of the sample domain (see Figure 6.11 and 6.12). The averaging method that is used is the traditional arithmetic phase volume average (Equations (5.2) and (5.5)). Note however that the used averaging method does not have an effect on the average residual saturation that can be reached.

As can be seen in Figure 6.23, the average residual wetting phase saturation that is reached for the homogeneous domain and the heterogeneous domain are more or less similar. The effect of heterogeneities on the residual saturation thus seems negligible, at least for heterogeneities with the intensity that is assumed to occur in a laboratory sample. However, it could also be that for different patterns and distributions of heterogeneities, the effect on the average residual wetting phase saturation is not negligible for the assumed intensity. The effect of heterogeneity distribution and pattern is not investigated in this thesis, but interested readers are referred to papers of for instance Das et al. (2004) and Ataie-Ashtiani et al. (2001, 2002). Note also that with increasing column length or width, the effect of heterogeneities could become larger.

![Figure 6.23: arithmetic phase volume average equilibrium $P_c - S_w$ relationship obtained for a homogeneous and heterogeneous domain, respectively. Simulation of primary static drainage experiment, including gravity.](image)

In Figure 6.24, the global average equilibrium $P_c - S_w$ curves are shown obtained for the homogeneous domain and the heterogeneous domain. The figure illustrates again that the difference between the average residual wetting phase saturations is negligible. As was already mentioned a couple of times before, with the global average, a capillary pressure-
saturation curve is obtained that is different from the analytical curve at low wetting phase saturations. Thus, it seems that the intensity of the heterogeneities used here is not strong enough to result in a higher average residual wetting phase saturation compared to a homogeneous situation. Therefore, also a simulation is performed for a heterogeneous domain with higher intensity heterogeneities. The procedure as described in Section 6.1.1 is used to obtain the permeability and entry pressure for each heterogeneity. The exact same procedure was followed, with the exception that now the mean and standard deviation of the used lognormal distribution are

\[ \mu = 3.63 \cdot 10^{-12} \text{ m}^2 \quad (6.16) \]

\[ \sigma = 4.75 \cdot 10^{-12} \text{ m}^2 \quad (6.17) \]

![Figure 6.24: global average equilibrium \( P_c - S_w \) relationship obtained for a homogeneous and heterogeneous domain, respectively.](image)

The random number generator in Matlab is seeded the same way as it was seeded in order to obtain the low intensity heterogeneous domain, so that the same distribution of heterogeneities with high and low entry pressures is obtained. Therefore, the only difference between the two heterogeneous domains is the intensity of the heterogeneities. Figure 6.25 shows the resulting heterogeneous domain. As can be seen, now the permeability varies between 0.27\( \cdot 10^{-12} \) m\(^2\) and 6.67\( \cdot 10^{-12} \) m\(^2\), which results in an entry pressure that varies between 3446 Pa and 17288 Pa. Just as for the low intensity heterogeneous domain, an analytical sample-scale equilibrium capillary pressure-saturation relationship is obtained by applying the assumption of capillary equilibrium (see Section 6.2). Moreover, a homogeneous simulation is performed for which the local curve is determined by fitting a curve through the heterogeneous analytical sample-scale equilibrium \( P_c - S_w \) relationship.
6.4 The Effect of Heterogeneities on the Average Residual Wetting Phase Saturation

Figure 6.25: 2D heterogeneous domain with stronger heterogeneities.

Figure 6.26: arithmetic phase volume average equilibrium $P_c S_w$ curves for a homogeneous domain (avg. over 2-phase domain), and a heterogeneous domain with strong heterogeneities (avg over whole domain).
In Figure 6.26, the obtained arithmetic phase volume average equilibrium capillary pressure-saturation relationships for both the homogeneous domain and the heterogeneous domain with strong heterogeneities are shown.

Figure 6.27: a) average capillary pressure as a function of applied nonwetting phase bottom boundary pressure; b) average wetting phase saturation as a function of applied nonwetting phase bottom boundary pressure

As can be seen, now the effect of the heterogeneities on the average residual wetting phase saturation that can be reached is significant. While for the homogeneous simulation an average residual wetting phase saturation of approximately 0.1 is reached, for the heterogeneous simulation the average wetting phase saturation only reaches a value of 0.36. Figure 6.27 shows the average capillary pressure and wetting phase saturation as a function of the applied nonwetting phase bottom boundary pressure. The figure shows that for the homogeneous domain, the average capillary pressure and wetting phase saturation keep changing throughout the simulation, and are still changing when the maximum applied nonwetting phase bottom boundary pressure is reached. However, for the heterogeneous domain, the capillary pressure and wetting phase saturation at some point do not change anymore even though the nonwetting phase pressure at the bottom boundary is increased. Thus, the residual wetting phase saturation that is reached really is the lowest saturation that can be reached in the domain with strong heterogeneities.

The difference between the residual average wetting phase saturations obtained for the homogeneous and heterogeneous domain is caused by the trapping of wetting phase in heterogeneities with high entry pressures. This is illustrated in Figure 6.28, which shows the final saturation distribution for the homogeneous and heterogeneous domain. Clearly, for the heterogeneous domain there are several heterogeneities that are not or only slightly infiltrated by the nonwetting phase, even though their entry pressure is far below the applied nonwetting phase boundary pressure of 27600 Pa. However, because the entry pressure of these heterogeneities is only reached when the surrounding heterogeneities are already infiltrated by the nonwetting phase, drainage of these heterogeneities is prevented and the wetting phase becomes trapped.

Note that as was discussed in Section 4.4.2, the strictness of the used equilibrium criterion has a large influence on the obtained average residual wetting phase saturation. With a very strict equilibrium criterion, it could be possible to obtain residual saturations that are close to the residual saturation defined for the analytical curve. However, in reality such equilibrium criteria are never used because then it would take too long to measure a complete capillary pressure-saturation relationship.
6.4 The Effect of Heterogeneities on the Average Residual Wetting Phase Saturation

Figure 6.28: Saturation distribution at an applied nonwetting phase bottom boundary pressure of 27600 Pa for a) the homogeneous domain; b) the heterogeneous domain. Note that for the heterogeneous domain, the applied nonwetting phase bottom boundary pressure surpasses the entry pressure of every heterogeneity in the domain, but despite this several heterogeneities are not or only slightly infiltrated by the nonwetting phase.

Therefore, the average residual wetting phase saturations obtained in this section by applying a relatively loose equilibrium criterion are considered to be representative of the residual wetting phase saturations that can be obtained in laboratory experiments.

Based on the simulations discussed in this section, it can be concluded that, at least for the specific heterogeneous domain used in these simulations, weak heterogeneities do not have a significant effect on the average residual wetting phase saturation that can be reached in a sample. However, strong heterogeneities are shown to have a significant effect. In addition, it should be added that different patterns or distributions of the heterogeneities may have a different effect on the obtained sample-scale capillary pressure-saturation relationship. In Chapter 7, the effect of heterogeneities in combination with the presence of a hydrophilic membrane used in static primary drainage experiments will be investigated further.

6.5 Summary and Conclusions

In this chapter, the effect of heterogeneities on the sample-scale equilibrium capillary pressure-saturation relationship is investigated. A heterogeneous domain is created by dividing a 3 cm × 6 cm 2-dimensional domain into 36 blocks of equal area. Subsequently, each block is assigned an intrinsic permeability randomly drawn from a lognormal distribution. The entry pressure then is determined using the Leverett J-function. For the constructed heterogeneous domain, an analytical sample-scale equilibrium capillary pressure-saturation relationship is determined by applying the assumption of capillary equilibrium. The average equilibrium capillary pressure-saturation relationship as obtained from simulation data is compared with the analytical curve. The following is concluded:

- The traditional arithmetic phase volume and phase volume averages return good results, both for simulations with and without gravity.
- The ‘new’ arithmetic phase volume and phase volume averages as defined in Equation (5.12), (5.13) and (5.14) give rise to significantly different capillary pressure-saturation relationships, both for simulations with and without gravity. This is simply
caused by the non-homogeneous saturation and pressure distributions that occur in a heterogeneous domain regardless of gravity effects.

- A simple arithmetic average over the whole domain for the capillary pressure results in an overestimation of the entry pressure in the obtained average P<sub>c</sub>-S<sub>w</sub> relationship. This is due to the numerical model, in which nodes that are not yet infiltrated by the nonwetting phase are assigned a nonwetting phase pressure equal to the wetting phase pressure plus the entry pressure of the heterogeneity the node is located in.

- As was found for a homogeneous domain, an average capillary pressure-saturation relationship based on a global average capillary pressure gives good correspondence with the analytical curve at high and intermediate average wetting phase saturations. At low wetting phase saturations, the global averaged capillary pressure is no longer related to the average capillary pressure inside the sample, and as a result the global averaged curve displays an fast increase in capillary pressure, while the average capillary pressure inside the sample stays constant.

- When heterogeneities are present in a sample, they can act to increase the residual wetting phase saturation that can be reached in a sample. However, the extent to which this occurs is dependent on the intensity of the heterogeneity pattern. For the particular heterogeneity pattern used in this chapter, it is shown that an intensity that is assumed to occur in a laboratory sample, there is no significant increase in the average residual wetting phase saturation that can be reached due to the presence of heterogeneities. Nonetheless, with increasing intensity the residual wetting phase saturation can increase significantly. Moreover, the effect of heterogeneities could also be dependent on the pattern or distribution of the heterogeneities.
Chapter 7

The use of a hydrophilic membrane in the measurement of $P_c$-$S_w$ relationships

In the previous chapters, it was shown that the capillary pressure-saturation relationship obtained at the sample scale is not necessarily an intrinsic property of the porous medium for which it is derived. The average $P_c$-$S_w$ curve can depend on for instance measurement techniques (e.g. measurement of pressures inside or outside of the sample), and, in case numerical simulations are performed, the averaging methods used. Moreover, it also depends on the strictness of the equilibrium criterion. Therefore, care should be taken when talking about ‘the’ capillary pressure-saturation relationship of a porous medium.

In this last chapter, the effect of the presence of a hydrophilic membrane on the sample-scale capillary pressure-saturation relationship will be investigated. As was mentioned in Chapter 2, in the laboratory measurement of a $P_c$-$S_w$ relationship, often membranes are used at the outflow of the laboratory sample to prevent either the nonwetting phase or wetting phase from leaving the sample. By making use of these membranes, the determination of the equilibrium $P_c$-$S_w$ curve takes considerably less time. When a drainage experiment is performed, the inflow of the sample is covered by a hydrophobic membrane, which prevents the wetting phase from leaving the sample through the inflow, while the outflow of the sample is covered with a hydrophilic membrane, preventing the nonwetting phase from leaving the sample when it reaches the outflow. When an imbibition experiment is performed, flow is reversed such that now the side of the sample with the hydrophilic membrane becomes the inflow of the sample, preventing the nonwetting phase from leaving through the inflow, while the hydrophobic membrane now is situated at the outflow, preventing the wetting phase from leaving the sample through the outflow.

The use of membranes that prevent either the nonwetting or wetting phase from leaving the sample make it possible to achieve a static equilibrium distribution of the fluids inside the sample for each applied boundary pressure. This means that both nonwetting and wetting phase fluxes approach zero as equilibrium is approached. However, in a lot of situations for which the capillary pressure-saturation relationship is obtained (e.g. the field), membranes are not present to prevent fluids from flowing, and steady-state or even dynamic flow conditions will prevail. As was discussed in Section 2.4, usually it is assumed that the capillary pressure-saturation relationship obtained under static conditions (i.e. by making use of hydrophilic/hydrophobic membranes) can be used in the description of two-phase flow systems were there is steady-state or transient flow. However, several researchers have shown that the capillary pressure-saturation relationship obtained under transient flow conditions is different from the capillary pressure-saturation relationship obtained under static conditions. This also follows from the extended formulation for capillary pressure proposed by Hassanizadeh and Gray (1993a) (Equation 2.55). According to this formulation, the dynamic capillary pressure is equal to the capillary pressure acquired under static conditions plus a term that is proportional to the rate of change of saturation. When there is no flow, or a steady-state flow, there are no changes in saturation through time, so that the dynamic capillary pressure becomes equal to the static or equilibrium capillary pressure. Thus, based on Equation (2.55), it can be expected that the capillary pressure-saturation relationship
obtained by performing a primary drainage experiment under static conditions is equal to the capillary pressure-saturation relationship obtained by performing a primary drainage experiment under steady-state conditions. This is also observed by several researchers, under which Topp et al. (1967) (see Figure 2.23). Even though in theory the capillary pressure-saturation relationships obtained under static and steady-state conditions should be equal, it could be expected that in reality the residual average wetting phase saturation that can be reached in a laboratory sample is dependent on whether a steady-state or static primary drainage experiment is performed. This is because the presence of a hydrophilic membrane prevents the nonwetting phase from leaving the sample, so that it will start accumulating below this membrane. Here it can prevent the wetting phase from leaving the sample. This effect is expected to be enhanced by the presence of heterogeneities.

In this final chapter, the following questions will be investigated:

- What is the effect of the presence of a hydrophilic membrane on the average residual wetting phase saturation that can be reached in a sample?
- What is the effect of heterogeneities in combination with a hydrophilic membrane on the average residual wetting phase saturation that can be reached in a sample?
- What other factors influence the average residual wetting phase saturation that can be reached in a sample?
- Is there a significant difference between how the capillary pressure-saturation relationship usually is measured in a laboratory sample, and how it alternatively could or should be measured?

Table 7.1 provides an overview of the simulations referred to in this chapter.

### Table 7.1: Overview of the simulations referred to in Chapter 7

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Description</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>1) static simulation, homogeneous domain, gravity</td>
<td>300 steps of 100 Pa</td>
<td>Input curve $P_d = 6000 \text{ Pa}$, $S_{wr} = 0.104$, $\lambda = 6.11$ Column of 18.2 cm length</td>
</tr>
<tr>
<td>2) steady-state simulation, homogeneous domain, gravity</td>
<td>300 steps of 100 Pa</td>
<td>Input curve $P_d = 6000 \text{ Pa}$, $S_{wr} = 0.104$, $\lambda = 6.11$ Column of 18.2 cm length</td>
</tr>
<tr>
<td>3) static simulation, homogeneous domain, gravity</td>
<td>300 steps of 100 Pa</td>
<td>Input curve $P_d = 6000 \text{ Pa}$, $S_{wr} = 0.104$, $\lambda = 6.11$ Column of 3 cm length</td>
</tr>
<tr>
<td>4) steady-state simulation, homogeneous domain, gravity</td>
<td>300 steps of 100 Pa</td>
<td>Input curve $P_d = 6000 \text{ Pa}$, $S_{wr} = 0.104$, $\lambda = 6.11$ Column of 3 cm length</td>
</tr>
<tr>
<td>5) static simulation, 2D heterogeneous domain, 3 cm × 6 cm, gravity</td>
<td>300 steps of 100 Pa</td>
<td>Low intensity heterogeneities</td>
</tr>
<tr>
<td>6) static simulation, 2D homogeneous domain, 3 cm × 6 cm, gravity</td>
<td>300 steps of 100 Pa</td>
<td>Input curve $P_d = 6168 \text{ Pa}$, $S_{wr} = 0.102$, $\lambda = 5.34$ (fit through heterogeneous analytical curve)</td>
</tr>
<tr>
<td>7) steady-state simulation, 2D heterogeneous domain, 3 cm × 6 cm, gravity</td>
<td>300 steps of 100 Pa</td>
<td>Low intensity heterogeneities</td>
</tr>
<tr>
<td>8) steady-state simulation, 2D homogeneous domain, 3 cm × 6 cm, gravity</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### 7.1 Procedure

The simulations referred to in this chapter are obtained with the Berentsen model, unless stated otherwise.

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Domain Type</th>
<th>Domain Dimensions</th>
<th>Boundary Conditions</th>
<th>Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>9) static simulation, 2D heterogeneous domain, 3 cm × 6 cm, gravity</td>
<td>2D heterogeneous domain</td>
<td>3 cm × 6 cm</td>
<td>300 steps of 100 Pa</td>
<td>High intensity heterogeneities</td>
</tr>
<tr>
<td>10) static simulation, 2D homogeneous domain, 3 cm × 6 cm, gravity</td>
<td>2D homogeneous domain</td>
<td>3 cm × 6 cm</td>
<td>300 steps of 100 Pa</td>
<td>High intensity heterogeneities</td>
</tr>
<tr>
<td>11) steady-state simulation, 2D heterogeneous domain, 3 cm × 6 cm, gravity</td>
<td>2D heterogeneous domain</td>
<td>3 cm × 6 cm</td>
<td>300 steps of 100 Pa</td>
<td>High intensity heterogeneities</td>
</tr>
<tr>
<td>12) steady-state simulation, 2D homogeneous domain, 3 cm × 6 cm, gravity</td>
<td>2D homogeneous domain</td>
<td>3 cm × 6 cm</td>
<td>300 steps of 100 Pa</td>
<td>High intensity heterogeneities</td>
</tr>
<tr>
<td>13) static simulation, homogeneous domain, gravity</td>
<td>Homogeneous domain</td>
<td></td>
<td>300 steps of 100 Pa</td>
<td>Column of 18.2 cm length, Flow from top to bottom</td>
</tr>
</tbody>
</table>

### 7.1.1 Domain description

In this chapter, simulations for both a homogeneous and a heterogeneous domain will be discussed. For the simulations using a homogeneous domain, the domain and medium properties are identical to the domain and medium properties described in Section 4.2.1. The domain and medium properties used in the simulations for a 2D heterogeneous domain are the same as the properties described in Section 6.1.1. Note that for the homogeneous simulations, a domain with a length of 18.2 cm is used, while for the heterogeneous domain, a 6 cm wide and 3 cm long domain is used. Therefore, the two types of simulations cannot be directly compared. The simulation results for the heterogeneous domain should be compared to results from a simulation for a 3 cm long homogeneous domain.

### 7.1.2 Boundary and initial conditions

The boundary and initial conditions applied in the simulations referred to in this chapter are identical to the conditions introduced in Section 4.2.2. Note that simulations for both a static and steady-state primary drainage experiment will be performed. As long as the nonwetting phase has not yet reached the outflow of the sample, a static primary drainage experiment is equal to a steady-state primary drainage experiment.

### 7.2 The effect of a hydrophilic membrane

In this section, the effect of the presence of a hydrophilic membrane on the sample-scale capillary pressure-saturation relationship is investigated. As was mentioned in the introduction of this chapter, it would be expected that the presence of such a membrane influences the average residual wetting phase saturation that can be reached in a sample,
because the nonwetting phase accumulates below the hydrophilic membrane during a drainage experiment. As a result, the wetting phase has difficulty leaving the sample through the outflow, as the relative permeability of the wetting phase just below the membrane becomes very low. In Section 7.2.1, first the effect of a hydrophilic membrane is investigated for a simple homogeneous domain. Subsequently, in Section 7.2.2, the same is done for a heterogeneous domain. In Section 7.2.3, an overview is given of all the factors found in this thesis that have an influence on the average residual wetting phase saturation that can be reached in a sample.

### 7.2.1 The effect of a hydrophilic membrane on the average $P_c$-$S_w$ curve in a homogeneous domain

In this subsection, the effect of the presence of a hydrophilic membrane on the sample-scale capillary pressure-saturation relationship in a homogeneous domain is investigated. For this purpose, simulation results of a static and steady-state primary drainage experiment are compared. Figure 7.1 illustrates the difference between the two types of experiments once again.

![Diagram of static and steady-state primary drainage experiments](image)

**Figure 7.1:** The difference between a static primary drainage experiment and a steady-state primary drainage experiment for a homogeneous domain.

For a static primary drainage experiment, the nonwetting phase is not allowed to leave the sample domain. As a result, when equilibrium is approached in the domain after an incremental pressure increase, both the wetting phase and nonwetting phase fluxes will approach zero. This type of equilibrium is called a static equilibrium. For a steady-state primary drainage experiment, both the wetting and nonwetting phase are allowed to flow out of the sample, as there is no membrane present. Before the nonwetting phase reaches the outflow of the sample, both the nonwetting phase and wetting phase fluxes inside the sample approach zero as equilibrium is approached, and the equilibrium is a static equilibrium. However, when the nonwetting phase reaches the outflow, it starts to flow out, and when equilibrium is approached the wetting phase flux becomes zero, while the nonwetting phase...
flux stays nonzero but approaches a constant value. This type of equilibrium is called a steady-state equilibrium, as the pressure and saturation distributions do not change anymore, but there still is a (constant) flux of nonwetting phase passing through the sample.

In Figure 7.2, the obtained average equilibrium capillary pressure-saturation relationships are shown for a simulation of a static primary drainage experiment, and a steady-state primary drainage experiment, respectively. Note that the column has a length of 18.2 cm, and a homogeneous domain is considered. The averaging of pressures and saturations has been done according to the ‘new’ arithmetic phase volume average (Equations 5.12 and 5.14). However, the type of averaging used does not have an influence on the residual saturation that is reached in the sample.

In Figure 7.2, two differences can be observed between the average $P_c$-$S_w$ relationship obtained for a static and a steady-state primary drainage experiment, respectively:

1. After the nonwetting phase reaches the outflow of the sample, which in this case occurs around an average wetting phase saturation of 0.6, the average $P_c$-$S_w$ curve obtained for the simulation of a steady-state primary drainage experiment begins to deviate from the reference curve. For the same average wetting phase saturation, the steady-state average $P_c$-$S_w$ curve gives a higher average capillary pressure than the reference curve. Also, the average $P_c$-$S_w$ curve obtained for a static primary drainage experiment stays close to the reference curve.

2. For the simulation of a steady-state primary drainage experiment, a lower average residual wetting phase saturation is reached compared to the simulation of a static primary drainage experiment. For this particular homogeneous domain of 18.2
cm length, and a final applied bottom boundary pressure of 30000 Pa, a residual wetting phase saturation of 0.172 is reached in the simulation of a static primary drainage experiment, while a residual wetting phase saturation of 0.145 is reached in the simulation of a steady-state primary drainage experiment. Note that the final average wetting phase saturation that is reached in a simulation also is dependent on simulation time and equilibrium criterion (see Section 4.4).

The first observation is caused by the difference in flow conditions when equilibrium is reached. Before the nonwetting phase reaches the outflow of the sample, flow conditions for both the static and steady-state primary drainage experiment are equal, because a static equilibrium is reached in both types of simulations. Before breakthrough of the nonwetting phase in a steady-state primary drainage experiment, there won’t be a steady-state flow of the nonwetting phase. After the nonwetting phase reaches the outflow however, for the simulation of a static primary drainage experiment still a static equilibrium is reached, while for the simulation of a steady-state primary drainage experiment now a steady-state equilibrium is reached. The flow of the nonwetting phase at steady-state equilibrium causes the gradients in pressure inside the sample to be different as there is an extra force caused by the constant flow of the nonwetting phase. This is illustrated in Figure 7.3, which shows the pressure distributions for an applied nonwetting phase bottom boundary pressure of 30000 Pa for the simulation of both a static and steady-state primary drainage experiment. As can be seen, the pressure distributions are very different, and as a result the average capillary pressure derived from these distributions is higher for a steady-state primary drainage experiment compared to a static primary drainage experiment.

![Pressure distribution at a P_{bottom} of 29998 Pa for both static and steady-state simulations](image)

**Figure 7.3:** Pressure distributions for both simulations of static and steady-state primary drainage experiments, and the derived average pressures, for an applied nonwetting phase bottom boundary pressure of 29998 Pa. (i.e. the end of the simulations).

As can be seen from Figure 7.3, the pressure gradients in a steady-state primary drainage experiment when equilibrium is reached are much steeper than in case of a static primary
drainage experiment. This is due to the difference in boundary conditions at the outflow of the sample.

The second observation that is made based on Figure 7.2 is that a lower average residual wetting phase saturation can be reached when a steady-state primary drainage experiment is simulated. This is also as is expected, as the hydrophilic membrane in the simulation of a static primary drainage experiment prevents the nonwetting phase from leaving the sample. As a result, the nonwetting phase will start to accumulate at the hydrophilic membrane, where it prevents the wetting phase from leaving the sample by decreasing the relative permeability of the wetting phase. This is shown in Figure 7.4, in which the nonwetting phase saturation
distribution at different moments in the drainage process is plotted, for both the simulation of a static and a steady-state primary drainage experiment.

Before the nonwetting phase reaches the outflow, the saturation distributions are approximately equal, as would be expected because in both cases a static equilibrium is reached. The small difference that can be observed is caused by the difference in the intrinsic permeability used for the bottom artificial layer (see also Section 4.2). After the nonwetting phase reaches the outflow, the distributions become significantly different. For the steady-state primary drainage experiment, the nonwetting phase is drawn out of the domain due to the boundary conditions imposed at the outflow, and as a result the nonwetting phase saturation drops as the outflow is approached. Alternatively, for the static primary drainage experiment, the nonwetting phase is not allowed to leave the column, and due to the accumulation of nonwetting phase below the hydrophilic membrane, the nonwetting phase saturation increases as the outflow is approached.

In Figure 7.5, the average wetting phase saturation is plotted as a function of the applied nonwetting phase bottom boundary pressure. For the simulation of a steady-state primary drainage experiment, the average wetting phase saturation is decreasing throughout the simulation, and is still decreasing when the final applied bottom boundary pressure of 29998 Pa is reached. This indicates that if the simulation would be continued by increasing the nonwetting phase boundary pressure further, even a lower average wetting phase saturation can be reached. However, for the simulation of a static primary drainage experiment, the average wetting phase saturation decreases initially, but becomes constant at an applied nonwetting phase bottom boundary pressure of approximately 14000 Pa. Thus, even though the nonwetting phase bottom boundary pressure is increased, the average wetting phase saturation does not change anymore. The same trend can be observed for the average capillary pressure, which still is increasing when the end of the simulation is approached in case of a steady-state primary drainage experiment, but has stabilised in case of a static primary drainage experiment.

The results discussed above indicate that with a steady-state primary drainage experiment, lower wetting phase saturations can be reached in a sample than with a static primary drainage experiment.
experiment. It could be possible that in the simulation of a steady-state primary drainage experiment, even a lower average residual wetting phase saturation can be reached, if the applied nonwetting phase bottom boundary pressure is increased sufficiently. For the static primary drainage experiment, a ‘true’ average residual wetting phase saturation is reached within the final applied bottom boundary pressure of 30000 Pa, and it is not possible to further decrease the wetting phase saturation in the sample. This residual saturation is significantly higher than the specified residual saturation for the porous medium.

The above discussion shows that the presence of a hydrophilic membrane has a significant influence on the residual wetting phase saturation that can be reached in a sample. Use of a hydrophilic membrane to prevent the nonwetting phase from leaving the sample can result in an overestimation of the residual wetting phase saturation. If a steady-state experiment is performed, lower residual saturations can be reached, which are closer to the intrinsic residual wetting phase saturation of the porous medium. However, the steady-state flow of the nonwetting phase when a steady-state equilibrium is reached does result in a deviation of the average $P_{c-S_w}$ curve from the reference curve after breakthrough.

Note that the effect of the hydrophilic membrane on the residual saturation that can be reached in a sample also is dependent on the sample column length. The longer the column, the stronger the effect of the hydrophilic membrane on the residual saturation that can be reached in the sample. With increasing column length, the residual wetting phase saturation in the column increases. This is illustrated in Figure 7.6.

![Figure 7.6: Average capillary pressure-saturation relationships obtained for simulation of a steady-state and static primary drainage experiment, respectively, using a column of either 18.2 cm or 3 cm.](image)

As can be seen, the difference between residual wetting phase saturations reached in a static and steady-state simulation is larger for the longer column of 18.2 cm, compared to the shorter column of 3 cm. For the simulation of a steady-state primary drainage experiment, the difference in residual saturation that can be reached in an 18.2 cm column and 3 cm column is
not very different. However, the obtained average $P_c$-$S_w$ curves do show a difference in the average capillary pressure compared to the reference curve. With decreasing column length, the average capillary pressure of the $P_c$-$S_w$ curve increases stronger after the nonwetting phase reaches the outflow of the sample, so that the deviation from the reference curve becomes larger. This is due to the steeper pressure gradients that are reached in a short column compared to a longer column.

Figure 7.7: Average wetting phase saturation as a function of the applied nonwetting phase bottom boundary pressure for a) simulation of static primary drainage experiment for column lengths of 18.2 and 3 cm, respectively; b) simulation of steady-state primary drainage experiment for column lengths of 18.2 cm and 3 cm, respectively.

In Figure 7.7, again the average wetting phase saturations are plotted as a function of the applied nonwetting phase bottom boundary pressure, now for the different column lengths. As can be seen, for the simulation of a static primary drainage experiment, for a shorter column, a lower residual wetting phase saturation can be reached. For the simulation of a steady-state primary drainage experiment, the average wetting phase saturation that is reached at the end of the simulation is approximately equal for both column lengths, and is still changing when the end of the simulation is reached.

Note however that in the discussion about column lengths, the same boundary conditions are applied for both the 3 cm and 18.2 cm column. As a result, there is a difference between the pressure gradients inside the columns. By using the same boundary conditions (i.e. the same applied nonwetting phase bottom boundary pressure), in the short column of 3 cm steeper gradients in pressure are reached than is the case for the long column of 18.2 cm. As a result, drainage is easier in the short column, especially when a static primary drainage experiment is considered. Thus, in order to truly investigate the effect of column length on the residual saturation that can be reached when performing a static or steady-state primary drainage experiment, the gradients in pressure should be kept constant for each column. This means that the boundary conditions need to be adapted. For instance, if for the simulation of a static primary drainage experiment in an 18.2 cm long column pressure increments of 100 Pa are used, for the same simulation in a 3 cm long column pressure increments of 100/6 Pa have to be used in order to create the same pressure gradient in both columns.
7.2.2 The effect of a hydrophilic membrane on the average $P_c$-$S_w$ curve in a heterogeneous domain

In this subsection, the influence of heterogeneities in combination with the use of a hydrophilic membrane is investigated. It would be expected that the presence of heterogeneities enhances the effect of a hydrophilic membrane. This is because with heterogeneities, it is possible that the nonwetting phase reaches the outflow by flow through the higher permeable heterogeneities. The low permeable heterogeneities however are not yet infiltrated by the nonwetting phase due to their higher entry pressure. If a hydrophilic membrane is present, the nonwetting phase accumulates below the membrane, and as a result it can prevent the lower permeable regions that only are drained at higher capillary pressures, from draining effectively. As a result, the presence of membranes in a heterogeneous sample could result in even higher residual wetting phase saturations than are observed in homogeneous samples where the same membranes are used. An illustration of this effect is given in Figure 7.8.

Figure 7.9 shows the obtained average $P_c$-$S_w$ relationships for the simulation of a steady-state and static primary drainage experiment in the 2D heterogeneous domain (see Section 6.1.1). Note that in the simulations discussed here, gravity is included, and an arithmetic phase volume average is used to obtain average pressures and saturations. This causes the average $P_c$-$S_w$ curves showed in Figure 7.9 to deviate slightly from the analytical curve at high average wetting phase saturations.

Just as was observed for a homogeneous domain, the average residual wetting phase saturation that can be obtained if a static primary drainage experiment is performed is higher than the average wetting phase saturation that can be obtained with a steady-state primary drainage experiment. Note that the difference is smaller as was observed in Section 7.2.1 for the homogeneous domain, but this is because the heterogeneous domain only has a length of 3 cm.

![Drainage experiment of heterogeneous porous medium](image_url)

Figure 7.8: Schematic of a drainage process in a heterogeneous porous medium on which a static primary drainage experiment is performed. The accentuated regions are heterogeneities with a lower permeability and thus higher entry pressure. If the nonwetting phase reaches the outflow, accumulation of this phase can inhibit the outflow of the wetting phase.
Figure 7.9: Average capillary pressure-saturation relationships obtained for a simulation of a static and a steady-state primary drainage experiment, respectively, for a 2D heterogeneous domain.

In Figure 7.10, the saturation distributions corresponding to an applied nonwetting phase bottom boundary pressure of 29998 Pa (i.e. the end of the simulation) are plotted. As can be seen, the difference between the distributions is not that pronounced because the heterogeneities are relatively weak. However, it does show that for the static primary drainage experiment, there are several heterogeneities that are drained to a lesser extent compared to the steady-state primary drainage experiment. Now, the question is whether the presence of the heterogeneities enhances the effect of the hydrophilic membrane. Thus, is the difference between the residual wetting phase saturation...
that can be reached in a static and steady-state primary drainage experiment more pronounced when a domain contains heterogeneities? In order to investigate this simulations of a steady-state and static primary drainage experiment for a homogeneous domain of 3 cm length are compared to simulations of a steady-state and static primary drainage experiment for a heterogeneous domain of 3 cm × 6 cm (see Section 6.1.1). Results are shown in Figure 7.11. At first sight, the differences between the residual saturations that are reached in the different simulations do not seem to be significant. By closer examination, the heterogeneities in both steady-state and static primary drainage experiments result in a slightly higher residual wetting phase saturation.

![Figure 7.11: Average capillary pressure-saturation relationships obtained from simulations of steady-state/static primary drainage experiments in a homogeneous/heterogeneous domain.](image)

Note however that for the steady-state primary drainage experiment, the difference between homogeneous and heterogeneous domain is much smaller than for a static primary drainage experiment. The difference between the residual saturation reached in a steady-state and static primary drainage experiment is slightly larger for a heterogeneous domain. This becomes more clear when Table 7.2 is considered, which contains the average residual wetting phase saturations that are reached at the end of each simulation (i.e. for $P_{n\text{bottom}} = 27578$ Pa). The table indicates that the difference in the average residual wetting phase saturation that is reached at the end of a simulation between a steady-state and a static primary drainage experiment for a homogeneous domain is 0.006, while for a heterogeneous domain this difference is 0.01. Thus, it seems that the presence of heterogeneities does enhance the effect of the hydrophilic membrane.

Of course, the differences discussed above are very small, but they could become more significant if more intense heterogeneities are present in the domain. This is investigated by comparing homogeneous simulations of steady-state and static primary drainage experiments with heterogeneous simulations of steady-state and static primary drainage experiments, where now more intense heterogeneities are used. The heterogeneous domain with more intense heterogeneities used here is the same as the domain that is introduced in Section 6.4.
Table 7.2: Average residual wetting phase saturation that is reached at the end of the simulation of a static/steady state primary drainage experiment in a homogeneous/weak heterogeneous domain

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Residual wetting phase saturation reached at end of simulation ($P_n^{\text{bottom}} = 27578 \text{ Pa}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Homogeneous domain of 3 cm Static primary drainage Input curve: $P_d = 6168 \text{ Pa}, S_w = 0.102, \lambda = 5.34$ (fit through heterogeneous analytical curve)</td>
<td>0.149</td>
</tr>
<tr>
<td>Homogeneous domain of 3 cm Steady-state primary drainage Input curve: $P_d = 6168 \text{ Pa}, S_w = 0.102, \lambda = 5.34$ (fit through heterogeneous analytical curve)</td>
<td>0.143</td>
</tr>
<tr>
<td>Heterogeneous domain of 3 cm $\times$ 6 cm Static primary drainage Low intensity heterogeneities</td>
<td>0.153</td>
</tr>
<tr>
<td>Heterogeneous domain of 3 cm $\times$ 6 cm Steady-state primary drainage Low intensity heterogeneities</td>
<td>0.143</td>
</tr>
</tbody>
</table>

Figure 7.12: Average capillary pressure-saturation relationships obtained for the simulation of a static and steady-state primary drainage experiment, for a 2D domain with strong heterogeneities.

In Figure 7.12, the average capillary pressure-saturation curve is shown for the simulation of a static and steady-state primary drainage experiment, for a heterogeneous domain with strong heterogeneities. The figure shows that for the stronger heterogeneities, there is a larger difference between the average residual wetting phase saturation that can be reached in a steady-state and static primary drainage experiment.
In Figure 7.13, the saturation distributions obtained in the simulation of a steady-state and static primary drainage experiment for an applied nonwetting phase bottom boundary pressure of 27578 Pa are shown. For a heterogeneous domain with stronger heterogeneities, clearly there are several heterogeneities that are not or only slightly infiltrated by the nonwetting phase. The saturation distribution obtained for a static primary drainage experiment shows a number of heterogeneities that are not or only slightly infiltrated by the nonwetting phase when a nonwetting phase bottom boundary pressure is reached of 27578 Pa. Moreover, the saturation distributions show that for the static primary drainage experiment, the heterogeneities just below the outflow of the sample are all saturated with nonwetting phase to high levels. Of course, this is due to the accumulation of the nonwetting phase below the hydrophilic membrane.

In Figure 7.14, the average capillary pressure-saturation relationships obtained for simulations of steady-state and static primary drainage experiments for both a homogeneous domain and the strong heterogeneous domain are compared, just as was done in Figure 7.11 for the weak heterogeneous domain. Note that for the homogeneous domain, an input curve is used that is obtained by fitting a Brooks-Corey relationship through the analytical $P_c-S_w$ relationship acquired for the strong heterogeneous domain by assuming capillary equilibrium. Table 7.3 contains the average residual wetting phase saturations that are reached within each simulation.

Interestingly, for the homogeneous domain, the average residual wetting phase saturation that can be reached in this case is higher for the simulation of a steady-state primary drainage experiment compared to the simulation of a static primary drainage experiment. This is opposite to what was observed before, where a steady-state primary drainage experiment led to a lower average wetting phase saturation than a static primary drainage experiment. However, a simple explanation for this observation is that in a steady-state primary drainage experiment, the domain is drained more slowly than is the case in a static primary drainage experiment. This can also be observed in Figure 7.15, in which the average wetting phase saturation is plotted as a function of the applied nonwetting phase bottom boundary pressure. Clearly, the average wetting phase saturation in the steady-state primary drainage experiment decreases more slowly compared to the static primary drainage experiment.
As a result, it is possible that at relatively ‘early’ stages in the drainage process in the static primary drainage experiment a lower average wetting phase saturation is obtained compared to the steady-state primary drainage experiment. If the simulations would be continued so that higher nonwetting phase boundary pressures are applied, the domain will drain gradually in case of a steady-state primary drainage experiment, while for a static primary drainage experiment at some point no more change in the average wetting phase saturation will occur. Therefore, if the drainage process is continued long enough, finally a lower average wetting phase saturation will be reached at the end of the simulation.
phase saturation will be reached in a steady-state primary drainage experiment compared to a static primary drainage experiment.

![Average Sw as a function of Pn bottom, simulations with gravity](image)

**Figure 7.15:** Average wetting phase saturation as a function of applied nonwetting phase bottom boundary pressure for simulations of a steady-state or static primary drainage experiment, and homogeneous or heterogeneous domains.

Note that for the homogeneous domain discussed in Section 7.2.1, the drainage process has progressed long enough for the column to reach a lower average wetting phase saturation when a steady-state primary drainage experiment is performed compared to a static primary drainage experiment. The difference between the homogeneous domain discussed in Section 7.2.1 and the equivalent homogeneous domain discussed in this section is the Brooks-Corey coefficient $\lambda$ that is used for the input curve. For the homogeneous domain discussed in Section 7.2.1, $\lambda$ has a value of 6.11, while for the homogeneous domain discussed here, $\lambda$ has a value of 1.51. A low value for the Brooks-Corey coefficient $\lambda$ means that the input $P_c$-$S_w$ curve is not very sharp, i.e. the change in capillary pressure with decreasing wetting phase saturation is more or less evenly distributed over the whole wetting phase saturation range (see also Figure 2.10). As a result, a higher applied nonwetting phase boundary pressure is needed for the average wetting phase saturation in the steady-state primary drainage experiment to become lower than the average wetting phase saturation in the static primary drainage experiment.

In Figure 7.16, the average capillary pressure-saturation relationships are shown for the simulation of a steady-state and static primary drainage experiment, for the homogeneous domain of 18.2 cm length discussed in Section 7.2.1 (i.e. with a reference curve with $P_d = 6000$ Pa, $S_{w0} = 0.104$, $\lambda = 6.11$). The curves are plotted for a final applied nonwetting phase bottom boundary pressure of 12000 Pa and 30000 Pa, respectively.

As can be seen, at an applied nonwetting phase bottom boundary pressure of 12000 Pa, the average wetting phase saturation obtained with the steady-state primary drainage experiment still is higher than the average wetting phase saturation obtained in the static primary drainage experiment, just as can be observed in Figure 7.14. However, if the nonwetting phase bottom boundary pressure is increased to 30000 Pa, the average wetting phase saturation in the steady-state primary drainage experiment has become lower than the average wetting phase...
saturation that is reached in the static primary drainage experiment. The same is expected to occur for the homogeneous domain discussed here, if the applied nonwetting phase bottom boundary pressure is increased further.

Because the average wetting phase saturation for the simulation of a steady-state primary drainage experiment is higher than the average wetting phase saturation for the simulation of a static primary drainage experiment in case of the homogeneous domain, it is difficult to compare the results obtained for the homogeneous domain with the ones obtained for the strongly heterogeneous domain. However, Table 7.3 does show that while for the homogeneous domain the average wetting phase saturation in the steady-state primary drainage experiment is still higher than the average wetting phase saturation in the static primary drainage experiment, for the strong heterogeneous domain in the steady-state primary drainage experiment a lower average wetting phase saturation is reached compared to the static primary drainage experiment. Moreover, the difference between the average wetting phase saturation that is reached in a static primary drainage experiment for a homogeneous and heterogeneous domain is 0.26, while for a steady-state primary drainage experiment this difference is 0.06. This indicates that these strong heterogeneities can enhance the effect of the hydrophilic membrane significantly, as the increase in average wetting phase saturation that is reached between the homogeneous and heterogeneous domain is larger if a static primary drainage experiment is performed.
7.2.3 Overview of factors influencing the average residual wetting phase saturation

Throughout this thesis, several factors have come up for discussion that were shown to influence the average residual wetting phase saturation that can be reached in a sample column. In this section, an overview of these factors is given.

1) Strictness of the equilibrium criterion. 
As was shown in Section 4.4.2, the strictness of the equilibrium criterion has a large influence on the residual wetting phase saturation that can be reached in a sample. If the equilibrium criterion is chosen strict enough, it is possible to reach the residual saturation that is intrinsic to the porous medium. However, a very strict equilibrium criterion also means that experimental times increase drastically, and in reality these very strict criterions can never be used. Thus, even though it would be possible to reach the intrinsic residual wetting phase saturation of a sample by choosing a strict enough equilibrium criterion, in reality this will never be used and looser equilibrium criteria result in a higher residual wetting phase saturation than is specified for the local or input curve.

2) The presence and intensity of heterogeneities. 
In Section 6.4, it was shown that when heterogeneities are present in a sample, the average residual wetting phase saturation that can be reached is higher compared to the average residual wetting phase saturation that would be reached in a homogeneous domain. However, for relatively weak heterogeneities that are assumed to occur in a laboratory sample, the effect is negligible. Only for stronger heterogeneities, the effect becomes significant. In this thesis, only one type of heterogeneity pattern was used, so it could be possible that different results will be obtained if a different heterogeneity pattern or distribution is applied.

3) Static primary drainage experiment vs. steady-state primary drainage experiment. 
As was shown above, the presence of a hydrophilic membrane in a static primary drainage experiment results in the increase of the average residual saturation that can be reached in a sample. This is because the nonwetting phase is prevented from leaving the sample, so that it starts accumulating below the hydrophilic membrane. The resulting decrease in the relative permeability of the wetting phase just below the membrane makes it more difficult or even impossible for the remaining wetting phase to leave the sample. Therefore, the average residual wetting phase saturation that can be reached in the sample will be higher compared to the residual saturation that can be reached when a steady-state primary drainage experiment is performed.
It was further shown that heterogeneities can act to enhance the effect of a hydrophilic membrane, though this is negligible for weak heterogeneities.

4) Column length. 
The effect of column length was discussed in Section 7.2.1. For the simulation of a static primary drainage experiment, it was shown that with increasing column length, the residual wetting phase saturation that can be reached in a sample increases. For the simulation of a steady-state primary drainage experiment, column length does not have a significant effect on the average residual wetting phase saturation that is reached in the domain.
Note however that in the simulations with different column length, the pressure gradients inside the columns are not the same. Because boundary conditions are kept equal, for the shorter column a steeper pressure gradient inside the sample is reached than for a longer column. This could also be causing the observed effect.
5) Flow direction.
In Section 5.9, it was shown that the direction of flow with respect to gravity influences the obtained average $P_c-S_w$ curve. The direction of flow can also be expected to have an influence on the average residual saturation that can be reached in a sample, especially when a hydrophilic membrane is used. When the direction of flow in the sample is parallel to the direction in which gravity forces act, the nonwetting phase will infiltrate the sample much faster than it would if it has to flow against gravity. This is also illustrated in Figure 5.36. As a result, the nonwetting phase reaches the outflow of the sample very fast, while the nonwetting phase saturation in the column still is relatively low. In case of a static primary drainage experiment, further outflow of the wetting phase is inhabited by the accumulation of nonwetting phase below the hydrophilic membrane, and as a result the residual wetting phase saturation that is reached in the sample will be much higher. This is shown in Figure 7.17, where the arithmetic phase volume average $P_c-S_w$ curves are plotted for a static primary drainage experiment where flow is either from top to bottom or from bottom to top in the sample.

![Figure 7.17: Average $P_c-S_w$ curves obtained for simulations of a static primary drainage experiment, with flow from the top of the sample to the bottom or vice versa, respectively. Averaging is done using an arithmetic phase volume average over the 2-phase domain.](image)

The used domain is homogeneous and 18.2 cm long. The figure shows that the average residual wetting phase saturation is much higher when the nonwetting phase infiltrates the sample from the top. In Figure 7.18 the same set of average $P_c-S_w$ curves is shown, but now for simulations of a steady-state primary drainage experiment. As can be seen, the effect of the direction of flow on the average residual wetting phase saturation that can be reached in the sample is much smaller when a steady-state primary drainage experiment is performed. This is because the nonwetting phase can easily flow out, so that it does not prevent the wetting phase from leaving the column.
7.2 THE EFFECT OF A HYDROPHILIC MEMBRANE

P_c vs. S_w curve, arithmetic phase volume avg over 2-phase domain, steady-state simulation

Figure 7.18: Average P_c-S_w curves obtained for simulations of a steady-state primary drainage experiment, with flow from the top of the sample to the bottom or vice versa, respectively. Averaging is done using an arithmetic phase volume average over the 2-phase domain.

Figure 7.19: Nonwetting phase saturation distributions for an applied nonwetting phase bottom boundary pressure of 29998 Pa, for both simulations were the nonwetting phase flows parallel or against the direction of gravity forces; a) nonwetting phase saturation distributions for simulations of a static primary drainage experiment; b) nonwetting phase saturation distributions for simulations of a steady-state primary drainage experiment.

In Figure 7.19, the nonwetting phase distributions are shown for an applied nonwetting phase bottom boundary pressure of 29998 Pa (i.e. the end of the simulation) after equilibrium is reached. As can be seen, there is a significant difference in the distributions when a static primary drainage experiment is performed. When the nonwetting phase infiltrates the sample from the top, the wetting phase clearly has more difficulty from leaving the sample because the nonwetting phase reaches the outflow fast, and it start accumulating there already, while the wetting phase saturation in the rest of the sample still is relatively high. On the other hand, the saturation distributions obtained for the simulation of a steady-state primary drainage
experiment are approximately equal, because the nonwetting phase can flow freely out of the sample.

Concluding this section, the average residual wetting phase saturation that can be reached in a sample is dependent on a number of factors. As a result, the obtained residual wetting phase saturation can be significantly different from the residual wetting phase saturation that is an intrinsic property of the porous medium.

7.3 A comparison between how the $Pc$-$Sw$ curve is measured and how it could be measured

To conclude this chapter, an attempt is made to investigate the traditional measurement of the $Pc$-$Sw$ curve. For this purpose, the $Pc$-$Sw$ curve as it is usually measured in the laboratory is compared to the $Pc$-$Sw$ curve that is obtained by making an ‘improvement’ to the traditional method. All this is done based on results from simulations.

The domain used in this section will be the 2D heterogeneous domain as discussed in Section 6.1.1. Thus, the domain is $3 \text{ cm} \times 6 \text{ cm}$, and contains weak heterogeneities. It is assumed these kind of weak heterogeneities are representative for the heterogeneities that are always present in laboratory samples, despite the fact that they are often assumed to be homogeneous. In Figure 7.20, an overview is given of the different methods that will be used to obtain an average $Pc$-$Sw$ curve.

Traditionally, the $Pc$-$Sw$ curve is determined in the laboratory by performing a static primary drainage experiment. Pressures of the wetting and nonwetting phase are usually measured with pore pressure transducers located in the fluid reservoirs outside the sample. Thus, the average capillary pressure of the sample is determined through:

$$Pc_{\text{sample}} = P_{w,\text{reservoir}} - P_{n,\text{reservoir}} = P_{w,\text{bottom}} - P_{w,\text{top}}$$ (7.1)

In addition, the saturation is measured through gravimetric or volumetric methods, and represents an average over the whole sample.

As an alternative for a static primary drainage experiment, a steady-state primary drainage experiment can be performed. This would perhaps represent reality better as in most settings (e.g. subsurface) hydrophilic membranes are not present to prevent the nonwetting phase from flowing, and therefore flow of the nonwetting phase often occurs. Note however that steady-state flow might not be very representative of reality either, as transient flow might be more common.

In combination with a steady-state primary drainage experiment, two different approaches are investigated to obtain average pressures and saturations. The first is to determine the nonwetting and wetting phase pressures and saturation by averaging over the whole length and width of the domain. The second approach is to determine the phase pressures and saturation from 1 cm sensors located inside the domain, at half the sample height. It is assumed the sensors ‘measure’ an average over the length of the sensor, and over the width of the whole sample.
7.3 A COMPARISON BETWEEN HOW THE PC-SW CURVE IS MEASURED AND HOW IT COULD BE MEASURED

Figure 7.20: Overview of how people usually determine the Pc-Sw curve in the laboratory, and some suggestions how this could be improved.

Figure 7.21 shows the comparison between the Pc-Sw curve as it would be obtained traditionally, and the Pc-Sw curve obtained by performing a steady-state primary drainage experiment, where the phase pressures and saturation are averaged over the whole sample domain. Note that averaging is done using an weighted phase volume average (Equation (5.2) and (5.6)). The figure shows that for high and intermediate average wetting phase saturations, both curves overestimate the capillary pressure relative to the analytical curve, though the ‘traditionally’ measured curve shows a larger overestimation. This overestimation is due to the use of Equation (7.1) to determine the average capillary pressure of the sample, as the nonwetting phase and wetting phase reservoir are not at the same height. Usually however, it is assumed that the effect of gravity can be neglected, and the capillary pressure is simply determined through Equation (7.1). Figure 7.21 shows that for a 3 cm high column, this can result in an overestimation of capillary pressure of approximately 500 Pa. Nevertheless, if the sensors are set to zero before the experiment starts, the effect of gravity is removed, and the overestimation of capillary pressure at high and intermediate wetting phase saturations will disappear. The average Pc-Sw curve obtained from the simulation of a steady-state primary drainage experiment, and averaging pressures and saturation over the whole domain also shows an overestimation of the capillary pressure relative to the analytical curve because an weighted phase volume average is used. In addition, at low average wetting phase saturations the curve deviates from the analytical curve because the experiment is steady-state (see also Section 7.2).

Another difference between the two curves occurs at low average wetting phase saturations. The traditionally determined Pc-Sw curve shows a fast increase in capillary pressure, while the alternative Pc-Sw curve does not show this increase. This is because for the alternative curve, the average phase pressures are determined based on pressures inside the sample as opposed to the traditionally measured pressures, which are determined outside the sample. There is a small difference in the average residual wetting phase saturation that can be reached due to the use of a static primary drainage experiment in the traditional determination of the Pc-Sw.
curve versus the use of a steady-state primary drainage experiment in the alternative
determination of a $P_c$-$S_w$ curve.

Figure 7.21: A comparison between the $P_c$-$S_w$ curve how it is usually determined, and the $P_c$-$S_w$ curve obtained by performing a steady-state primary drainage experiment, and averaging phase pressures and saturation over the whole sample domain; a) full $P_c$-$S_w$ curves; b) the $P_c$-$S_w$ curves between an average capillary pressure of 4000 Pa and 15000 Pa.

In Figure 7.22, the average $P_c$-$S_w$ curve as it is usually measured (i.e. static primary drainage experiment, pressures determined outside the sample) is compared to the average $P_c$-$S_w$ curve
obtained for the simulation of a steady-state primary drainage experiment, where the phase pressures and saturation are averaged over a sensor of 1 cm, situated at half the column height. As can be seen, this alternative $P_c$-$S_w$ curve slightly underestimates the capillary pressure compared to the analytical curve, but this difference is not very large. At low wetting phase saturations again the alternative curve shows relatively low capillary pressures and stays close to the analytical curve. Moreover, this curve reaches a significantly lower average residual wetting phase saturation than follows from the traditionally determined $P_c$-$S_w$ curve.

Thus, based on Figure 7.21 and 7.22, there can be significant differences between the $P_c$-$S_w$ relationship as it is usually determined, and how it could or should alternatively be determined. The most important differences are an overestimation of capillary pressure along the whole range of the wetting phase saturation, due to the measurement of the phase pressures in the fluid phase reservoirs, which usually are not at equal heights. As a result, the nonwetting phase pressure measured in the nonwetting phase fluid reservoir is overestimated because it includes an oligostatic pressure, while the wetting phase pressure in the wetting phase reservoir does not include this pressure. Note that this only is the case when the nonwetting phase flows from the bottom of the sample towards the top, and the nonwetting phase reservoir thus is situated at the bottom of the sample. Moreover, this effect is easily overcome by setting the sensors to zero before the experiment starts, so that the hydrostatic pressure is not taken into account by the sensor situated in the reservoir connected to the bottom of the sample. In addition, at low average wetting phase saturations, the average capillary pressure for the traditionally measured curve, using a ‘global’ capillary pressure, increases strongly. This is not observed in the alternative curves, which stay close to the reference curve of the porous medium.

Another important difference that can be observed is the average residual wetting phase saturation that can be reached in the sample. With the traditional measurement of the capillary pressure-saturation relationship, the average residual wetting phase saturation can be overestimated. This overestimation seems to be stronger if the traditionally determined $P_c$-$S_w$ curve is compared with an alternative $P_c$-$S_w$ curve obtained by simulating a steady-state primary drainage experiment, in which phase pressures and saturation are determined by averaging over a volume in the sample that is representative of a volume that would be measured by a sensor such as a PPT (for pressure) or TDR (for saturation).

Note also that if the simulations would be continued for a longer period of time, i.e. if the applied nonwetting phase bottom boundary pressure is increased beyond 30000 Pa, an even larger difference between the average residual wetting phase saturations that can be reached for the traditional curve and the alternative curves would occur. As was shown in Section 7.2 (e.g. Figure 7.15), in the static primary drainage experiment, even if the applied nonwetting phase bottom boundary pressure would be further increased, the average residual wetting phase saturation will not change anymore. On the other hand, in the steady-state primary drainage experiment, a further increase in applied nonwetting phase bottom boundary pressure would result in a further decrease of the average wetting phase saturation. Therefore, the difference between the two average curves plotted in Figure 7.21 and 7.22 could potentially be larger if the applied nonwetting phase bottom boundary pressure would be allowed to increase to values beyond 30000 Pa.
7.4 Summary and conclusions

In this chapter, the effect of the presence of a hydrophilic membrane in static primary drainage experiments on the obtained average $P_c$-$S_w$ curve is investigated. In order to do this, the average capillary pressure-saturation relationship obtained by performing a simulation of a static primary drainage experiment is compared to the average capillary pressure-saturation relationship.
relationship obtained by performing a simulation of a steady-state primary drainage experiment. While in a static primary drainage experiment the nonwetting phase is prevented from leaving the sample by the presence of a hydrophilic membrane at the outflow, in a steady-state primary drainage experiment the nonwetting phase is allowed to flow out. Static experiments have the advantage that a shorter time is needed to obtain a capillary pressure-saturation relationship. The effect of the hydrophilic membrane on the average $P_c$-$S_w$ curve was investigated for both a homogeneous and a heterogeneous domain. Further, a comparison was made between the $P_c$-$S_w$ curve as it is traditionally determined, and how it could alternatively be determined. This means a comparison was made between a $P_c$-$S_w$ curve obtained from the simulation of a static primary drainage experiment, with the average capillary pressure determined from pressures outside the sample and saturation averaged over the whole domain, and a $P_c$-$S_w$ curve obtained from the simulation of a steady-state primary drainage experiment, where either both pressures and saturation are averaged over the whole domain, or are averaged over a volume (or in this 2D case an area) that represents the volume a 1 cm sensor would be measuring.

The following is concluded:

- With a static primary drainage experiment, the average residual wetting phase saturation that can be reached in a sample can be overestimated. With a steady-state primary drainage experiment, significantly lower average residual wetting phase saturations can be reached, given that the drainage process is allowed to proceed long enough.
- The presence of heterogeneities can enhance the effect of the hydrophilic membrane used in static primary drainage experiments. However, for weak heterogeneities and the particular heterogeneity pattern and distribution used in this chapter this effect is not significant. If stronger heterogeneities are used, the effect becomes more significant.
- The presence of a hydrophilic membrane in a static primary drainage experiment is not the only factor influencing the average residual saturation that can be reached in a sample. Other factors that are shown to have an influence are the strictness of the equilibrium criterion, presence and intensity of heterogeneities, column length, and flow direction. These factors also influence the effect of each other on the average residual wetting phase saturation.
- There can be some significant differences between the $P_c$-$S_w$ relationship as it is usually determined, and how it could or should alternatively be determined. The measurement of pressures outside the sample can result in a fast increase in average capillary pressure at low wetting phase saturations, which is not observed inside the sample. Moreover, the use of a static primary drainage experiment can result in the overestimation of the residual wetting phase saturation.
Chapter 8

Summary and conclusions

8.1 Summary and conclusions

In this thesis, the average equilibrium capillary pressure-saturation relationship in two-phase flow in porous media is investigated. Two-phase flow is of importance in many natural and industrial porous media. It plays a role in many aspects of daily life, from environmental problems to industrial processes. Therefore, the correct description of two-phase flow in porous media is very important. For this correct description, constitutive relationships such as the capillary pressure-saturation relationship are needed. These constitutive relationships close the set of governing equations needed to describe two-phase flow in porous media.

Commonly, the capillary pressure-saturation relationship is determined in the laboratory as it cannot be derived directly from physical considerations. The capillary-pressure saturation relationship obtained from such laboratory experiments is assumed to be an intrinsic property of the porous medium under consideration. Thus, it is assumed to be independent of the methods that were used to obtain it.

The main aim of this thesis is to investigate whether this assumption is valid. First, the effect of upscaling the equilibrium \( P_c-S_w \) curve from the local scale to the sample scale using averaging methods is investigated. In addition, the effect of heterogeneities in combination with this upscaling is investigated. Finally, the effect of the use of a hydrophilic membrane in the traditional measurement of the \( P_c-S_w \) curve is investigated. Below, a short summary of each chapter is given, together with the main conclusions of that chapter.

In Chapter 2, first a general background is given on the theory of two-phase flow, for both the micro- and macroscale.

In Chapter 3, the numerical models that are used in this thesis are introduced. The numerical simulations discussed in this thesis are mainly performed with a model provided by dr. ir. C. Berentsen. The model MUFTE-UG from Universität Stuttgart is used to a lesser extent.

In Chapter 4, preliminary numerical experiments are discussed that are performed to determine the value of three parameters that are needed to perform simulations of steady-state and static primary drainage experiments. It is found that a mesh size of 0.4 mm gives numerically accurate results. Moreover, an equilibrium criterion for the maximum wetting phase flux of \( 10^{-8} \) m/s is chosen to represent equilibrium conditions, while a pressure increment of 100 Pa is chosen to simulate a static or steady-state primary drainage experiment.

In Chapter 5, the effect of different averaging methods on the obtained average \( P_c-S_w \) curve is investigated for the simulation of a static primary drainage experiment in a homogeneous domain, including gravity. Several averaging methods are investigated, under which the arithmetic phase volume and phase volume averages, the centroid phase average, and the ‘global’ average. It is found that the used averaging method can have a significant effect on the obtained average \( P_c-S_w \) curve, and that therefore care should be taken when averaging
pressures and saturations, especially in the presence of gravity forces. In addition, it was shown that the use of pressures outside the sample to determine an average capillary pressure (global $P_c$) results in a fast increase in average capillary pressure at low wetting phase saturations, something that is not observed when pressures inside the sample are used to obtain an average capillary pressure.

In Chapter 6, the effect of heterogeneities on the average equilibrium capillary pressure-saturation relationship is investigated. For this purpose, a 3 cm × 6 cm heterogeneous domain is used, that consisted out of 36 heterogeneities of equal volume. An analytical capillary pressure-saturation relationship is determined by applying the assumption of equilibrium. The main conclusion from this chapter is that averaging should be performed over the whole domain, as the wetting phase saturations for the analytical curve also are obtained by averaging over all 36 heterogeneities. In addition, it is found that heterogeneities can act to increase the average residual wetting phase saturation that can be reached in a sample. However, the extent to which this occurs is dependent on the intensity of the heterogeneities.

In Chapter 7, the effect of the presence of a hydrophilic membrane used during static primary drainage experiments on the obtained average $P_c$-$S_w$ curve is investigated. It is concluded that with a static primary drainage experiment, the average residual wetting phase saturation that can be reached in a sample can be overestimated because the nonwetting phase accumulates below the hydrophilic membrane and inhibits the flow of wetting phase out of the sample. With a steady-state primary drainage experiment, significantly lower average residual wetting phase saturations can be reached, given that the drainage process is allowed to proceed long enough. Further it is shown that heterogeneities can act to enhance the effect of a hydrophilic membrane. Finally, it is shown that there can be a significant difference between the $P_c$-$S_w$ curve as it is usually determined (i.e. static primary drainage experiment, pressures outside the sample) and how it could be measured alternatively. The most important differences are an overestimation of the capillary pressure, especially at low wetting phase saturations, and an overestimation of the average residual wetting phase saturation that can be reached in the sample.

The main conclusion of this thesis is that the average $P_c$-$S_w$ curve at the sample scale is not necessarily an intrinsic property of the porous medium. It is dependent on for instance boundary conditions (steady-state versus static primary drainage experiment), measurement methods (measurement of the pressures and saturation, equilibrium criterion), and, in case numerical experiments are performed, the averaging methods used to obtain the average capillary pressure and saturation. This is an important conclusion to keep in mind when talking about the capillary pressure-saturation relationship as an intrinsic property of a porous medium.

8.2 Remarks and Suggestions

The simulations in this thesis only were performed for a water-DNAPL system, and mostly for flow of the nonwetting phase from bottom to top. In addition, a particular set of boundary conditions was used. In case of the heterogeneous domain, a particular distribution and shape and size of heterogeneities were used. However, different patterns and distributions of heterogeneities might influence the results. Thus, the results discussed in this thesis only are valid for the conditions under which they were obtained, and different results might be found under other other conditions.
The simulation of a steady-state primary drainage experiment was performed by using a Dirichlet boundary condition for both the wetting and nonwetting phase pressure at the outflow of the domain. Alternatively however, also a freeflow boundary condition could be used. A freeflow boundary conditions is a Neumann boundary condition for which the flux is not specified. This means the flux of the nonwetting phase at the outflow is free to vary. The flux is computed within each timestep, which requires a Dirichlet boundary condition for the nonwetting phase (Manthey, 2006). The use of a freeflow boundary condition might give rise to different results.

Something that was not investigated in this thesis, but could be a suggestion for future work, is the effect of using sample-scale capillary pressure-saturation relationships in numerical simulations of larger domains. For this purpose, the following approach could be used (see also Figure 8.1):

- First, a large heterogeneous domain (scale of meters) is created.
- This large scale heterogeneous domain can be subdivided into several coarse-scale gridblocks. Each of these gridblocks represents a sample-scale domain, contained micro-heterogeneities. These sample-scale domains are similar to the ones described in Chapter 6.
- For each of these coarse-scale gridblocks, an average equilibrium $P_c$-$S_w$ relationship can be determined by performing a simulation of a primary drainage experiment, and by averaging the pressures and saturations obtained from the simulation data. For the averaging, one of the methods described in Chapter 5 and 6 can be used.
- The obtained average $P_c$-$S_w$ curves for the coarse-scale gridblocks represent the $P_c$-$S_w$ curves that would be measured for a sample taken in the field and analysed in the lab.
- Now the obtained average $P_c$-$S_w$ relationship for each coarse scale gridblock can be used to perform a simulation of for instance a DNAPL spill in the large-scale domain. In this simulation, the obtained average $P_c$-$S_w$ curves for the coarse-scale gridblocks are used as ‘local’ input curves for the coarse scale gridblocks.
- In addition, the same simulation also can be performed for a situation where the micro-heterogeneities inside the coarse-scale gridblocks are not upscales, so that the fine-scale heterogeneity distribution is kept intact. Results from this simulation can be used to represent ‘reality’. The results from the upscaled simulation on the other hand represent what would be simulated with a numerical model when only sample-scale average $P_c$-$S_w$ relationships are known measured in the laboratory. Ideally, the results should be the same.
Figure 8.1: Illustration of proposed approach to investigate the effect of using sample-scale capillary pressure-saturation relationships in larger scale simulations. Ideally, both the fine-scale simulation (representing ‘reality’) containing micro-heterogeneities and the coarse scale simulation in which the micro-heterogeneities are upscaled result in the same evolution of the saturation and pressure distributions.
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Appendix A

Discretising a 1-D mass balance equation using the finite volume method

In this appendix, the finite volume method is illustrated by the discretisation of a 1-D mass balance equation. In a 1-D situation, the numerical domain is discretised as is shown in Figure A.1. The node $i$ is situated in the middle of the control volume $V_i$. The fluxes across the boundary of the control volume are denoted as $q_i^{-\frac{1}{2}}$ and $q_i^{+\frac{1}{2}}$. Note that these fluxes are only in the x-direction as this is a 1-D domain.

First of all, a local mass balance is written for each control volume $V_i$ inside the discretised domain. The local mass balance used here is for the nonwetting phase, but similar discretisation steps can be performed for the mass balance of the wetting phase:

$$\frac{\partial n \rho_n S_n^i(x,t)}{\partial t} + \frac{\partial \rho_n q_n^i(x,t)}{\partial x} = 0$$  \hspace{1cm} (A.1)

where $n$ is the control volume porosity, assumed to be constant, $\rho_n$ is the nonwetting phase density, which is assumed to be constant as well, $S_n^i$ is the saturation of the nonwetting phase inside the control volume, and $q_n^i$ is the flux inside the control volume. Note that both $S_n^i$ and $q_n^i$ are dependent on time and position inside the control volume.

Equation (A.1) can be integrated over the control volume $V_i$, so that an integral form of the local mass balance is obtained:

$$\int_{V_i} \frac{\partial n \rho_n S_n^i(x,t)}{\partial t} dV + \int_{V_i} \frac{\partial \rho_n q_n^i(x,t)}{\partial x} dV = 0$$  \hspace{1cm} (A.2)

Equation (A.2) can be rewritten as:
\[ n \frac{\partial}{\partial t} \int_{V_i} S_n^i(x, t) dV - \int_{V_i} \frac{\partial q_n^i(x, t)}{\partial x} dV = 0 \] (A.3)

The second term on the left hand side of Equation (A.3) can be transformed into a surface integral using the Divergence Theorem (Gauss’s Theorem) which states that:

\[ \int \nabla \cdot F dV = \oint_F F dS \] (A.4)

Using this theorem, Equation (A.3) becomes:

\[ n \frac{\partial}{\partial t} \int_{V_i} S_n^i(x, t) dV - \oint_{\partial V_i} q_n^i(x, t) dS = 0 \] (A.5)

Moreover, the volume averaged nonwetting phase saturation over the control volume is defined as:

\[ \langle S_n^i \rangle(t) = \frac{1}{V_i} \int_{V_i} S_n^i(x, t) dV \] (A.6)

Equation (A.6) thus can be substituted into equation (A.5):

\[ nV_i \frac{\partial \langle S_n^i \rangle(t)}{\partial t} - \int_{\partial V_i} q_n^i(x, t) dS = 0 \] (A.7)

Finally, because this is a 1D situation, the surface integral can be written as the difference between the flux at the outflow boundary of the control volume \( V_i \) and the flux at the inflow boundary of the control volume \( V_i \):

\[ \oint_{\partial V_i} q_n^i(x, t) dS = A \left( q_n^{i+\frac{1}{2}} - q_n^{i-\frac{1}{2}} \right) \] (A.8)

where \( A \) is the surface area of the inflow boundary (which is equal to the surface area of the outflow boundary. Applying an implicit discretisation scheme for the time derivative, and substituting Equation (A.8) into equation (A.7), finally the following discretised form of the local mass-balance equation for control volume \( V_i \) is obtained:

\[ n \frac{\langle S_n^i \rangle^{k+1} - \langle S_n^i \rangle^k}{\Delta t} = \frac{1}{L_i} \left( \left[ q_n^{i+\frac{1}{2}} \right]^{k+1} - \left[ q_n^{i-\frac{1}{2}} \right]^{k+1} \right) \] (A.9)

where \( L_i \) is the length of the control volume, which follows from \( L_i = V_i / A \).

\( \langle S_n^i \rangle \) is the averaged nonwetting phase saturation over the control volume. As can be seen from Equation (A.9), the finite volume method relates the nonwetting phase saturation, averaged over the control volume, to the fluxes of the nonwetting phase at the boundaries of the control volume. Equation (A.9) can now be solved for the unknown quantity \( \langle S_n^i \rangle^{k+1} \), if
the fluxes $q_n^{i+1/2}$ and $q_n^{i-1/2}$ are known. Therefore, this equation needs to be coupled to other equations to include the phase potential $\Phi_n$. 
Appendix B

The Newton-Raphson method

The Newton-Raphson method is a root-finding algorithm that uses the first terms of the Taylor series of a function \( f(x) \) in the vicinity of a suspected root. In this case, the function \( f(x) \) is dependent on the three main variables \( S_n, \Phi_n \) and \( \Phi_w \). Moreover, the discretisation used makes it necessary to consider the function \( f \) at three positions in the domain at the same time, thus:

\[
\begin{align*}
\alpha & = S_n, \Phi_n, \Phi_w \sum_{i=1}^{k+1} \left[ S_n, \Phi_n, \Phi_w \right]_{i-1}^{k+1} \left[ S_n, \Phi_n, \Phi_w \right]_{i}^{k+1} = 0 \\
\beta & = S_n, \Phi_n, \Phi_w \sum_{i=1}^{k+1} \left[ S_n, \Phi_n, \Phi_w \right]_{i-1}^{k+1} \left[ S_n, \Phi_n, \Phi_w \right]_{i}^{k+1} = 0 \\
\gamma & = S_n, \Phi_n, \Phi_w \sum_{i=1}^{k+1} \left[ S_n, \Phi_n, \Phi_w \right]_{i-1}^{k+1} \left[ S_n, \Phi_n, \Phi_w \right]_{i}^{k+1} = 0
\end{align*}
\] (B.1)

where \( \alpha, \beta \) and \( \gamma \) represent the three discretised governing equations that need to be solved. Thus, \( \alpha, \beta \) and \( \gamma \) are all dependent on \( S_n, \Phi_n, \Phi_w \) and use information from positions \( i-1, i, \) and \( i+1 \). This means that each of these three functions depend nonlinearly on all three main variables in all three points, at least hypothetically. The above set of equations can also be written in vector form as:

\[
f_i = f_i(\mathbf{v}) \quad i = 1, 2, 3
\] (B.2)

where \( \mathbf{v} \) represents the vector \( (v_1, v_2, v_3) \), with

\[
\begin{align*}
v_1 & = S_n \\
v_2 & = \Phi_n \\
v_3 & = \Phi_w
\end{align*}
\] (B.3)

Now, in order to solve the above set of equations for a certain timestep, first the equations are expanded with a Taylor series. The Taylor series expansion of \( f_i(\mathbf{v}) \) around the point \( \mathbf{v} = \mathbf{v}_0 + \Delta \mathbf{v} \) is given by:

\[
f_i(\mathbf{v}_0 + \Delta \mathbf{v}) = f_i(\mathbf{v}_0) + \sum_j \frac{\partial f_i}{\partial v_j} \Delta v_j + \frac{1}{2} \sum_j \sum_k \frac{\partial^2 f_i}{\partial v_j \partial v_k} (\Delta v_j)^2 + O((\Delta v_j)^3) + \mathbf{K} \quad i = 1, 2, 3 \quad j = 1, 2, 3
\] (B.4)

where \( O((\Delta v_j)^3) \) represents terms of third order and higher. Only taking the first order terms into account gives:

\[
f_i(\mathbf{v}_0 + \Delta \mathbf{v}) \approx f_i(\mathbf{v}_0) + \sum_j \frac{\partial f_i}{\partial v_j} \Delta v_j \quad i = 1, 2, 3 \quad j = 1, 2, 3
\] (B.5)
here $\Sigma \partial f_i/\partial v_j$ represents a matrix of partial derivatives, which is also known as the Jacobian:

$$J_{ij} = \frac{\partial f_i}{\partial v_j} \quad i=1,2,3 \quad j=1,2,3 \quad (B.6)$$

Rewriting Equation (B.5) in matrix notation gives:

$$f(v_0 + \delta v) \approx f(v_0) + J \cdot \delta v \quad (B.7)$$

Where $f$ is the entire vector of functions $f_i$, and $J$ is the Jacobian matrix. Now, a first guess for the root is made. For this guess, usually the values of the variables for the previous timestep are taken. Thus, it is assumed that:

$$f(v_0 + \delta v)^0 = 0 \quad (B.8)$$

where the index 0 refers to the initial guess. With Equation (B.8), a new guess for the position of the root can be calculated. The basics of this method are shown in Figure B.1. The initial guess is assumed to be close to the actual root, with an offset of $\delta v$. Note that the initial guess cannot be too far away from the true root because in the Taylor expansion above only the first order terms were taken into account, so that the function $f_i$ is assumed to be linear. The more non-linear the functions $f_i$ are, the less accurate the first order approximation of the Taylor series will be.

Figure B. 1: basics of the Newton-Raphson method (in 1-D). $\delta S_n^0$ is the first correction/iteration to the saturation of the nonwetting phase that brings the function $f_i$ closer to 0. Similar graphs can be drawn for the potentials.

Equation (B.7) and (B.8) can be combined to create a set of linear equations for the term $\delta v$, which brings the initial guess closer to the analytical root of the equations:

$$J^0 \cdot \delta v^0 = -f(v_0)^0 \quad (B.9)$$
With Equation (B.9), the term $\delta v^0$ can be found. With this term, the initial guess vector can be corrected to bring it close to the analytical root:

$$v^1 = v^0 + \delta v^0$$  \hspace{1cm} (B.10)

Thus, Equation (B.10) results in a new estimation of the three main variables $S_n$, $\Phi_n$, and $\Phi_w$. Now, the whole procedure can be repeated to find $v^2$ and further estimates in an iteration procedure. If the initial estimate is chosen at a good position, the iteration will lead to a rapid convergence. The algorithm is assumed to have converged when the fractional accuracy becomes less than some prescribed value. The fractional accuracy can be given by:

$$\lambda = \frac{v^{n+1} - v^n}{v^{n+1}}$$  \hspace{1cm} (B.11)
# Appendix C

An overview of the different averaging approaches discussed in Chapter 5

<table>
<thead>
<tr>
<th>Averaging method</th>
<th>Section</th>
<th>Equations</th>
<th>Average pressure</th>
<th>Average saturation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Traditional arithmetic phase volume average</td>
<td>5.3</td>
<td>(5.8) (5.12)</td>
<td>$\bar{P}<em>a = \frac{\sum</em>{i=1}^{N} P^i_a n^i_a}{n_{a&gt;0}}$</td>
<td>$\bar{S}<em>a = \frac{\sum</em>{i=1}^{N} S^i_a}{N}$</td>
</tr>
<tr>
<td>Traditional phase volume average</td>
<td>5.3</td>
<td>(5.9) (5.12)</td>
<td>$\langle P_a \rangle = \frac{\sum_{i=1}^{N} S^i_a P^i_a}{\sum_{i=1}^{N} S^i_a}$</td>
<td>$\langle S_a \rangle = \frac{\sum_{i=1}^{N} S^i_a}{N}$</td>
</tr>
<tr>
<td>Arithmetic phase volume average over 2-phase system</td>
<td>5.3</td>
<td>(5.17) (5.19)</td>
<td>$\bar{P}^{\text{new}}<em>a = \frac{\sum</em>{i=1}^{N} P^i_a (S^i_a &gt; 0)}{\sum_{i=1}^{N} n^i (S^i_a &gt; 0)}$</td>
<td>$\bar{S}^{\text{new}}<em>a = \frac{\sum</em>{i=1}^{N} S^i_a (S^i_a &gt; 0)}{\sum_{i=1}^{N} n^i (S^i_a &gt; 0)}$</td>
</tr>
<tr>
<td>Arithmetic phase volume average over 2-phase system</td>
<td>5.3</td>
<td>(5.18) (5.19)</td>
<td>$\langle P^{\text{new}}<em>a \rangle = \frac{\sum</em>{i=1}^{N} S^i_a P^i_a (S^i_a &gt; 0)}{\sum_{i=1}^{N} S^i_a (S^i_a &gt; 0)}$</td>
<td>$\langle S^{\text{new}}<em>a \rangle = \frac{\sum</em>{i=1}^{N} S^i_a (S^i_a &gt; 0)}{\sum_{i=1}^{N} n^i (S^i_a &gt; 0)}$</td>
</tr>
<tr>
<td>Centroid phase average</td>
<td>5.4</td>
<td>(5.31) (5.12)</td>
<td>$[P_a] = \langle P_a \rangle + \frac{1}{\nabla \langle z_a \rangle} (\mathbf{z} - \langle \mathbf{z}_a \rangle)$</td>
<td>$\bar{S}<em>a = \frac{\sum</em>{i=1}^{N} S^i_a}{N}$</td>
</tr>
<tr>
<td>Simple arithmetic average</td>
<td>5.5</td>
<td>(5.36) (5.37)</td>
<td>$\langle P^i_a \rangle^{\text{wholedom}} = \frac{\sum_{i=1}^{N} P^i_a}{N}$</td>
<td>$\langle S^i_a \rangle^{\text{wholedom}} = \bar{S}<em>a = \frac{\sum</em>{i=1}^{N} S^i_a}{N}$</td>
</tr>
</tbody>
</table>

With

1) $P_n = P_n^{\text{simulation}}$

2) $P_n = P_w = P_w^{\text{simulation}}$

or

2) $P_n = P_w = \rho_w g h$

for $S_n = 0$
### C.II An Overview of the Different Averaging Approaches Discussed in Chapter 5

<table>
<thead>
<tr>
<th>Global average</th>
<th>5.6</th>
<th>( P_n = P_n^{\text{simulation}} ) for ( S_n &gt; 0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>( P_w = P_w^{\text{simulation}} )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[ \langle P \rangle_{\text{global}}^{\text{corrected}} = P_{n}^{\text{bottom}} + \frac{1}{2} (\rho_w - \rho_n) g z_{\text{front}} - \rho_n g h ]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[ \langle P \rangle_{\text{corrected}}^{\text{global}} = P_{n}^{\text{bottom}} - P_{w}^{\text{top}} ]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[ \langle P \rangle_{\text{global}}^{\text{corrected}} = P_n^{\text{bottom}} + \frac{1}{2} (\rho_w - \rho_n) g z_{\text{front}} - \rho_n g h ]</td>
</tr>
</tbody>
</table>

\[ S_{\alpha} = \frac{\sum_{i=1}^{N} S'_n}{N} \]

or

\[ S_{\alpha}^{\text{new}} = \frac{\sum_{i=1}^{N} S'^i_n (S'_n > 0)}{\sum_{i=1}^{N} n(S'_n > 0)} \]
Cao, Y. / Eikemo, B. / Helmig, R.: Fractional flow formulation for two-phase flow in porous media

Korteland, S.-A., The average equilibrium capillary pressure-saturation relationship in two-phase flow in porous media