Imperial College Consortium on Pore-Scale Modelling

Final Report

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Executive Summary

This is the final report of Phase 1 of the Imperial College Consortium on Pore-Scale Modelling. In the last three years the consortium had developed state-of-the-art software to model two- and three-phase flow in mixed-wet porous media. The codes have been tested through extensive validation against experiment and we have demonstrated that a physically-based methodology to predict multiphase flow properties has a field-scale impact on predicted oil recovery.

The two PhD students who started their research funded by the Consortium three years ago have now graduated: Per Valvatne defended his thesis in November and is now working for Shell in the Netherlands; and Mohammad Piri who defended in December and who will be staying at Imperial College as a post-doctoral Research Associate. Their work represents the main thrust of the research – the development of network modelling codes to simulate two- and three-phase flow.

This final report contains two major sections that are the PhD theses of the two students: Section 1 contains Per Valvatne’s thesis on two-phase flow, while section 2 describes Mohammad Piri’s thesis on three-phase flow.

Under the consortium, further research has been performed on the field-scale consequences of using physically-based relative permeabilities, upscaling, developing three-dimensional pore-space images from two-dimensional thin sections, non-Newtonian flow in porous media and rate dependent effects. The results of this work have already been presented in previous reports.

We are now launching Phase 2 of the consortium for a further three years, where the emphasis will be on developing and validating a predictive methodology for predicting relative permeability with further research on pore space characterization, with particular application to carbonates, three-phase flow and upscaling.

The current researchers in the group are:

Martin Blunt, Professor of Petroleum Engineering – overall supervision and fundamental studies of three-phase flow.


Mohammed Al-Gharbi, 3rd year PhD student – modelling of rate dependent effects.

Xavier Lopez, 3rd year PhD student – pore-scale modelling of non-Newtonian flows.

Hiroshi Okabe, 2nd year PhD student – pore-space reconstruction.

Anwar Al-Kharusi, 1st year PhD student – analysis of carbonates.
Sander Suicmez, 1st year PhD student – three-phase flow.

Hu Dong – 1st year PhD student – to be decided.

All our publications, theses, reports and presentations are available on our Website: http://www.ese.ic.ac.uk/general.php?GenID=407

Project publications
Journal publications

Conference Proceedings

I would like to thank you all for your continued support that allows us to fund so many students and without which this research would not be possible.

Martin Blunt
London, December 2003
PREDICTIVE PORE-SCALE MODELLING OF MULTIPHASE FLOW

A DISSERTATION
SUBMITTED TO THE DEPARTMENT OF EARTH SCIENCE AND ENGINEERING OF IMPERIAL COLLEGE LONDON IN PARTIAL FULFILMENT OF THE REQUIREMENTS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

Per Henrik Valvatne
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Abstract

I show how to predict flow properties for a variety of porous media using pore-scale modelling with geologically realistic networks. A state of the art pore-scale network model is developed for this purpose. It combines topologically disordered networks that represent real systems with detailed displacement mechanisms for any sequence of water and oil flooding, and any wettability. The model is verified by successfully predicting experimental relative permeability from a well described water-wet Berea sandstone. More complex experimental data are subsequently investigated. By developing a methodology combining realistic network topology with network properties tuned to easily obtainable experimental data such as mercury injection capillary pressures, I successfully predict flow properties for several porous media, initially applied to a water-wet sand pack. The wettability of the porous medium is recognized as being important for multiphase properties. I will first reproduce the surprising experimental trend whereby maximum oil recovery is achieved for systems with Amott wettability index around zero, and explain this behaviour from a pore-scale perspective. Subsequently I will combine careful wettability characterization with the methodology for modifying networks to successfully predict relative permeability for both oil- and mixed-wet datasets. For water flooding I introduce a method for assigning contact angles to match measured wettability indices. The aim of this work is not simply to match experiments, but to use easily acquired data to predict difficult-to-measure properties. Furthermore, the variation of these properties in the field, due to wettability trends and different pore structures, can now be predicted reliably.
Acknowledgements

I would like to thank my advisor Professor Martin J. Blunt for his constant support, guidance and encouragement during this study. Without his assistance, this work would have not been accomplished. Statoil, and in particular Dr. Pål-Eric Øren, is thanked for many helpful discussions, both during my stay at the Statoil research centre in Trondheim and during his visits to Imperial College. If it had not been for Statoil kindly letting me use some of their networks, this work would certainly not have turned out this successful. As the title suggests, the focus of this thesis is on predictive pore-scale modelling, something that is not possible without comparison to real data. It has been very much appreciated that both Shell and Statoil have given us access to complete datasets, something that has made this work stronger than if I would had to rely only on published material. I look forward to continue research into pore-scale modelling, something that has been made possible by Shell deciding to employ me. Dr. Xudong Jing is thus thanked for championing the cause of pore-scale modelling within Shell, and for being extremely helpful in finding good experimental data for us to use. Financial support from the sponsors of the Imperial College Consortium on Pore-Scale Modelling is gratefully acknowledged.
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Chapter 1

Introduction

The understanding of multiphase flow in porous media is of great importance in many fields such as hydrology, contaminant cleanup and petroleum engineering. Macroscopic properties – principally capillary pressure and relative permeability – are often needed when modelling flow and transport at the continuum scale, whether it be transport of non-aqueous phase liquids (NAPL) in contaminant clean-up or the production of oil during reservoir water flooding. These macroscopic properties are, however, difficult to obtain. It is possible to conduct physical experiments on samples of the reservoir, but this will only reflect one set of conditions. Furthermore, the scale of the reservoir itself is so much larger that a few experiments are unlikely to describe the variation likely to be present. Hence, there is a need to develop physically-based models that can predict multiphase flow and transport properties and their likely variation in a reservoir setting, based on readily available experimental data.

Though many models have been suggested over the years, the focus of this thesis will be on network modelling wherein the void space of the porous medium is represented at the microscopic scale by a lattice of pores connected by throats. By applying rules that govern the transport and arrangement of fluids in pores and throats, macroscopic properties, for instance capillary pressure or relative permeability, can then be estimated across the network, which typically consists of several thousand pores and throats representing a rock sample of a few millimetres cubed.

In Chapter 2 I will conduct a literature review of the current state of network modelling, with special emphasis on the use of network models to predict experimental data. This has mainly become possible through the use of networks that
are realistic representations of porous media, and a better understanding of wettability effects on the pore-scale. Two main approaches to generate realistic networks have been reported in the literature. From a voxel-based representation of the porous medium, either numerically constructed or directly imaged, a topologically equivalent network can be directly generated. Alternatively, one can use a regular network but map the statistical properties of the porous medium, obtained from image or experimental data, onto it. Both of these methods will be reviewed.

Chapter 3 will describe the mathematical details and assumptions made that are at the foundations of the computer code that has been written as part of this thesis to simulate multiphase flow in network models. Details about generating the networks themselves will however be ignored, as this does not form part of this thesis. The computer code is written in such a way that no assumptions are made about the topology of the network.

The computer code described in Chapter 3 will then be subsequently used to predict experimental data. In Chapter 4 only water-wet media will be considered. As wettability is easier to characterise in this case, it will allow us to focus on verifying the details of the implemented network model. We will also introduce a methodology for modifying networks using easily obtainable experimental data. A network originally constructed to represent a Berea sandstone will be modified to predict multiphase properties of a sand pack.

Very few porous media are in fact water-wet, and the influence of wettability on predicted flow properties will be investigated in Chapter 5. First, we will try to predict production characteristics of mixed-wet systems for which we have a specific realistic network. Subsequently we will combine the methodology for modifying networks with prediction of different mixed-wet and oil-wet media. Experimental capillary pressure and relative permeability data from both reservoir sandstones and carbonates will be used. We will also introduce a new method for distributing mixed wetting at the pore-scale, and show how this improves the predictions of a reservoir sandstone. Finally, in Chapter 6 we will summarize the important findings of this work, and give some thoughts about the application and future direction of predictive pore-scale modelling.
The following articles have all been either based on material presented in this thesis, or used the computer code developed for this thesis:


Chapter 2

Literature Review

Modelling flow behaviour using network models was pioneered by Fatt in the 1950s [1956a; 1956b; 1956c]. By distributing the pores and throats on a regular 2D lattice and sequentially filling them in order of inscribed radius using the Young-Laplace equation, he was able to produce capillary pressure and relative permeability curves for drainage (as a function of average saturation) that had the same characteristics as those obtained experimentally. He investigated the effects of different network lattices (square, triangular, honeycomb and double-hexagonal) and found that these gave results that were closer to experimental measurements than assuming that the porous medium could be modelled as a bundle of parallel tubes. The pore size distribution was found to be more important for the results than were differences between lattices. Fatt computed the flow properties using an equivalent physical network of electrical resistors, since at the time (1956), numerical solution of the flow/conductance equations was not possible.

Further advances in network modelling didn’t occur until the late 1970s when computer processing power became more readily available. Chatzis and Dullien [1977] focused on the assumptions made earlier by Fatt. They noted that 2D networks could not reliably predict the behaviour in 3D, which until then had been a common assumption. The percolation threshold, when one phase spanned the system, was found to be highly dependent on the dimensionality of the problem, as predicted by percolation theory. They also noted the importance of coordination number $z$ (the number of throats connected to a pore), with breakthrough occurring later with reduction in average $z$. Their networks consisted of both pores and throats, both of which had assigned volumes. The invading fluid was injected from the inlet face and filled pores and throats in order of radius, in a similar process to that
described by Wilkinson and Willemsen [1983] who introduced the concept of invasion percolation, which is the theoretical foundation for drainage, and will be described in detail later. They also allowed clusters of defending fluid to become surrounded by the invader and become trapped. Trapping was further investigated by Dias and Wilkinson [1986].

Micro-model experiments of drainage and imbibition allowed the pore-scale physics of displacement to be understood. Lenormand et al. [1983] used models with rectangular cross-section capillaries to observe and describe the displacement processes in imbibition that still are at the foundations for network modelling – piston-like displacement, snap-off and cooperative pore-body filling. The details of these processes will be described later.

2.1 Description of the Pore Space

Until recently most networks were based on a regular lattice. The coordination number can vary depending on the chosen lattice (e.g. 5 for a honeycombed lattice or 6 for a regular cubic lattice). Chatzis and Dullien [1977] compared their results from regular networks to experimental mercury intrusion data from sandstones, and noted that regular networks combined with circular capillaries did not yield a realistic description of real sandstones.

Jerauld and Salter [1990] performed an extensive study of relative permeability and explained the trends seen using pore-scale network modelling. Using a cubic lattice with circular capillaries they were able to reproduce the features of relative permeability curves seen in experiments. They found that the most important structural property of the network was the size aspect ratio between pore-bodies and throats. This was found to influence significantly the amount of relative permeability hysteresis between flooding cycles as well as the shape of the curves. Also influencing the shape was the spatial correlation of pore and throat sizes, and to some degree the pore size distribution.

In order to match the coordination number of a given rock sample, which typically is between 3 and 8 [Jerauld and Salter, 1990], it is possible to remove throats from a lattice of higher coordination number. Dixit et al. [1997], again using a regular cubic lattice, found that in less well-connected media, with an average
coordination number of 4 rather than 6, the size aspect ratio between pore-bodies and throats had less influence on the relative permeability. The reduced connectivity of the network was found to dominate the relative permeability hysteresis.

To better reflect real porous media it is possible to randomly distribute points within the model area and then construct a network from the triangulation of these points. Jerauld et al. [1984a; 1984b] constructed random networks from Voroni diagrams. These networks had an initial coordination number of more than 15. This was subsequently reduced by removing the longest throats until an average coordination number of 6 were achieved. However, little difference in relative permeability was observed when comparing to regular networks [Jerauld and Salter, 1990]. Blunt and King [1990; 1991] constructed networks using a similar approach. These were then used to investigate the influence of both capillary and viscous forces on pore-scale displacements.

All the methods described so far fail to capture any of the statistics associated with real porous media. The use of networks derived from a real porous medium was pioneered by Bryant et al. [1992; 1993a; 1993b]. They extracted their networks from a random close packing of equally-sized spheres in which all sphere coordinates had been measured. They included compaction effects (by moving the sphere centres closer together vertically) and cementation (by increasing the spheres radii without moving their coordinates). They were able to show that the hydraulic conductivities of the network were spatially correlated and made good predictions of the trend in permeability with porosity for Fontainebleau sandstone. In contrast, using a statistically equivalent but uncorrelated network, the permeability was over-predicted by a factor of two [Bryant et al., 1993b]. This finding shows the crucial importance of using geologically realistic networks when predicting flow behaviour. Other transport properties, such as relative permeability and electrical conductivity, as well as capillary pressure, were also compared successfully with experimental results from sand packs, bead packs and a simple sandstone. However, since their networks were based on a pack of equally-sized spheres, resulting in a constant coordination number of 4, the application to more complex sandstones was limited.

In order to capture the connectivity of a real rock and reproduce this in the subsequent network representation, the rock itself has to be analyzed. It is common to do this in a two-step approach. First a 3D voxel-based representation (typically in
a binary format where 0 indicates matrix and 1 void space) of the pore space is
created that should capture the statistics of the real rock, from which an equivalent
network (in terms of topology, pore volume, throat radii, clay content, etc) is then
extracted. Neither of these steps is exclusive to the field of network modelling, and
both can be treated independently.

Figure 2.1: Comparison between different 3D voxel representations of a
Fontainebleau sandstone [Biswal et al., 1999], generated using different
reconstruction techniques. The side length of each sample is 2.25 mm. (a) X-ray
microtomography. (b) Object-based modelling. (c) Gaussian field technique. (d)
Simulated annealing.

The pore space description can be generated directly using X-ray
microtomography [Dunsmuir et al., 1991; Spanne et al., 1994; Coker et al., 1996],
where the rock is imaged at resolutions of around a few microns. This can be done
due to the differences in X-ray absorption of rock matrix and void space. A 3D
image of a Fontainebleau sandstone is shown in Figure 2.1 (a) along with a 2D cross-
section in Figure 2.2 (a). This method has the advantage of directly reconstructing the pore space, but due to the specialized scanners required, it is not readily available and also very costly. It is, however, very useful for validating numerical reconstruction techniques of the microstructure, described below.

Figure 2.2: Comparison between different 2D cross-sections of a Fontainebleau sandstone [Biswal et al., 1999], generated using different reconstruction techniques. The side length of each sample is 2.25 mm. (a) X-ray microtomography. (b) Object-based modelling. (c) Gaussian field technique. (d) Simulated annealing.

It is possible to generate a 3D model of the pore space by reproducing statistical information measured on 2D thin sections, of which an example is shown in Figure 2.3. Porosity, also called the one-point correlation function, and the two-point correlation function, measuring the probability of finding two points separated
by a distance $u$ within the same phase, pore or matrix, are the most basic quantities used to characterize porous media. However, both of these methods fail to incorporate any information about the underlying topology of the porous medium. The lineal-path function is the probability of finding a line segment of length $L$ completely within either the pore space or matrix [Lu and Torquato, 1992]. This provides more characterization of the structure of the medium as the function can be evaluated on a specific phase (pore space or matrix). It also has the benefit of being relatively quick to evaluate.

Figure 2.3: 2D thin section image of a Berea sandstone, generated using back scattered electron (BSE) imaging. The pore space is black, matrix is light grey and clay minerals are dark grey [Øren and Bakke, 2003].

Hilfer [1991] introduced the concepts of local porosity distribution and local percolation probability to improve the geometric characterization of porous media. Local porosity distribution is the probability density of finding the local porosity $\phi$ in the range $\phi \pm \Delta \phi$ in a cell of side lengths $L$. From the resulting histogram and porosity variance it is possible to get an indication of the level of heterogeneity within the investigated volume. Local percolation probability is a measure of the connectivity of the sample, measuring the fraction of cells with side length $L$ that percolate in a given direction (a continuous path through the cell exists). This is clearly an important characteristic of the reconstructed porous medium as it has a direct relation
to the transport properties, something that is not captured by the other quantitative measures.

Most stochastic reconstruction algorithms are based on thresholded Gaussian field techniques. Adler and Thovert [1998] have written an extensive review article on these. They are based on porosity and two-point correlation functions, both of which can be readily obtained by image analysis of 2D thin sections. The technique is similar to that used in geostatistics. A continuous correlated field is generated using Fourier transform methods and thresholded to retrieve the binary phases (pore space and matrix) with the correct porosity and correlation function, Figure 2.2 (c) and Figure 2.3 (c). This method can also be extended to include more phases, such as clays.

Realising that the earlier Gaussian based methods were not very good at reproducing the underlying particulate structures of the porous media, as evident from Figure 2.3 (c), Yeong et al. [1998b; 1998a] developed a stochastic method based on simulated annealing, later extended by Manwart et al. [2000]. Rather than being restricted to one- and two-point correlation functions, the objective function used can be made to match additional quantities such as multi-point correlation functions, lineal-path function or pore size distribution function to name a few. Since the method is based on moving pore-space voxels around to minimize the objective function, the correct porosity is always retained. They subsequently reconstructed a 3D Fontainebleau and Berea sandstones from 2D sections using an objective function based on both two-point correlation function and either lineal-path or pore size distribution function, Figure 2.2 (d) and Figure 2.3 (d). The estimated percolation probability was closer to the reference than when only using the two-point correlation function. Incorporating more higher-order information into the objective function, such as the local percolation probability, would most likely improve the reconstruction further, but that would also increase the computational cost of the method significantly.

Another technique is the use of object-based modelling whereby the actual rock-forming process is simulated. Packing algorithms for spheres are well established [Adler and Thovert, 1998] and algorithms for arbitrary shapes have also been presented by several authors [Coelho et al., 1997; Pilotti, 2000; Jia and Williams, 2001; Latham et al., 2001; Latham et al., 2002]. An algorithm that takes
into account the whole rock-forming process where primary grain sedimentation is followed by compaction and diagenesis has been presented by Bakke and Øren [1997; 2002] and later by Jin et al. [2003]. A grain size distribution is determined from image analysis of thin sections. Grains are then randomly picked from this distribution during the sedimentation process. Compaction is modelled by moving the centre of each grain down in proportion to its original vertical position. Finally, diagenetic processes are modelled. Quartz overgrowth is modelled by increasing the radii of the grains, and clays are precipitated on quartz surfaces. The amount of diagenesis to include is also determined from thin section analysis. Though this reconstruction method does not guarantee that statistical geometrical parameters such as the two-point correlation functions are honoured, it is assumed that these will be adequately reproduced since the actual rock-forming process is simulated, Figure 2.2 (b) and Figure 2.3 (b).

Biswal et al. [1999] performed a quantitative comparison of three reconstruction methods (Gaussian field, simulated annealing and object-based) on a Fontainebleau sandstone, where the reference, containing 300³ voxels, was obtained using microtomography. They found that the object-based technique reproduced the two-point correlation function reasonably well. When comparing connectivity using local percolation probability it was clear that the object-based technique was far superior to the statistical techniques. This agrees with analysis performed by Øren and Bakke [2002] and Hilfer [2000].

Recently several statistical reconstruction techniques have been suggested that try to improve on the deficiencies of the Gaussian field techniques, while not being as computationally demanding as simulated annealing. Thovert et al. [2001] introduced a method that is a hybrid between the statistical and object-based methods. Their technique is statistical, using only porosity and two-point correlation function, but conditioned to an underlying granular structure, defined using a pore size distribution derived from the two-point correlation function. This is based on a Poissonian penetrable sphere model. They verified their method using a 3D Fontainebleau sample and reported good agreement with the reference, even for the percolation probability. Hilfer and Manswart [2001; 2002] also developed a hybrid between statistical and object-based method. Initially a close packing of spheres is laid down. Matrix voxels are then randomly distributed in the pore space until a
prescribed porosity is attained. The configuration of the added matrix voxels are then updated using simulated annealing, matching the two-point correlation function. They also verified their method using a 3D Fontainebleau sample and the local percolation probability was found to be significantly better than traditional simulated annealing though not quite as good as a traditional object-based method.

For many types of porous media it might, however, be difficult to define the structures that make up the matrix. In carbonate rocks post-depositional diagenesis often completely dominates the matrix structure [Lucia, 1999], making object-based techniques difficult to use. In field-scale reservoir characterization the same problems are often experienced where there are multiple facies with distinctive connected geometries; for example, in fluvial reservoirs. Gaussian field techniques will not reproduce the channel connectivity whereas object-based methods rely on the facies geometries being easily parameterized. Strebelle [2002] suggested a statistical algorithm in which the multiple-point statistics were inferred from exhaustive 2D training images of equivalent reservoir structures and then used to reconstruct the reservoir, adhering to any conditioning data. This method was applied successfully to both fluvial and more complex patterned reservoirs. The ability to reproduce any pattern makes this method highly attractive for reconstructing complex porous media like carbonates. Okabe et al. [2003] have used this algorithm to reconstruct a 3D Fontainebleau sandstone from a 2D training image. Although the granular structure is not as well reproduced as in object-based methods, the local percolation probability is significantly better reproduced than that achieved by other statistical methods such as Gaussian field techniques.

2.2 Methods to predict transport properties

When estimating single phase transport properties like absolute permeability it is possible to conduct flow experiments directly on the 3D reconstructed sample. Many authors have reported good agreement with experimentally obtained values when solving the Stokes equation for single phase flow using finite difference methods [Roberts et al., 1996; Adler and Thovert, 1998; Hilfer and Manwart, 2001; Manwart and Hilfer, 2002; Øren and Bakke, 2002] or the Lattice-Boltzmann method [Manwart et al., 2002]. The importance of reproducing long-range connectivity in any reconstruction technique is clearly evident from calculations of absolute
permeability. Whereas object-based methods reproduce permeability values within a few percentage points, traditional Gaussian field techniques and simulated annealing typically under-predict permeability by about a factor of ten for low porosity systems that are close to the percolation threshold [Hilfer and Manwart, 2001; Manwart et al., 2002; Manwart and Hilfer, 2002; Øren and Bakke, 2002]. For higher porosity systems, the statistical methods generally perform somewhat better at reproducing the local percolation probability [Manwart et al., 2000], with permeability predicted within a factor of about five [Øren and Bakke, 2003].

Even single phase simulations conducted directly on the 3D reconstructed sample are computationally very expensive. A common way to model both single and multiphase flow quickly on large systems is to represent complex porous media by an equivalent network of pores and connecting throats. Absolute permeability has been successfully predicted, as already mentioned, by Bryant et al. [1993b] using this method. Another approach is to skip the 3D reconstruction process and estimate absolute permeability directly from the 2D thin sections. Lock et al. [2002] computed a distribution of fluid conductances by recoding pore areas and perimeter lengths. From this a single effective conductance was found using effective medium theory, resulting in a direct estimate of absolute permeability. This approach was applied to a number of sandstone thin sections with predicted absolute permeabilities generally within a factor of 2 of the measured values.

For multiphase flow it is possible to use Lattice-Boltzmann techniques [Gunstensen and Rothman, 1993; Chen and Doolen, 1998; Hazlett et al., 1998] to solve the transport equations on the 3D reconstructed sample. Being computationally very demanding, their use in multiphase flow problems is, however, limited to relatively small systems. As a consequence their applications are more tailored towards understanding the fundamental physics of flow in complex systems rather than for quantitative predictions.

A whole range of empirical or semi-empirical methods for predicting relative permeability have suggested over the last five decades [Dullien, 1992]. One of the most widely used is found by combining the model by van Genuchten [1980], relating effective wetting saturation to capillary pressure, with the model for relative permeability by Mualem [1976]. Empirical fitting parameters are found by matching the van Genuchten model to experimental capillary pressure. These parameters are
subsequently used for the relative permeability predictions. However, what most of these models have in common is that they are only applicable for strongly water-wet data, and many of them also rely on difficult to define parameters such as tortuosity exponents.

In this work, the approach chosen for predicting multiphase flow properties is pore-scale network modelling. In the following section we will therefore review in some detail the aspects for constructing and modelling flow through such networks.

2.3 Networks, pore shapes and wetting layers

2.3.1 Constructing networks

In cases where the matrix is just made up of a random packing of equal spheres, an equivalent network of pores and connecting throats can be created by tessellating the pack into tetrahedral cells. The pores will then be the cells, with throats being where cells share a common face [Bryant et al., 1993b]. This method can, however, not be used in more complex voxel-based representations of the pore space. In those cases the skeleton of the pore space is first created, consisting of the centre-lines of the pore space.

Lindquist et al. [1996; 1999; 2000] extended a thinning algorithm [Lee et al., 1994] in which the pore space is eroded until only the centre-lines remain. Though they didn’t create networks on which to perform fluid flow simulations, they did analyze geometric properties such as connectivity and tortuosity of skeletons generated from various micro-CT imaged rock samples. Liang et al. [1998] proposed an improvement to the existing thinning algorithms. This method was applied to statistically reconstructed samples of Berea sandstone and chalk [Talukdar et al., 2002]. One cause of concern was however that the level of smoothing applied to the reconstructed sample gave rise to significant differences in the topology of the skeleton [Liang et al., 2000]

The problem with pore space thinning algorithms is that pore space irregularities can create additional line segments and multiple vertices often have to be merged into a single pore. This can easily result in the subsequent network becoming too tortuous [Bakke and Øren, 1997]. When generating networks from object-based reconstruction methods, one is aided by being able to easily identify the
separate grains. By dilating each grain until adjacent grains meet, a Voroni diagram is created. The skeleton is then simply the points on the boundary surfaces that have neighbouring voxels from three or more grains with pore locations being points with four or more neighbouring grains [Bakke and Øren, 1997]. The area, perimeter and radius of each throat are defined by rotating a vector about the pore space centreline in the reconstructed medium, recording the values at the narrowest constriction and the averages. For pore bodies the vector is rotated about the centre point, using the average of the recorded values. Volumes are calculated by simply counting the voxels. A network constructed using this method is shown in Figure 2.4 (b).

Figure 2.4: Different network lattices consisting of 512 pore bodies. (a) A regular cubic lattice with a constant coordination number of 6. (b) From a 3D voxel-based representation of the pore space it is possible to construct a topologically equivalent network [Bakke and Øren, 1997]. The average coordination number in this case is 3.6.

An alternative to the thinning and dilation approaches has been suggested by Delerue et al. [1999; 2002] whereby the skeleton is created from the Voronoi diagram of the pore space. Although this method does not ensure the connectivity of the skeleton, as the others methods do, good agreement with experimentally obtained conductivity was reported for a soil that had been imaged with microtomography.

When using pore-scale modelling to predict experimental data, it is clearly important that the underlying network is representative of the rock. However, if the exact rock type has to be used for the network construction, the application of
predictive pore-scale modelling will be severely limited due to the complexity and cost of methods such as X-ray microtomography. How much information about the rock is needed in the network representation in order to make good predictions of experimental data thus becomes an important question. Chatzis and Dullien [1977] noted the importance of coordination number on flow behaviour while Bryant et al. [1992; 1993a; 1993b] could only get good predictions of permeability when spatially correlating the geometric properties of the network elements.

2.3.2 Calibrating networks using capillary pressure

Capillary pressure as a function of wetting phase saturation has commonly been used as a tool to calibrate the network model due to the close relationship to the distribution of inscribed radii [Dullien, 1992]. Wise [1992] used measured capillary pressure combined with the Laplace equation to randomly distribute the radii on a regular cubic lattice, of which an example is shown in Figure 2.4 (a). The throats with the smallest radii were subsequently removed from the network until a match with the absolute permeability was achieved, resulting in a network with coordination number less than six.

Rajarman et al. [1997] also conducted simulations on cubic networks but the throat radii were both spatially correlated in a given direction as well as cross correlated between throats connected to a single pore. Cross correlation was found to influence both the capillary pressure response and relative permeability more than did the spatial correlation. Both the pore size distribution and correlation parameters were subsequently optimized to obtain a best possible match between predicted and experimental capillary pressures for various unconsolidated soils. These networks were then used to predict primary drainage wetting phase relative permeability with some encouraging results.

Fischer and Celia [1999] calibrated their networks to capillary pressure very similarly to Rajarman et al. [1997]. Experimental data from a wide range of unconsolidated soils were used to test the methodology, with relative permeabilities available for both water and gas. The matches with capillary pressures were generally good, as were the predicted absolute and water relative permeabilities. For gas relative permeability the hysteresis between secondary drainage and tertiary imbibition was under predicted, resulting in relatively poor predictions. They noted
that additional structural components were needed in the network topology if improvement in the predictions were to be achieved.

An alternative to using capillary pressure when calibrating network models is to infer the properties from the reconstructed sample of the sandstone. In this approach the network is not constructed directly from the voxel representation, but rather its statistical properties are mapped onto a regular grid. This approach is motivated not just by the fact that capillary pressure might not always be available, but also by the observation that the optimized pore size distribution obtained in the previous methods is not unique [Vogel, 2000]. Depending how the pore sizes were spatially correlated, a good match with the reference capillary pressure could be obtained with significantly different pore size distributions.

Vogel and Roth [1997; 1998; 2001] obtained pore size distribution and pore connectivity from reconstructed samples of unconsolidated soils. The reconstruction was obtained by multiple 2D thin sections. Rather than obtaining a continuous pore size distribution, the range of pore sizes was divided into set number of bins (typically 10), obtained using an erosion-dilation approach. At each size interval the connectivity of pores larger than that size is quantitatively measured. When subsequently constructing the network representation, a face-centred cubic lattice with a maximum coordination number of 12, and the same pore size distribution and pore connectivity measure was imposed. The pore connectivity will affect both the distribution of pore sizes as well as the effective coordination number. Predicted primary drainage capillary pressures and hydraulic conductivities were then compared against experimental results. Though the predictions clearly were worse than those obtained by Fischer and Celia [1999], they were considerably better than those obtained when excluding the effects of pore connectivity in the network construction.

Hilpert et al. [2003] used a similar approach to that of Vogel and Roth, though using a regular cubic lattice rather than a face-centred one and explicitly modelling pore bodies as well as throats. By also introducing cross correlation between throats sizes connected to a single pore they were able to predict both experimental primary drainage and imbibition capillary pressures for different sphere packs with reasonable accuracy.
Tsakiroglou and Paytakes [2000] combined extracting statistical properties from reconstructed samples with conditioning to capillary pressures from mercury intrusion and retraction. First pore size distribution and connectivity information is extracted from thin section analysis with throat size distribution estimated from the experimental capillary pressures. These parameters are then optimized along with the coordination number distribution using a regular cubic lattice until a satisfactory match with both intrusion and extraction capillary pressures are obtained. The performance of the method was however only measured by the match to capillary pressure and predicted absolute permeability, both of which were quite good. No additional transport properties were predicted.

Using reconstructed samples of Fontainebleau sandstones, obtained by microtomography, Sok et al. [2002] compared transport predictions from topologically equivalent networks to those based on a face-centred cubic lattice with the same statistical properties. Even when including spatial and cross correlation for pore and throat sizes as well as the correct distribution of coordination numbers, the regular lattices gave poor predictions of both invasion pattern and residual saturations. Their conclusion was that those statistical parameters that can be easily obtained from the reconstructed medium are not sufficient for reliable predictions of transport properties and that additional higher-order topological information is needed.

The predicted transport properties are obviously not just a function of lattice topology and pore size distribution but also how each individual pore element is represented and the amount of pore-scale physics they can accommodate. Most of the network models described so far have been modelled as a collection of cylindrical tubes representing the throats, though in the work by Fischer and Celia [1999] the throats had a biconical shape rather than a uniform cylinder. It was argued by Reeves and Celia [1996] that this allowed for more accurate calculation of volumes and interfacial area as the location of possible fluid interfaces in throats could be accurately resolved. It also helped minimize trapping of wetting fluid in throats during drainage with the throats being allowed to drain if the interface from each side touched.

If pores were explicitly included they were often modelled as spheres or cylinders. In the work of Bryant et al. [1992; 1993a; 1993b] the throats were
assumed to control flow through the network, with the pores contributing volume. McDougall and Sorbie [1995; 1997] used a similar approach but only assigned volume to the throats. In some finer textured soils it was argued by Vogel [2000] that this was a better representation of the pore morphology than placing all the volume in pore bodies.

### 2.3.3 Wetting layers

The major restriction from only using circular tubes in network modelling is their inability to contain more than one fluid. The pore space in real rock is highly irregular with wetting fluid remaining in grooves and crevices due to capillary forces, even after the centre has been occupied by non-wetting fluid. This behaviour has been extensively observed in micromodel experiments where the flow channels typically have a square cross-section [Lenormand et al., 1983] The wetting layers might not be more than a few microns in thickness, with little effect on overall saturation or flow. Their contribution to wetting phase connectivity is however of vital importance, ensuring low residual wetting phase saturation due to the prevention of trapping. Wetting films, as observed by Dullien et al. [1989] in smooth bead packs, are only nanometers in thickness, stabilized by molecular forces. These covered the smooth beads but were found not to conduct hydraulically and contributed negligibly to saturation. The wetting fluid was trapped in pendular rings between the beads, resulting in a residual saturation of 9 percent. Once the beads were etched in acid, creating grooves in the surface, the residual wetting phase saturation fell to 1 percent as a result of flow in layers.

It is clear that a network model consisting exclusively of circular tubes will not capture this behaviour, resulting in wrong predictions for residual saturation, transport properties and hysteresis effects. Kovscek et al. [1993] suggested using star shaped tubes in order to capture the effects of wetting layers. This is the same cross-sectional shape as that resulting from using grain boundary shaped throats, as used by for example Man and Jing [1999; 2000; 2001]. Other popular pore shapes include squares [Blunt, 1997a, 1998; Fenwick and Blunt, 1998; Dillard and Blunt, 2000] and equilateral triangles [Hui and Blunt, 2000]. These different shapes are illustrated in Figure 2.5.
Figure 2.5: Popular pore shapes used in network modelling studies include circular (a), square (b), star shaped (c) and triangular (d). The throats can either have a constant radius (e) or vary smoothly (f).

When using networks based on reconstructed sandstones one would like to relate the individual pore shape to that observed in the reconstructed medium, which one cannot do when using a single cross-sectional shape. Since the real pore space is highly irregular it is not feasible to reproduce it exactly, but one can still include the measured quantities (cross-sectional area, radius and perimeter length) through the use of a dimensionless shape factor $G$, as suggested by Mason and Morrow [1991]. This is defined as the average cross-sectional area divided by the perimeter squared. Once the shape factor has been measured on the reconstructed medium an equivalent (in terms of $G$) irregular triangle can be defined, where $G$ varies from 0 for a slit-shaped pore to $\sqrt{3}/36$ for an equilateral triangle. A highly irregular pore will thus
have a low shape factor, resulting in the equivalent triangle having sharp corners, with more wetting fluid retained and higher conductivity in the wetting layers. A further advantage of this approach is that not only will it correct for layer volume and conductivity, but calculated capillary entry pressure will now be a direct function of the pore shape using expressions derived by several authors [Mason and Morrow, 1991; Ma et al., 1996; Øren et al., 1998]. In the few cases where pore shapes are in fact quite regular in the reconstructed medium one can use other equivalent pore shapes like squares ($G = 1/16$) or circles ($G = 1/4\pi$). It is assumed that the wetting fluid residing in corners is connected to those of adjacent pores and throats, with the result that the wetting fluid generally spans the entire network (excluding possible elements with circular cross-section). This is the approach used by Øren et al. [1998], Patzek [2001] and will also be followed by the work presented here.

### 2.4 Wettability effects

The wetting condition of the porous medium is of great importance in defining the flow characteristics. The oil-water contact angle $\theta_{ow}$ is defined as the angle of contact of oil and water on a solid surface measured through the denser (water) phase, as illustrated in Figure 2.6 (a). Three broad classifications can be identified – water-wet, oil-wet or intermediate-wet, where the contact angles are less than 90°, greater than 90° or close to 90°, respectively. A combination of these wetting conditions is also possible. I will refer to this latter condition as mixed-wet – most hydrocarbon bearing reservoirs are found to fall into this category [Anderson, 1986a].

![Figure 2.6](image-url)

Figure 2.6: (a) The oil-water contact angle $\theta_{ow}$ is measured through the denser phase (water). (b) On rough surfaces the advancing contact angle $\theta_a$ (increase in water saturation) is typically found to be significantly larger than the receding contact angle $\theta_r$ (reduction in water saturation). The intrinsic contact angle $\theta_i$ is that measured at rest on a smooth surface [Morrow, 1975].
Consider that initially the rock is water-saturated and strongly water-wet. Following primary oil flooding it is assumed that the part of the rock in direct contact with hydrocarbon will alter its wettability, whereas the crevices and small throats still containing water will remain strongly water-wet. Initially a thin water film protects the pore walls from the asphaltenes in the oil that can make the pore walls become oil-wet [Kovscek et al., 1993]. In some pores this film might collapse, allowing the pore to become oil-wet. Some wettability alteration might still occur in pores where the film remains as a result of asphaltenes diffusing across the water film [Kaminsky and Radke, 1997]. The rock might therefore end up with three distinctively different simultaneous wetting populations – strongly water-wet where oil has not invaded, strongly oil-wet where the water films have collapsed and intermediate-wet where the films remain. This type of wetting condition has indeed been observed experimentally [Masalmeh, 2003]. The same wettability state is likely to occur in groundwater situations where non-aqueous phase liquids have been in contact with the soil for many months or years.

In addition to wettability alteration, contact angles are affected by the direction of flow. Due to surface roughness, advancing contact angles $\theta_a$ (increase in water saturation) are typically found to be significantly larger than receding contact angles $\theta_r$ (reduction in water saturation), Figure 2.6 (b). Morrow [1975] developed several models for this contact angle hysteresis by measuring both advancing and receding angles in a number of smooth and roughened Teflon tubes and relating these to the intrinsic contact angle as measured at rest on a smooth surface. Although one would expect to see no difference between advancing and receding contact angles in completely smooth tubes (referred to as Class I model), some hysteresis was observed (Class II model). Morrow explained this by minor inaccuracies in the tube manufacturing process. Following roughening of the tubes, substantially more hysteresis was observed (Class III model). The amount of hysteresis experienced in real porous media is still, however, highly uncertain due to the difficulty of measuring and classifying results from non-ideal systems where both mineralogy and fluid composition can have large influences [Buckley et al., 1998]. Xie et al. [2002] measured both advancing and receding contact angles on a quartz surface during repeated flooding cycles. The receding contact angle was generally found to remain stable. Depending on which of the 10 crude oil samples were used, the advancing
contact angle was found to either remain stable (four crude oils) or decrease somewhat with flooding cycle. The amount of hysteresis was generally found to be between 40 and 70 degrees, somewhat less than the Class III model but considerably more than the Class II model, as suggested by Morrow [1975].

The flow behaviour when large parts of the rock surface are strongly oil-wet is found to be significantly different from intermediate and water-wet conditions. Salathiel [1973] conducted flooding experiments on a range of cores with different wettability. He found that oil production continued long after initial water breakthrough in mixed-wet cores with very low residual oil saturation obtained as a result. However, a very large number of injected pore volumes of water were needed to achieve these low saturations. Salathiel suggested that oil escaped through connected layers that could exist in strongly oil-wet pores. Kovscek et al. [1993] suggested this behaviour could be captured in network models using the above-mentioned star shaped network elements. Following drainage only the part of the pore wall in direct contact with oil would become oil-wet with the corners remaining water-wet. The oil-water interface in the corners would initially remain pinned during water flooding, allowing oil layers to become sandwiched between water in the corners and that in the centre. With this pore level scenario he was able to reproduce the experimental trends observed by Salathiel.

From Amott core-flood tests and nuclear magnetic resonance (NMR) it is possible to obtain a bulk indication of the wettability [Anderson, 1986b]. How the mixed wettability is distributed on the pore-scale is, however, much more difficult to evaluate. Kovscek et al. [1993] proposed a theoretical model where the smaller pores become oil-wet while the larger ones remain water-wet. Using cryo- and environmental scanning electron microscopy it is possible to visualize directly the distribution of fluids at the pore-scale [Fassi-Fihri et al., 1991; Combes et al., 1998; Durand and Rosenberg, 1998]. These studies suggested that the distribution of clay, in particular kaolinite, plays a very important role in determining what parts of the rock becomes oil-wet.

The impact of wettability on relative permeability has been extensively studied using pore-scale network modelling. McDougall and Sorbie [1995; 1997] investigated trends in relative permeability as well as recovery efficiency. Even with a fairly simple network model that didn’t explicitly include wetting layers they were
able to predict trends in recovery that indicated that optimum recovery would be obtained with about half the pore space being oil-wet, something that had been previously observed experimentally [Jadhunandan and Morrow, 1995].

Dixit et al. [1998; 1999; 2000] used the same simple network model as McDougall and Sorbie [1995] to introduce a wettability classification system, relating recovery from mixed-wet systems to aging and fraction of oil-wet pores. They also developed analytical expressions relating different wettability indices to different mixed-wetting scenarios and compared these to network modelling predictions [2000]. It was suggested that if experimental capillary pressures were available for different flooding cycles, it should be possible to determine whether oil-wet pores were correlated to pore size or just randomly distributed.

Blunt [1997b; 1998] used square elements for both pores and throats. This allowed him to explicitly model wetting layers and from simple geometrical considerations develop capillary pressure expressions for the different filling events described by Lenormand et al. [1983]. In each element multiple wetting conditions were allowed to exist, with the corners remaining water-wet while the centre becoming oil-wet in a similar approach to that of Kovscek et al. [1993]. The effects on relative permeability from a wide range of wetting conditions were investigated and although the main conclusions were the same as those reached using simpler network models [Dixit et al., 1997; McDougall and Sorbie, 1997; Dixit et al., 1998] an improved understanding of strongly oil-wet systems was made possible.

Only very limited mixed-wet experimental relative permeability data have been predicted using pore-scale network modelling. Only recently when combining geologically realistic networks with improved understanding of pore level physics have some promising results been shown by Øren et al. [1998] who predicted relative permeability for a water-wet Bentheimer sandstone and for a mixed-wet reservoir sandstone. Jadhunandan and Morrow [1995] measured oil recovery from a series of Berea cores. Mixed-wetting conditions where achieved primarily by varying the initial water saturation. Maximum recovery was achieved in cores where the Amott wettability index was close to zero, corresponding to intermediate initial water saturations. Using geologically realistic networks from reconstructed samples of Berea sandstone both the trend [Jackson et al., 2003] and a quantitative match [Øren and Bakke, 2003] with experimental recoveries have been predicted. Jackson
et al. [2003] assumed that all invaded pores following primary drainage become oil-wet. The experimentally measured wettability indices were then matched by varying the distribution of oil-water contact angles. We will pursue a similar but more thorough approach in this thesis. Øren and Bakke [2003] introduced a method for estimating the oil-wet fraction and contact angle distributions using the measured wettability indices. They were able to obtain a quantitative match with experiments using several different schemes for selecting the oil-wet pores.

2.5 Discussion

Pore-scale network modelling has been an active field of research for more than two decades. However, its main application has been constricted to better understanding pore-scale physics and explaining general displacement trends rather than a tool to predict the flow behaviour of a specific porous medium. The reason for this is simple: flow in real porous media is a complex problem. A pore-scale network model with predictive capabilities will need to carefully address both the statistical and topological properties of the porous medium, the physics of fluid transport at the pore-scale, and wettability characterization. Recent advances in these three areas have thus been the focus of this literature survey.

It seems clear that using a regular lattice structure to represent real porous media is not feasible if the network model is to have predictive capabilities. Even when mapping most of the morphological properties of a sandstone onto the lattice Sok et al. [2002] were unable to satisfactorily predict the transport properties of the sandstone. Another approach used in conjunction with regular lattices is to use easily obtainable macroscopic properties such as experimental capillary pressure to populate the properties of the lattice. This is then used to predict other macroscopic properties like relative permeability that are more difficult to obtain experimentally. Though Fischer and Celia [1999] managed to predict relative permeability for individual flooding cycles quite well, they were unable to predict hysteresis trends between different cycles. The experimental data they tried to predict will in fact be revisited in Chapter 4 of this thesis.

One approach that has shown itself to be successful in predicting experimental transport properties is that pioneered by Øren and co-workers at Statoil [1997; 1998; 2002]. By obtaining the lattice structure directly from a voxel-based representation
of the porous media they are able to capture both the relevant statistical and topological properties of the media. Combining this with a network model that is able to model all the relevant pore-scale physics has progressed network modelling to the stage where it now can be used to reliably predict transport properties of real systems. This approach will indeed be followed in this thesis. However, there are still remaining issues, some of which will be addressed in this work. The approach as presented by Øren et al. assumes that lattice and subsequent flow predictions are specific to the properties of the porous medium used in the voxel-based reconstruction. I will present in Chapter 4 a methodology for combining realistic networks, originally constructed to represent one particular porous medium, with conditioning to easily obtainable experimental data to predict flow properties of a variety of different porous media.

Predictive pore-scale modelling of systems with complex wetting behaviour is something that is almost completely absent from the literature. One reason for this is the high degree of uncertainty relating to the characterization of mixed wettability on the pore-scale. Relatively simple theoretically based scenarios for mixed wetting [Kovscek et al., 1993] are found to inadequately describe real systems [Durand and Rosenberg, 1998]. However, if some degree of confidence can be attached to the basics of the pore-scale network model, i.e. lattice properties and implemented pore-scale physics, valuable insight into the displacement process can be achieved by comparing experimental data to network model predictions [Jackson et al., 2003; Øren and Bakke, 2003]. This is something that will be investigated in further detail in Chapter 5.
Chapter 3

Network Model

In this section we will outline the mathematical details and assumptions made when simulating multiphase flow in network models. This broadly follows the work of Øren et al. [1998], Patzek [2001] and Al-Futaisi and Patzek [2003]. The most basic assumption made is that the flow is capillary dominated (quasi-static) with the viscous pressure drop in the model being insignificant in comparison to the capillary pressure. The capillary number $N_{cap}$ (ratio of viscous to capillary forces) should be less than $10^{-4}$ [Blunt and Scher, 1995], as defined by

$$N_{cap} = \frac{\mu v}{\sigma},$$

(3.1)

where $\mu$ is viscosity, $\sigma$ is interfacial tension and $v$ is fluid velocity. What this means in practice is that all interfaces are kept static throughout the network with the exception of a single displacement event.

We will refer to the initial wetting phase as water and the non-wetting phase as oil (unless experimental data is based on other fluids). Also, since mixed-wet systems make the terms drainage (non-wetting phase invasion) and imbibition (wetting-phase invasion) ambiguous, we will refer to these processes as oil and water flooding, respectively.

3.1 Description of the pore space

A 3D voxel representation of Berea sandstone is the basis for the networks used in this paper, Figure 1. A topologically equivalent network of pores and throats is then generated with properties (radius, volume, etc) extracted from the original voxel representation.
Figure 3.1: (a) 3D image of a sandstone along with (b) a topologically equivalent network representation [Bakke and Øren, 1997].

The individual network elements are uniform ducts with circular, triangular or square cross-sectional shapes. These have the same shape factor [Mason and Morrow, 1991], \( G = A/P^2 \), as the voxel representation, where \( A \) is the cross-sectional area and \( P \) the perimeter length, as illustrated in Figure 3.2. In the voxel representation these are average values recorded along the throat and at the pore centre. As the pore space becomes more irregular the shape factor decreases. A circle and a square have shape factors of \( 1/16 \) and \( 1/4\pi \), respectively. For a triangle the
shape factor will range from zero for a slit shaped triangle to 3/36 for an equilateral triangle.

$$G = \frac{A}{P^2}$$

$$G = \frac{1}{4\pi}$$

$$G = \frac{1}{16}$$

Figure 3.2: The network elements (triangular, circular or square cross-section) have the same shape factor [Mason and Morrow, 1991] as that measured on the irregular voxel representation.

For a given shape factor the corner half angles $\beta$ can take on a range of values where $\beta_1 \leq \beta_2 \leq \beta_3$. First $\beta_2$ is chosen randomly within the allowed range

$$\beta_{2,\text{min}} = \arctan \left( \frac{2}{\sqrt{3}} \cos \left( \frac{\arccos \left( -\frac{12\sqrt{3}G}{3} \right) + 4\pi}{3} \right) \right)$$

(3.2)

and

$$\beta_{2,\text{max}} = \arctan \left( \frac{2}{\sqrt{3}} \cos \left( \frac{\arccos \left( -\frac{12\sqrt{3}G}{3} \right)}{3} \right) \right),$$

(3.3)

with $\beta_1$ subsequently given by

$$\beta_1 = -\frac{1}{2} \beta_2 + \frac{1}{2} \arcsin \left( \frac{\tan \beta_2 + 4G}{\tan \beta_2 - 4G} \right),$$

(3.4)

and finally $\beta_3 = \pi/2 - \beta_1 - \beta_2$ [Patzek, 2001]. Compared to the voxel image the network elements are obviously only idealized representations. However, by maintaining the measured shape factor a quantitative measure of the irregular pore space is maintained. Fairly smooth pores with high shape factors will be represented by network elements with circular cross-sections, whereas more irregular pore
shapes will be represented by triangular cross-sections, possibly with very sharp corners.

Using square or triangular shaped network elements allows for the explicit modelling of wetting layers (water or oil depending on the wetting state), whereby non-wetting phase occupies the centre of the element and wetting phase remains in the corners. The pore space in real rock is highly irregular with water remaining in grooves and crevices after primary oil flooding, due to capillary forces. This behaviour has been observed in micromodel experiments where flow channels typically have a square cross-section [Lenormand et al., 1983]. The wetting layers might not be more than a few microns in thickness, with little effect on the overall saturation or flow. Their contribution to wetting phase connectivity is, however, of vital importance, ensuring low residual wetting phase saturation by preventing trapping.

Micro-porosity and water saturated clays will typically not be drained during core analysis. Rather than explicitly including this in the network representation, a constant clay volume that remains water-filled is associated with each element.

### 3.2 Primary oil flooding

Since all the elements (pores and throats) in the network model initially only contain water, displacement can only occur through piston-like displacement whereby the centre of an element can only be filled if it has an adjacent element containing oil. The capillary pressure required for the oil meniscus to invade a water-filled element is given by the Young-Laplace equation

\[ P_{cow} = P_o - P_w = \sigma_{ow} \left( \frac{1}{R_1} + \frac{1}{R_2} \right), \tag{3.5} \]

where \( \sigma_{ow} \) is the oil-water interfacial tension and \( R_1 \) and \( R_2 \) are the principal radii of curvature of the interface. When we know the shape of the pore and the contact angle at which the interface hits the solid surface we can use expressions that are easier to evaluate. For a circular pore it is simply

\[ P_{cow} = \frac{2\sigma_{ow}\cos\theta_{ow}}{R}, \tag{3.6} \]
where $\theta_{owr}$ is the receding oil-water contact angle and $r$ is the inscribed radius [Dullien, 1992]. Gravity effects can be included easily by subtracting $\Delta \rho_{ow}gh$ from the capillary entry pressure expressions, where $\Delta \rho_{ow}$ is the density difference between oil and water, $g$ is the gravitational constant and $h$ is the height above datum of the element. For the remaining part of this thesis I will omit the oil-water subscript.

Figure 3.3: View of oil (transparent) displacing water in a triangular duct during piston-like displacement.

Figure 3.4: Cross-sectional view of a single corner in a polygonal shaped element.

Only a very small fraction of network elements will have a circular cross-section. For polygonal shaped elements the capillary entry pressure expressions become complex as the wetting fluid remains in the corners as arc menisci (AMs). Entry pressures are found by calculating the force balance acting on the interface in the duct, as illustrated in Figure 3.3. This method has become known as the Mayer, Stowe and Princen (MS-P) method [Mason and Morrow, 1991] and we follow Øren et al.’s [1998] generalization of it, given by

$$P_c = \frac{\sigma \cos \theta_r (1 + 2/\pi G)}{r} F_d(\theta_r, G, \beta),$$

(3.7)
where $F_d$ is a dimensionless correction factor for wetting fluid that might be retained in the corners. For a polygonal shaped element, for which one corner is shown in Figure 3.4, it can be calculated by considering a small displacement $dx$ of the AM. This must be balanced by the change in surface free energy,

$$P_c A_{eff} = (L_{ow} \sigma_{ow} + L_{os} \sigma_{os} + L_{os} \sigma_{ws}) dx,$$  (3.8)

where $A_{eff}$ is effective area occupied by oil, $L_{os}$ is the length of the oil-surface interface and $L_{ow}$ is the length of the oil-water interface. A horizontal force balance gives the Young equation,

$$\sigma_{os} = \sigma_{ws} + \sigma_{os} \cos \theta_{owr},$$  (3.9)

that allows us to simplify (3.8),

$$\frac{P_c}{\sigma_{ow}} = \frac{1}{R} \left( \frac{L_{ow} + L_{os} \cos \theta_{owr}}{A_{eff}} \right),$$  (3.10)

where $R$ is the radius of curvature. The interface lengths can be determined from elementary geometry,

$$A_{eff} = A - R^2 \sum_{i=1}^{n} \left[ \frac{\cos \theta_r \cos(\theta_r + \beta_i)}{\sin \beta_i} + \theta_r + \beta_i - \frac{\pi}{2} \right] = \frac{r^2}{4G} - R^2 S_1,$$  (3.11)

$$L_{os} = \frac{r}{2G} - 2R \sum_{i=1}^{n} \frac{\cos(\theta_r + \beta_i)}{\sin \beta_i} = \frac{r}{2G} - 2RS_2,$$  (3.12)

$$L_{ow} = 2R \sum_{i=1}^{n} \left( \frac{\pi}{2} - \theta_r - \beta_i \right) = RS_3,$$  (3.13)

where $n$ is the total number of corners containing AM’s ($\beta < \pi/2 - \theta_r$) and $A = r^2 / (4G)$ is the total polygon area. A quadratic expression for the curvature radius is then given by,

$$R = \frac{r \cos \theta_r \left( -1 \pm \sqrt{1 + \frac{4GD}{\cos^2 \theta_r}} \right)}{4GD},$$  (3.14)

$$D = S_1 - 2S_2 \cos \theta_r + S_3.$$  (3.15)
The sign in (3.14) must be chosen so that the curvature radius that is less than the inscribed radius. The dimensionless correction factor in (3.7) is therefore given by

\[ F_d(\theta_r, G, \beta) = \frac{1 + \sqrt{1 + \frac{4GD}{\cos^2 \theta_r}}}{1 + 2\pi G}. \tag{3.16} \]

In the case of a circular tube where there are no corners, \( F_d \) will be 1 and (3.7) will simplify to (3.6).

The throats along the inlet face of the network model are all assumed to be connected to a reservoir of oil. The pressure in the oil phase \( P_o \) is then increased while the water phase pressure \( P_w \) is kept constant throughout the network, resulting in increased capillary pressure \( P_c \). The elements are filled in order of increasing capillary entry pressure (assuming they have an oil-filled neighbour). This process continues until some predefined saturation is reached, or all elements have been filled by oil. Once a polygonal element has been filled by oil, water still remains in the corners. This will ensure that water, as the wetting phase, will remain connected throughout primary oil flooding, since escape to the outlet is always possible through wetting layers.

### 3.3 Secondary water flooding

The part of the rock in direct contact with oil will have its wettability altered following primary oil flooding, whereas the corners and elements still only containing water will remain strongly water-wet, Figure 3.5. In addition to wettability alteration, contact angles are affected by the direction of flow due to surface roughness. Contact angle hysteresis between the flooding cycles is thus modelled using the Class III model suggested by Morrow [1975]. By defining a distribution of intrinsic contact angles, the receding \( \theta_r \) (reduction in water saturation) and advancing \( \theta_a \) (increase in water saturation) values can be found using the relationship illustrated in Figure 3.6.
Figure 3.5: Possible fluid configurations. (a) Initially the element is water-filled and strongly water-wet. (b) Following primary oil flooding the part of the element in contact with oil will alter its wettability. (c) During water flooding the element might again become completely water-filled. (d) If wettability alteration was large enough, oil might become sandwiched as a layer between water in the corner and the centre.

Figure 3.6: Relationship between receding and advancing contact angles on a rough surface, as a function of intrinsic contact angle measured at rest on a smooth surface [Morrow, 1975].
With wettability alteration and water in corners the mechanisms by which water can displace oil become more complex [Lenormand et al., 1983]. The three main processes are piston-like displacement, pore body filling and snap-off.

### 3.3.1 Piston-like displacement

As the capillary pressure drops, the oil-water interface in corner \( i \) will initially remain pinned at the last position \( b_i \) obtained during primary oil flooding, Figure 3.7 (a).

![Figure 3.7: Fluid configurations in corners. (a) A pinned interface hinges between receding and advancing contact angles. (b) Oil might become sandwiched between water in corners and water in the centre.](image)

In order to maintain capillary equilibrium, the contact angle \( \theta_{h,i} \) will hinge at this position in order to maintain capillary equilibrium. Therefore,

\[
\begin{align*}
    b_i &= R_{\text{min}} \frac{\cos(\theta_r + \beta_i)}{\sin \beta_i}, \\
    \theta_{h,i} &= \arccos \left( \frac{b_i \sin \beta_i}{R} \right) - \beta_i,
\end{align*}
\]

where \( R = \sigma / P_c \) is the radius of curvature and \( R_{\text{min}} \) is the smallest radius of curvature obtained during primary oil flooding. Only when reaching the advancing contact angle \( \theta_a \) will the interface start to move along the pore surface. During spontaneous (positive capillary pressure) piston-like displacement the capillary entry pressure is again found by calculating the force balance acting on the interface. Since the hinging contact angle is a function of capillary pressure, the following equations are solved iteratively to obtain the solution for the curvature radius corresponding to the capillary entry pressure:

\[
R = \frac{A_{\text{eff}}}{L_{\text{ow}} + L_{\text{os}} \cos \theta_a},
\]
\[ A_{\text{eff}} = A - R^2 \sum_{i=1}^{n} \left[ \frac{\cos \theta_{h,i} \cos(\theta_{h,i} + \beta_i)}{\sin \beta_i} + \theta_{h,i} + \beta_i - \frac{\pi}{2} \right], \quad (3.20) \]

\[ L_{os} = \frac{r}{2G} - 2 \sum_{i=1}^{n} b_i, \quad (3.21) \]

\[ L_{ow} = 2R \sum_{i=1}^{n} \sin \left( \frac{b_i \sin \beta_i}{R} \right). \quad (3.22) \]

If the hinging contact angles have all reached the limiting advancing value, the expression for the capillary entry pressure will be the same as that during primary oil flooding with the receding contact angle replaced by the advancing one. In the case where one or more of the interfaces have reached the advancing contact angle the expression for \( b_i (3.17) \) is simply replaced by

\[ b_i = R \frac{\cos(\theta_r + \beta_i)}{\sin \beta_i}. \quad (3.23) \]

From these expressions it is clear that spontaneous displacement might occur for advancing contact angles greater than 90°, with the maximum angle given by

\[ \cos \theta_{a,\text{max}} \approx \frac{-4G \sum_{i=1}^{n} \cos(\theta_r + \beta_i)}{r - \cos \theta_r + 12G \sin \theta_r}. \quad (3.24) \]

During forced water invasion (negative capillary pressure) the absolute entry pressure is simply given by (3.7) with \( \theta_r \) replaced by \( \pi - \theta_a \).

### 3.3.2 Pore body filling

The capillary entry pressure for filling a pore body during spontaneous water flooding is limited by the largest radius of curvature that can be achieved. This will depend on the number of adjacent oil-filled throats [Lenormand et al., 1983], as shown in Figure 3.8.
Figure 3.8: Pore body filling processes. The capillary entry pressure will be lower when several connecting throats (b) are filled with oil compared to when only a single throat is oil-filled (a).

A pore body with coordination number $z$ can thus be filled by $z-1$ possible events, $I_1$ to $I_{z-1}$, each occurring at a separate capillary pressure. If only a single adjacent throat is filled with oil ($I_1$ mechanism) the process is similar to piston-like displacement, with the entry pressure found using the approach outlined in the previous section. Since the exact spatial location of the oil-filled throats is difficult to estimate, it is common to express the capillary entry pressure as a parametric model [Blunt, 1998]:

$$P_c = \frac{2\sigma \cos \theta}{r} - \sigma \sum_{i=1}^{n} A_i x_i,$$

where $n$ is the number of connecting oil-filled throats, $A_i$ are arbitrary numbers and $x_i$ are random numbers between zero and one. Since $A_i$ have dimensions of m$^{-1}$ we chose to relate it to permeability,

$$A_2 - A_n = \frac{0.03}{\sqrt{K}},$$

where the permeability $K$ is measured in m$^2$. This approximately reproduces the results by Blunt [1998]. When only one connecting throat contains oil ($I_1$ event) the process is similar to piston-like displacement and hence $A_1 = 0.0$ µm$^{-1}$. This is also the most favoured event. During forced water invasion the capillary entry pressure is not dependent on the number of adjacent oil-filled throats and the filling process is again similar to piston-like displacement.
The choice of weights will clearly have an impact on what type of displacement will be most favoured. Larger weights will reduce the capillary entry pressure when the pore body is surrounded by multiple oil-filled throats, making other displacement events, like snap-off, more favourable. This effect will be similar to that achieved by having a smaller advancing contact angle or a larger size aspect ratio between pore bodies and throats, both of which make snap-off more likely to occur compared to pore body filling.

### 3.3.3 Snap-off

In snap-off an element is filled with water as the result of corner water layers swelling so much that the fluid/fluid interface becomes unstable. Snap-off will only occur if there is no adjacent element whose centre is filled with water. If \( \theta_a < \pi/2 - \beta_1 \) the arc menisci will advance smoothly along the pore wall once \( \theta_a \) has been reached. Once two menisci meet, there no longer is an oil-water-solid contact, resulting in the oil-water interface becoming unstable with spontaneous water filling as the result, as shown in Figure 3.9 (a). The capillary pressure at which this occurs depends on whether one or several menisci have started to advance along the pore wall. If two or more menisci have started to move, the menisci in the sharpest corners will meet at a capillary pressure

\[
P_c = \frac{\sigma}{r} \left( \cos \theta_a - \frac{2 \sin \theta_a}{\cot \beta_1 + \cot \beta_2} \right),
\]

whereas if only the meniscus in the sharpest corner has started to advance, it will meet the pinned meniscus in the most oblique corner at a capillary pressure

\[
P_c = \frac{\sigma}{r} \left( \frac{\cos \theta_a \cot \beta_1 - \sin \theta_a + \cos \theta_{h,3} \cot \beta_3 - \sin \theta_{h,3}}{\cot \beta_1 + \cot \beta_2} \right).
\]

The event with the highest capillary pressure will be the one that occurs.
Figure 3.9: Snap-off events. (a) During spontaneous water injection snap-off will occur once water in corners meet along the pore wall. (b) During forced water injection snap-off will occur as soon as the advancing contact angle is reached.

During forced water invasion snap-off will occur as soon as $\theta_{h,1}$ has reached $\theta_a$ or $\theta_a - \beta_1$ in the case where $\theta_a > \pi - \beta_1$. Once the arc meniscus starts advancing along the pore wall, the absolute negative curvature will decrease, making it unstable with spontaneous filling as the result, Figure 3.9 (b), with the entry pressure given by

$$P_c = \frac{\sigma \cos(\theta_a + \beta_1)}{R_{\text{min}} \cos(\theta_r + \beta_1)} \quad \theta_a \leq \pi - \beta_1 \tag{3.29}$$

or

$$P_c = -\frac{\sigma}{R_{\text{min}} \cos(\theta_r + \beta_1)} \quad \theta_a > \pi - \beta_1. \tag{3.30}$$

Piston-like displacement is always favoured (occurring at a higher capillary pressure) to snap-off wherever piston-like displacement is topologically possible. Snap-off can, however, still be an extremely important displacement process as it does not require any adjacent elements being water-filled. Hence, it can occur anywhere where the oil is connected to the outlet.
3.3.4 Oil layers

When the water interface enters the element during forced invasion a layer of oil, Figure 3.7 (b), might become sandwiched between water in the corner and that in the centre if

$$\theta_a > \frac{\pi}{2} + \beta_i.$$ (3.31)

This can occur because the inner oil-water interface has a hinging contact angle that might be much less than the advancing contact angle associated with the outer interface. Stable oil layers can significantly increase recovery as they increase oil connectivity in much the same way that water layers influence primary oil flooding. The oil layer will collapse once the two interfaces meet, which if the capillary pressure is the same across the two interfaces, is given by the condition

$$P_c = \frac{\sigma \cos(\alpha \cos(2 \sin \beta_i + \cos \theta_a) + \beta_i)}{b_i \sin \beta_i}. \hspace{1cm} (3.32)$$

3.3.5 Displacement process

At the beginning of water flooding the reservoir is at some given initial water saturation and capillary pressure. Water is then injected by increasing the water phase pressure, keeping the oil phase pressure constant through the outlet reservoir, resulting in a reduced capillary pressure. All possible displacement events are sorted in terms of capillary entry pressure, with the event with the highest capillary pressure executed first. The initial list of possible events is much bigger than it was during oil flooding. Not only are elements with adjacent water included, but also all possible snap-off events.

During primary oil flooding trapping was unimportant (though possible because oil-filled elements with a circular cross-section do not contain water layers) as water in corners ensured global connectivity, whereas during water flooding it becomes crucial. Once an element is filled from spontaneous invasion, it no longer conducts oil, since it is completely water-filled. Snap-off events, which typically occur in small throats, will reduce oil connectivity even further. Once a cluster of oil-filled elements becomes trapped it no longer is in pressure communication with the outlet. The capillary pressure within that cluster is frozen and the oil within it cannot
be displaced. If the model is primarily oil-wet, trapping again becomes less important as the oil can escape through oil layers.

### 3.4 Subsequent flooding cycles

We assume that no further wettability alteration takes place following that occurring after primary oil flooding. Secondary oil flooding might thus become a spontaneous process. The possible displacement events occurring are the same as those described for water flooding. If oil layers are present we assume that the capillary entry pressure is only affected by the outer oil-water interface, which initially is pinned at the last position attained during water flooding. The entry pressure is calculated analogously to spontaneous piston-like water invasion. If no oil layers are present the entry pressure is simply given by (3.7) with $F_d = 1$. Oil snap-off is also possible as long as water and oil is not trapped.

![Possible layer configurations](image)

**Figure 3.10:** Possible layer configurations that might occur in network elements. (a) During secondary water flooding the layer will collapse once the two interfaces meet at the crest of the interface. (b) During higher order flooding cycles several more layer configurations are available. If water either in the centre or in the layers is trapped, the capillary pressure across the interfaces might not be equal. (c) Depending on the capillary pressures the layer might collapse as the interfaces meet at the base rather than at the crest.

If secondary water flooding progressed down to residual oil saturation, most oil layers will typically have collapsed, though we assume a molecular film of oil will remain. As the capillary pressure increases during secondary oil flooding these layers will reform if a neighbouring element contains non-trapped oil either in layers or in the centre. The capillary pressure at which this happens will depend on whether any of the water, either in the corners or in the centre, is trapped. If none is trapped the capillary pressure is given by (3.32) and we assume that the outer interface will
subsequently hinge at the last position before the layer collapsed. If none of the
water is trapped, but both the inner $\theta_{ih,j}$ and outer $\theta_{oh,j}$ contact angles for a given
corner $j$ are hinging, as depicted in Figure 3.10 (a), the collapsing capillary pressure
can be found by iteratively solving the following equations:

$$\frac{\cos \theta_{ih,j} - \cos \theta_{oh,j}}{\sin \beta} = 2, \quad (3.33)$$

$$\cos (\cos \theta_{ih,j} + \beta_j) = \frac{b_{ij} \sin \beta_j}{R}, \quad (3.34)$$

$$\cos (\cos \theta_{oh,j} - \beta_j) = \frac{b_{oj} \sin \beta_j}{R}, \quad (3.35)$$

where $b_{ij}$ and $b_{oj}$ are the pinned apex distances for the inner and outer interfaces.

If water in the corner is trapped, the inner interface has a constant radius of
curvature $R_i$ and inner hinging contact angle $\theta_{ih,j}$, fixed in position the moment water
got trapped. If the outer interface is not hinging, the oil layer will collapse at a radius
of curvature

$$R = \frac{R_i (\cos \theta_{ih,j} - \sin \beta_j)}{\cos \theta_{a} + \sin \beta_j}, \quad (3.36)$$

whereas if the outer interface is hinging, the radius of curvature can be found by
iteratively solving (3.35) in combination with (3.36), replacing $\theta_a$ with $\theta_{oh,j}$.

Similarly, if water in the centre is trapped, the outer interface has a constant
radius of curvature $R_o$. The collapsing radius of curvature is found iteratively by
solving (3.34) in combination with,

$$R = \frac{R_o (\cos \theta_{a} + \sin \beta_j)}{\cos \theta_{ih,j} - \sin \beta_j}. \quad (3.37)$$

If outer interface in hinging, replace $\theta_a$ with $\theta_{oh,j}$.

In some cases the layer might collapse once the interfaces touch at the base
rather than the crest of the interface, Figure 3.10 (c). This is possible if water in the
corner is trapped with $\theta_{ih,j} < \pi - \theta_a$. The radius of curvature is then given by

$$R = \frac{b_{ij} \sin \beta_j}{\cos (\theta_{a} - \beta_j)}. \quad (3.38)$$
3.5 Calculation of transport properties

Estimation of transport properties can be done at any point during the displacement. Saturation is calculated using the prevailing maximum in capillary pressure (or minimum in the case of water injection) to compute the radius of curvature of the fluid interfaces. It is assumed that fluid flow in each phase is independent of the other phase and that the network configuration, i.e. the location of all the fluid interfaces is frozen in place. The absolute permeability $K$ of the network is found from Darcy’s law,

$$K = \frac{\mu_p q_{\text{top}} L}{A(\Phi_{\text{inlet}} - \Phi_{\text{outlet}})}, \quad (3.39)$$

when the network is fully saturated with a single phase $p$ of viscosity $\mu_p$. The total single-phase flow rate $q_{\text{top}}$ through the network is found by imposing a potential drop $(\Phi_{\text{inlet}} - \Phi_{\text{outlet}})$ across its length $L$, with $A$ being the cross-sectional area of the model. Potential is defined as $\Phi = P - \rho_p gh$, where $P$ is the pressure, $\rho_p$ is the phase density, $g$ is the gravitational constant and $h$ is the height above datum. The relative permeability $k_{rp}$ is then given by

$$k_{rp} = \frac{q_{\text{mp}}}{q_{\text{top}}}, \quad (3.40)$$

where $q_{\text{mp}}$ is the total flow rate of phase $p$ in multiphase conditions with the same imposed pressure drop. The total flow rate is found by solving for the pressure everywhere, imposing mass conservation at every pore $i$,

$$\sum_j q_{p,ij} = 0, \quad (3.41)$$

where $j$ runs over all the throats connected to pore $i$. For this to be valid we must assume the flow to be incompressible and that the viscous pressure drops are insignificant compared to the capillary pressure. This is consistent with the previously stated assumptions about capillary dominance. The flow rate $q_p$ between two pores $i$ and $j$ is given by

$$q_{p,ij} = \frac{\sigma_{p,ij}}{L_{ij} (\Phi_{p,i} - \Phi_{p,j})}, \quad (3.42)$$
where $g_p$ is the fluid conductance, $L$ is the length between the pore centres and $\Phi_p$ is the phase potential. The conductance between two pore bodies $g_{p,i,j}$ is taken to be the harmonic mean of each individual conductance,

$$
\frac{L_{ij}}{g_{p,ij}} = \frac{L_i}{g_{p,i}} + \frac{L_t}{g_{p,t}} + \frac{L_j}{g_{p,j}},
$$

(3.43)

where $t$ indicates the connecting throat. The pore body lengths, $L_i$ and $L_j$, are the lengths from the pore-throat interface to the pore centre, as illustrated in Figure 3.11. A linear set of equations can be defined from (3.41) and (3.42) that can be solved in terms of pore pressures. This is done using an algebraic multigrid solver [Ruge and Stueben, 1987]. With the pressures known at either side of any cross-sectional plane within the network model, the total flow rate can be computed from (3.42). To prevent boundary effects influencing relative permeability predictions, only the last half of the network is used for these calculations.

For single-phase laminar flow in a circular tube the conductance $g_p$ is given analytically by the Hagen-Poiseuille formula,

$$
g_p = k \frac{A^2 G}{\mu_p} = \frac{1}{2} \frac{A^2 G}{\mu_p}.
$$

(3.44)

Analytical expressions for equilateral triangles and squares can also be developed [Patzek and Silin, 2001] with $k$ being 3/5 and 0.5623 respectively. From numerical simulations Øren et al. [1998] found that the conductance for an irregular triangle was closely approximated by (3.44), using the same constant $k$ as for an equilateral triangle, 3/5.
In multiphase conditions an individual polygonal network element might contain both oil and water. Expressions for flow in element centres (where the corners contain a different phase) and flow in water and oil layers are all needed. These expressions are typically derived empirically from numerical simulations of flow in arbitrarily shaped ducts. For flow in the centre we continue to use (3.44) but multiply it by the fraction of the cross-section occupied by the phase in the centre, whereas flow in layers require separate expressions as the geometry becomes more complex. There are a number of variables affecting the shape of the corners and layers (Figure 3.12) – half angle $\beta$, contact angles $\theta$ and meniscus apex distances $b$.

The boundary condition for the fluid interface is clearly very important. Here we assume infinite surface shear viscosity (no-slip boundary condition) which should be valid for a surfactant-laden water-oil interface.

### 3.5.1 Conductance of water layers

For flow in corners we use the correlation proposed by Øren et al. [1998], given by

$$A_c = \left(\frac{b_i \sin \beta}{\cos(\theta_i + \beta)}\right)^2 \left(\frac{\cos \theta_i \cos(\theta_i + \beta)}{\sin \beta} \cos(\theta_i + \beta) + \theta_i + \beta - \frac{\pi}{2}\right),$$  

$$G_c = \frac{A_c}{4b_i^2 \left(1 - \frac{\sin \beta}{\cos(\theta_i + \beta)} \left(\theta_i + \beta - \frac{\pi}{2}\right)\right)^2},$$  

$$G^* = \frac{\sin \beta \cos \beta}{4(1 + \sin \beta)^2},$$  

$$C = 0.364 + 0.28 \frac{G^*}{G_c},$$
\[ g_{pc} = C \frac{A_c^2 G_c}{\mu_p}, \]  

(3.49)

where \( G_c \) is the shape factor for the corner section containing the fluid, \( G^* \) is the shape factor without any curvature on the fluid interface and \( A_c \) is the corner area.

The performance of the correlation was tested using a 2D finite element code for incompressible laminar flow. For a variety of corner configurations it was found to predict the conductance well within a ten percent error margin (Figure 3.13) with a mean absolute error of 4.9 percent. It was also found to compare favourably to correlations proposed by Patzek and Kristensen [2001] and Zhou et al. [1997].

![Figure 3.13: Performance of the layer conductance correlation suggested by Øren et al. [1998] when compared to numerical finite element simulations.](image)

3.5.2 Conductance of oil layers

Predicting the conductance of oil layers is more difficult than water layers since there are two interfaces to include, Figure 3.12 (b). No correlation in the literature was found to adequately predict the hydraulic conductance. Numerical simulations, using a 2D finite element code for incompressible laminar flow (using an internal Statoil research code), were conducted, with the grid containing 4000 elements. 1035 different configurations were investigated, with the outer contact angle \( \theta_o \) was varied between 120 and 180 degrees, the meniscus apex distance ratio between 0.01 and 0.6 and layer shape factor between 0.002 and 0.048, resulting in a variation of corner
half angles from 3 to 62 degrees. Based on these simulations we suggest the following correlation:

\[ \tilde{b}_i = \frac{b_i}{b_o}, \quad (3.50) \]

\[ \bar{A}_o = \left( \frac{\sin \beta}{\cos(\theta_o - \beta)} \right)^2 \left( \frac{\cos \theta_o \cos(\theta_o - \beta)}{\sin \beta} - \theta_o + \beta + \frac{\pi}{2} \right), \quad (3.51) \]

\[ \bar{A}_i = \left( \frac{\tilde{b}_i \sin \beta}{\cos(\theta_i + \beta)} \right)^2 \left( \frac{\cos \theta_i \cos(\theta_i + \beta)}{\sin \beta} + \theta_i + \beta - \frac{\pi}{2} \right), \quad (3.52) \]

\[ \bar{A}_l = \bar{A}_o - \bar{A}_i, \quad (3.53) \]

\[ \bar{L}_{oow} = \frac{2 \sin \beta}{\cos(\theta_o - \beta)} \left( \frac{\pi}{2} - \theta_o + \beta \right), \quad (3.54) \]

\[ \bar{L}_{iow} = \frac{2 \tilde{b}_i \sin \beta}{\cos(\theta_i + \beta)} \left( \frac{\pi}{2} - \theta_i - \beta \right), \quad (3.55) \]

\[ G_l = \frac{\bar{A}_l}{(\bar{L}_{oow} + \bar{L}_{iow} + 2 (1 - \tilde{b}_i))^2}, \quad (3.56) \]

\[ \ln \tilde{g}_l = a_1 \ln \left( \tilde{A}_l^3 G_l \right) + a_2 \ln(\tilde{A}_l^3 G_l) + a_3, \quad (3.57) \]

\[ g_{pl} = \frac{b_o \tilde{g}_l}{\mu_p}, \quad (3.58) \]

where \( \bar{A}_l \) is the dimensionless area of the layer, \( \bar{A}_o \) and \( \bar{A}_i \) are the outer and inner dimensionless corner areas, \( \bar{L}_{oow} \) and \( \bar{L}_{iow} \) are the dimensionless oil-water interface lengths, \( G_l \) is the layer shape factor and \( \tilde{g}_l \) is the dimensionless layer conductance. The constants \( a_1 \) to \( a_3 \), tabulated in Table 3.1 are found from a polynomial fit to the numerical results shown in Figure 3.14.
Table 3.1: Tabulation of polynomial fit parameters as a function of corner half angle.

<table>
<thead>
<tr>
<th>Half angle, $\beta$</th>
<th>$a_1$</th>
<th>$a_2$</th>
<th>$a_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Global fit</td>
<td>-2.401E-02</td>
<td>2.840E-01</td>
<td>-2.953</td>
</tr>
<tr>
<td>0-10</td>
<td>-1.061E-02</td>
<td>5.161E-01</td>
<td>-2.065</td>
</tr>
<tr>
<td>10-20</td>
<td>-2.681E-02</td>
<td>1.867E-01</td>
<td>-3.598</td>
</tr>
<tr>
<td>20-30</td>
<td>-4.402E-02</td>
<td>-6.320E-02</td>
<td>-4.375</td>
</tr>
<tr>
<td>30-40</td>
<td>-3.152E-02</td>
<td>1.695E-01</td>
<td>-3.360</td>
</tr>
<tr>
<td>40-50</td>
<td>-3.137E-02</td>
<td>1.933E-01</td>
<td>-3.267</td>
</tr>
<tr>
<td>50-60</td>
<td>-2.320E-02</td>
<td>3.118E-01</td>
<td>-2.925</td>
</tr>
<tr>
<td>60-</td>
<td>-3.576E-02</td>
<td>-6.537E-04</td>
<td>-4.702</td>
</tr>
</tbody>
</table>

Figure 3.14: Basis for the polynomial fit to data. The dimensionless conductivity can be approximated from the dimensionless layer area and shape factor.

The performance of the correlation, when compared to numerical simulation results, is shown in Figure 3.15. The mean absolute error is 8.7 percent when using a global polynomial fit to the data and 7.1 percent when using a separate fit for 7 intervals of corner half angles. The largest errors occur in the wider corners but this is not such a problem as the combined layer conductance for a network element will typically be dominated by the sharpest corner. It is clear that the proposed correlation compares
favourably to that suggested by Hui and Blunt [2000] that has a mean absolute error of 24.7 percent with the largest errors occurring in the important sharp corners, as evident from Figure 3.15 (c). In this work we use separate polynomial fits when calculating oil layer conductance.

Figure 3.15: Performance of layer conductance correlations when compared to numerical finite element simulations. (a) Proposed correlation with a global polynomial fit. (b) Proposed correlation with separate polynomial fits for different corner half angles. (c) Correlation proposed by Hui and Blunt [2000].
3.6 Electrical properties

Because Poiseuille’s law is closely related to Ohm’s law, \( a = g_e V \), flow of electrical current is analogous to fluid flow, with pressure replaced by voltage \( V \), fluid flow replaced by electrical current \( a \) and hydraulic conductance replaced by electrical conductance \( g_e \). This property was used extensively by Fatt [1956c] who generated relative permeability curves by flowing current though an equivalent network of resistors. The electrical analogy to absolute permeability is formation factor \( F \),

\[
F = \frac{R_o}{R_w},
\]

where \( R_o \) is the computed resistivity at 100 percent water saturation and \( R_w \) is the water resistivity. Since the rock matrix is non-conductive, formation factor will vary inversely with absolute permeability. The resistivity of the network is found from Ohm’s law,

\[
R_o = \frac{A\Delta V}{a_s L},
\]

where \( A \) is the cross-sectional area \( \Delta V \) is the imposed voltage drop, \( a_s \) is the total single phase flow of current and \( L \) is the length of the model. The electrical conductance between two pore bodies is assumed to only be a function of the cross-sectional area occupied by the conducting water,

\[
g_e = \frac{A_w}{R_w}.
\]

The potential field is calculated completely analogous to the pressure field, using equations (3.41) to (3.43) to solve for the potential in all pores and subsequently computing total current flow across any cross-sectional plane from (3.42). Clays are typically found to also conduct electricity, though this has not been investigated any further in this thesis. The electrical analogy to relative permeability is resistivity index \( I \), given by

\[
I = \frac{R_i}{R_o},
\]

where \( R_i \) is the resistivity at some given saturation. We assume that only water conducts electricity.
Chapter 4

Predicting Water-Wet Experimental Data

To validate the model we need to compare it against experimental results. In this section we will focus on water-wet experimental data, where the pore-level wettability is fairly easily characterized. We will start with data from Berea sandstones, where we know we have an appropriate network, allowing us to validate the basic network model. Subsequently we will investigate flow in sand packs. This poses a challenge since we have to modify our network to be representative of the porous medium.

As pore-scale network modelling has grown in complexity the amount of possible input parameters has grown. However, for this work the only parameters we will modify are the networks, through a well-defined process, and the pore-level wetting state, defined by the intrinsic contact angle $\theta_i$. All other parameters are kept fixed for all predictions. Most of the experimental data we analyze are based on steady-state measurements. Unsteady-state data, though more abundant, require additional numerical simulations to calculate relative permeability, increasing experimental uncertainty.

4.1 Description of network

In this section we will be using a network generated from reconstructed Berea sandstone [Lerdahl et al., 2000] to predict a wide range of experimental data conducted on several types of porous media. The network covers a rock volume of $3^3$ mm$^3$, consisting of 12,349 pores and 26,146 throats. 6.5 percent of the elements were squares, 1.2 percent were circular with the rest being irregular triangles. The connection numbers varies between 1 and 19, with an average of 4.19. The porosity of the network is 0.24 with an absolute permeability of 2.5 Darcy. The distributions
of inscribed radii are shown in Figure 4.1, with the main statistics tabulated in Table 4.1. As expected, there is a clear correlation between the radius of a given pore and the radii of the connecting throats, as seen from Figure 4.2. The correlation coefficient is 0.72.

![Histograms of inscribed radii for Berea sandstone. (a) Pores. (b) Throats.](image_url)

Figure 4.1: Distribution of inscribed radii for Berea sandstone. (a) Pores. (b) Throats.
Table 4.1: Statistical properties of network constructed from Berea sandstone.

<table>
<thead>
<tr>
<th></th>
<th>Pore radii</th>
<th>Throat radii</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean (µm)</td>
<td>19.2</td>
<td>11.0</td>
</tr>
<tr>
<td>Standard deviation (µm)</td>
<td>8.5</td>
<td>7.0</td>
</tr>
<tr>
<td>Minimum (µm)</td>
<td>3.6</td>
<td>0.9</td>
</tr>
<tr>
<td>Maximum (µm)</td>
<td>73.5</td>
<td>56.9</td>
</tr>
</tbody>
</table>

Figure 4.2: Correlation between radii of pores and connecting throats.

4.2 Berea sandstone

Predicted relative permeability for primary and secondary flooding cycles are compared to steady-state experimental data by Oak [1990] for water-oil (Figure 4.3) and oil-gas (Figure 4.4). During the primary flooding cycle the network is assumed to be strongly wetted by the wetting phase (water for the water-oil system and oil for the oil-gas system) with a receding contact angle of 0 degrees. There are no other parameters to adjust, with all geometric network properties (connection numbers, radii, shape factors, etc) defined in the sandstone reconstruction process. During the secondary flooding cycle the advancing contact angles will be larger, due to roughness of the surface and minor wettability alteration. The predictions shown in
Figure 4.3 (b) and Figure 4.4 (b) were obtained with intrinsic contact angles uniformly distributed between 50 and 60 degrees for the water-oil system and between 30 and 40 degrees for the oil-gas system.

Figure 4.3: Predicted primary oil flooding (a) and secondary water flooding (b) relative permeability for water-wet Berea sandstone (lines) compared to experimental data by Oak [1990] (circles). The predicted results are the mean of 20 realizations and the length of the error bars is twice the standard deviation.
Figure 4.4: Predicted primary gas flooding (a) and secondary oil flooding (b) relative permeability for Berea sandstone (lines) compared to experimental data by Oak [1990] (circles). The predicted results are the mean of 20 realizations and the length of the error bars is twice the standard deviation.

The corresponding advancing contact angles can be found from Figure 3.6. Small changes in the distribution of contact angles did not significantly affect the results, as long as the contact angles were less than 90 degrees. Additional fluid and rock parameters are given in Table 4.2. The predictions are the mean of 20 realizations with the length of the error bars being twice the standard deviation. The network topology and the pore and throat sizes are the same for all realizations. The statistical variation is mainly the result of contact angles being randomly distributed. During
the primary flooding cycle there is hardly any variation as contact angles are kept at a constant 0 degrees, though there is some small variation in the network due to the random assignment of the intermediate corner half angle. All predictions generally agree very well with the experimental data, with the exception of gas relative permeability in the primary oil flooding cycle. Oak [Oak, 1990] noted that this gas relative permeability was highly affected by the flooding rates used, and this might thus be the cause of the observed difference between experimental and predicted results.

Table 4.2: Fluid and rock properties used in predictions of experimental data by Oak [1990].

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Connate water saturation</td>
<td>0.22</td>
</tr>
<tr>
<td>Surface tension, $\sigma$ ($10^{-3}$ N/m)</td>
<td>30.0</td>
</tr>
<tr>
<td>Water viscosity, $\mu_w$ ($10^{-3}$ Pa/s)</td>
<td>1.05</td>
</tr>
<tr>
<td>Oil viscosity, $\mu_o$ ($10^{-3}$ Pa/s)</td>
<td>1.39</td>
</tr>
<tr>
<td>Gas viscosity, $\mu_g$ ($10^{-5}$ Pa/s)</td>
<td>1.87</td>
</tr>
</tbody>
</table>

4.3 Sand pack

When using pore-scale modelling to predict experimental data it is clearly important that the underlying network is representative of the rock. However, if the exact rock type has to be used for the network construction the application of predictive pore-scale modelling will be severely limited due to the complexity and cost of methods such as X-ray microtomography. In this section we will use the topological information of the Berea network (relative pore locations and connection numbers) while tuning the properties of the individual network elements using capillary pressure data. This modified network will be used to predict the flow properties of a sand pack (Table 4.3) as measured by Dury et al. [1997; 1998]. The experimental data are based on air-water with capillary pressure and air relative permeability available for secondary air flooding and tertiary water flooding, also referred to as the main flooding cycles. The relative permeabilities were obtained using the stationary liquid method. In this case air is the non-wetting phase, and is treated identically to oil.
Table 4.3: Rock properties of sand pack used in experiments by Dury et al. [1998].

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity</td>
<td>0.356</td>
</tr>
<tr>
<td>Grain size distribution (mm)</td>
<td>0.08–1.2</td>
</tr>
<tr>
<td>Column length (cm)</td>
<td>15</td>
</tr>
</tbody>
</table>

The capillary pressures for the sand pack are shown in Figure 4.6 (b). By assuming the network to be a bundle of capillary tubes it is possible to obtain an initial estimate of the throat size distribution using the air flooding capillary pressures and (3.6). Intrinsic contact angles used in the network model are consistent with experimentally measured values (Table 4.4) and during air flooding the model is strongly water-wet. Individual network throats are assigned inscribed radii from this target distribution. This is done by first sorting all throats according to their radius. Each throat in the list, starting with the largest, are then assigned a new inscribed radius from the target distribution by simply doing a table lookup with cumulative throat volume used as input, as illustrated in Figure 4.5. This will preserve their rank order – that is the largest throat in the network is given the largest radius from the target distribution and so on, which should ensure that size correlations between individual elements and on larger scales are maintained.

Figure 4.5: Throat elements are assigned new radii from the target distribution by doing a table lookup, using cumulative throat volume as input.
From Figure 4.6 (b) it is, however, clear that the predicted capillary pressure is not close to the experimental data. This indicates the difficulty of predicting multiphase data – the capillary pressure and relative permeabilities are influenced by the spatial distribution of pores and throats and their connectivity, something that cannot be captured using a bundle of capillary tubes assumption. The target distribution of throat sizes is subsequently modified iteratively until an adequate pressure match is obtained against the experimental air flooding data (Figure 4.7). Modifications to the throat size distribution at each iteration step were done by hand rather than by any optimization technique. The results are insensitive to the details of how the throat sizes are adjusted.

Table 4.4: Fluid properties used in predictions of experimental data by Dury et al. [1998].

<table>
<thead>
<tr>
<th>Property</th>
<th>Water (10^3 N/m)</th>
<th>Air (kg/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface tension, $\sigma$</td>
<td>70.25</td>
<td>—</td>
</tr>
<tr>
<td>Measured adv. contact angle, $\theta_a$ (deg)$^a$</td>
<td>19.9</td>
<td>—</td>
</tr>
<tr>
<td>Measured rec. contact angle, $\theta_r$ (deg)$^a$</td>
<td>13.5</td>
<td>—</td>
</tr>
<tr>
<td>Intrinsic contact angles used, $\theta_i$ (deg)</td>
<td>30 - 40</td>
<td>—</td>
</tr>
<tr>
<td>Density, $\rho$ (kg/m³)</td>
<td>1000</td>
<td>1.22</td>
</tr>
<tr>
<td>Viscosity, $\mu$ (10^3 Pa/s)</td>
<td>0.97</td>
<td>0.018</td>
</tr>
</tbody>
</table>

$^a$ Measured using Wilhelmy plate method.
Figure 4.6: Comparison between predicted properties and experimental data by Dury et al. [1998]. (a) Using the experimental capillary pressure and a bundle of capillary tubes assumption an initial estimate for the throat size distribution can be made. However, the predictions for capillary pressure (b) and relative permeability (c) are poor, indicating that the pore size distribution needs to be adjusted to match the data.
Figure 4.7: Comparison between predicted properties and experimental data by Dury et al. [1998] following a network modification process to match the capillary pressure data. (a) The match to experimental capillary pressure is excellent, except at high water saturations. (b) Predictions of air relative permeability are also improved.
Figure 4.8: Distribution of pore body to throat radius aspect ratio for original Berea network (a) and modified network (b). The latter is used for predictions of experimental data by Dury et al. [1998].

Capillary pressure hysteresis is a function of both the contrast between pore body and throat radii and the contact angle hysteresis. The radii of the pore bodies is determined from

$$r_p = \max \left( \frac{\sum_{i=1}^{n} r_i}{n}, \max(r_i) \right), \quad (4.1)$$
where \( n \) is the connection number and \( \alpha \) is the aspect ratio between the pore body radius \( r_p \) and connecting throat radii \( r_i \). A good match to experimental water flood capillary pressure is achieved by distributing the aspect ratios between 1.0 and 5.0 with a mean of 2.0. This distribution is very similar to that of the original Berea network (Figure 4.8), though with a lower maximum value, which in the original network was close to 50. This is expected since an unconsolidated sand pack would typically have smaller aspect ratios than a consolidated Berea sandstone. The absolute size of the model, defining individual pore and throat lengths, is adjusted such that the average ratio of throat length to radius is maintained from the original network. Pore and throat volumes were adjusted such that the target porosity was achieved, again maintaining the rank order. The final pore body and throat size distributions are shown in Figure 4.6 (a). Both distributions are shifted towards smaller values compared to the initial estimates.

In Figure 4.7 (b) the predicted air relative permeability for secondary air flooding and tertiary water flooding are compared to experimental data by Dury et al. [1998]. For experimental convenience the relative permeability was calculated using the air flow rate at connate water saturation \( S_{wc} \) rather than that at single phase conditions as defined by (3.40). This has, however, little influence on the results since our computed air relative permeability is 0.99 at \( S_{wc} \). Both the relative permeability hysteresis and the extinction point (where air no longer flows across the model) following water flooding are well predicted.

From the capillary pressure curve we appear to predict much higher residual gas saturation than in the experiments. Dury [1997] suggested that the large difference in saturation between where all remaining air is trapped and where it is able to flow across the pack could be partly related to air compressibility but more likely is due to the displacement of clusters of air not spanning the network. In the network model this difference is in the order of a few percentage points, rather than the almost 20 percent seen in the experiments.

The large experimental difference between the emergence point (where air is first able to flow across the model during air flooding) and the extinction point, something that is not observed in the network model, is difficult to explain physically. Using a network originally constructed to represent a consolidated Berea sandstone, it is possible that the contrast in size between pore bodies and connecting
throats is still over-predicted. This could result in snap-off becoming too dominant, resulting in too high predictions of residual oil. However, this is unlikely to explain why the network model predicts considerably smaller difference between the emergence and extinction points. With snap-off being less dominant, the number of trapped clusters following water flooding should be smaller. It would be naturally to expect that fewer forced displacement events are needed before a gas cluster once again spans the network. Hence, an over-prediction of the size contrast between pore bodies and throats should, if anything, lead to an over-prediction of the difference between emergence and extinction points.

The methodology of tuning the properties of the network to experimental capillary pressure, which is fairly easy to obtain, in order to match transport properties such as relative permeability, which undoubtedly is more difficult to obtain, has been attempted by several authors [Wise, 1992; Rajaram et al., 1997; Fischer and Celia, 1999]. What distinguishes this method is that we use networks that are constructed directly from realistic images of porous media. Our assumption is that the higher order topological information, that Sok et al. [2002] found were crucially important if reliable predictions of transport properties were to be made, are less specific to a given system than are properties such as pore size distribution. By preserving the rank order of the individual network elements we not only maintain topological information but we also go some way towards resolving the problem of non-uniqueness as noted by Vogel [2000]. Fischer and Celia [1999] also attempted to predict this data [Dury et al., 1998]. Although the relative permeability for the water flooding cycle was reasonably well predicted, they were unable to predict the observed hysteresis, resulting in a poor prediction for the gas flooding cycle. With the approach presented here we have been able to successfully predict relative permeability for both flooding cycles.
Chapter 5

Wettability Effects on Experimental Data

Most hydrocarbon-bearing reservoir rocks are found to be mixed-wet, where parts of the grain surface have become oil-wet while the rest remains water-wet \cite{Anderson, 1986a}. We will first predict data from mixed-wet Berea cores. Though the network geometry should still be valid, pore-level wettability and residual saturations are more uncertain. We will subsequently try to predict mixed-wet relative permeability for other rock types. This poses a challenge since we have to modify our network while at the same time try to characterize the pore-level wetting state.

The wetting states of the cores are typically determined using the Amott method \cite{Anderson, 1986b}, measuring the fraction of each phase \( p \) that spontaneously imbibes,

\[
I_p = \frac{\Delta S_{ps}}{\Delta S_{ps} + \Delta S_{pf}},
\]

where \( \Delta S_{ps} \) and \( \Delta S_{pf} \) are the spontaneous and forced parts of the displacement. It is typical to report the wetting state through a combined water-oil index \( I_{w-o} = I_w - I_o \), where \( I_w \) and \( I_o \) are the water and oil indices.

5.1 Mixed-wet Berea sandstone

The influence of wettability on oil recovery during water flooding has been extensively investigated by Jadhunandan and Morrow \cite{1995}. Experiments were conducted on 50 Berea core samples. Following primary oil flooding to some initial water saturation, between 7.9 and 32 percent, the cores were aged, during which the wettability was altered, and then subsequently water flooded until 20 pore volumes had been injected.
Using the network model combined with Buckley-Leverett analysis [Dullien, 1992] the experiments were reproduced to see if the same trends and results could be predicted. All cores were assumed to have connate water saturation $S_{wc}$ of 7.9 percent, equal to the lowest initial saturation in the experiments. Following primary oil flooding to some initial water saturation $S_{wi}$, all network elements contacted by oil were assumed to have their wettability altered. Oil recovery was determined from the secondary water flooding cycle. Finally the Amott wettability indices were determined with additional oil and water flooding cycles. All cycles except primary oil flooding were terminated following 20 pore volumes injected with the corresponding residual saturation and oil recoveries determined from a one-dimensional Buckley-Leverett analysis using the predicted network relative permeability and ignoring capillary pressure. Fluid parameters are given in Table 5.1.

Table 5.1: Fluid properties used in predictions of experimental data by Jadhunandan and Morrow [1995]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value (10(^{-3}) N/m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface tension, $\sigma$</td>
<td>12.0</td>
</tr>
<tr>
<td>Water viscosity, $\mu_w$</td>
<td>0.99</td>
</tr>
<tr>
<td>Oil viscosity, $\mu_o$</td>
<td>5.23</td>
</tr>
</tbody>
</table>

Careful attention to wettability characterization and displacement processes is needed to explain the surprising experimental results shown in 5.1 (a), where as $S_{wi}$ increases recovery initially increases but then decreases again for the largest values. The simplest scenario is that for a given crude oil, brine and rock condition the distribution of contact angles in pores contacted by oil during primary oil flooding is similar regardless of initial water saturation [Jackson et al., 2003]. The wettability variation observed through the Amott indices is then just a function of $S_{wi}$, with the rock becoming less oil-wet as $S_{wi}$ increases, since fewer pores have their wettability altered. By matching the observed wettability indices at a given initial water saturation it should then be possible to predict the trends in recovery and wettability as $S_{wi}$ is varied. With connate water saturation chosen as the reference case the wetting state was reasonably well matched with intrinsic contact angles in wettability-altered pores uniformly distributed between 85 and 120 degrees. The
Amott water $I_w$ and oil $I_o$ indices were calculated to be 0.00 and 0.47, the same as the experimental values.

Figure 5.1: Oil recovery for different initial water saturations. (a) Experimental data from Jadhunandan and Morrow [1995]. (b) Predicted recoveries using pore-scale modelling with a fixed distribution of intrinsic contact angles between 85 and 120 degrees. (c) Predictions where fewer pores become oil-wet for $S_{wi}$ above 0.20.
Oil recovery is a direct function of the fractional water flow $f_w$, which in the one-dimensional Buckley-Leverett analysis is given by

$$f_w(S_w) = \frac{1}{1 + \frac{k_{ro}(S_o)}{k_{rw}(S_w)} \mu_w}$$

(5.2)

From (5.2) it is clear that the relative permeability being low for water and high for oil is advantageous to oil recovery. Relative permeability curves for different $S_{wi}$ are shown in Figure 5.3, along with water fractional flow curves and capillary pressures. Although snap-off is possible, it is highly unfavourable compared to piston-like displacement in oil-wet conditions. Hence, water will typically enter the model through piston-like displacement from existing water-filled elements. If $S_{wi}$ is low there are relatively few of these left following primary oil flooding, resulting in water entering the model though large well-connected clusters. To illustrate this we ran a 2D network simulation with the same distribution of contact angles and the results are shown in Figure 5.2 (a). As $S_{wi}$ increases, the number of initially water-filled elements will increase rapidly, Figure 5.2 (b). These are typically isolated elements, resulting in water entering the system through many clusters only connected through layers. This behaviour has significant influence on relative permeability, since flow conductance in layers is typically orders of magnitude less than that in pore centres. In cases where there are many initial clusters, water has to repeatedly flow through layers to connect from inlet to outlet, resulting in low relative permeability, as evident from the $S_{wi} = 0.18$ case in Figure 5.3. Since the initially oil-filled elements are oil-wet, water preferentially fills the larger pores and throats. This results in a large increase in water saturation with little change in water connectivity and hence water relative permeability, Figure 5.2 (c). Only at high water saturations, around 0.7, will the water clusters start to coalesce, resulting in a rapid increase in water relative permeability. In the limiting case where $S_{wi} = S_{wc}$ there is only a single water cluster originating from the inlet reservoir, which rapidly establishes a connected path of water-filled elements across the network giving a more gradual increase in $k_{rw}$. 
Figure 5.2: Distribution of water-filled elements during water flooding. (a) When $S_{wi} = S_{wc} = 0.08$ very few elements remain water-filled following primary oil flooding. During water flooding there will only be a few well connected clusters, even at $S_w = 0.40$ as shown. Water spans the network through completely filled elements, resulting in a high relative permeability. (b) When $S_{wi} = 0.18$ many throats will remain water-filled at the shown initial condition. (c) As water is injected, each water-filled throat will allow for piston-like displacement into a neighbouring pore body, resulting in rapid increase in water saturation without much change in the overall network conductivity, even at the shown saturation of 0.40, giving a very low water relative permeability. (d) When $S_{wi} = 0.31$ connected water clusters will remain at the shown initial conditions, resulting once again in increased water relative permeability.
Figure 5.3: Influence of $S_{wi}$ on macroscopic flow properties during secondary water flooding. We have assumed that all pores contacted by oil after primary oil flooding have a fixed distribution of intrinsic contact angles between 85 and 120 degrees, corresponding to the predictions shown in 5.1 (b). Each flooding cycle is terminated after 20 pore volumes have been injected. (a) Water relative permeability. (b) Oil relative permeability. (c) Fractional water flow. (d) Capillary pressure during secondary oil flooding and tertiary water.

There is less effect of $S_{wi}$ on the oil relative permeability. The last elements to be filled during primary oil flooding are the smallest ones that also contribute the least to oil conductance, whereas the first elements filled during water flooding in oil-wet conditions are the largest, resulting in large oil relative permeability hysteresis. The oil relative permeability for a given $S_{wi}$ will thus lie above those starting from a lower $S_{wi}$.

The effects on both oil and water relative permeability combine to give lower fractional water flow, and subsequently higher recovery, as $S_{wi}$ increases. There is, however, an optimal $S_{wi}$ above which recovery again starts to decrease, as evident
from Figures 5.1 and 5.3 (c). Elements filled by water during water flooding still conduct oil due to oil layers, which is not the case for elements that remain water-filled from primary oil flooding. This results in increased oil trapping with $S_{wi}$, reducing oil relative permeability. Also, at some point so many elements still contain water at the beginning of water flooding that large water clusters can easily form, increasing the water relative permeability, as illustrated in Figure 5.2 (d). Whereas relative permeability and fractional flow show a non-uniform trend with $S_{wi}$, this is not the case for the Amott wettability indices (Table 5.2), calculated from the capillary pressures as shown in Figure 5.3 (d).

Table 5.2: Variation in Amott wettability indices for different initial water saturations.

<table>
<thead>
<tr>
<th>$S_{wi}$</th>
<th>Experimental Data</th>
<th>Fixed wettability</th>
<th>Variable wettability</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$I_w$</td>
<td>$I_o$</td>
<td>$I_w$</td>
</tr>
<tr>
<td>0.079</td>
<td>0.00</td>
<td>0.47</td>
<td>0.00</td>
</tr>
<tr>
<td>0.180</td>
<td>0.02</td>
<td>0.20</td>
<td>0.06</td>
</tr>
<tr>
<td>0.240</td>
<td>0.20</td>
<td>0.07</td>
<td>0.13</td>
</tr>
<tr>
<td>0.311</td>
<td>0.34</td>
<td>0.00</td>
<td>0.19</td>
</tr>
</tbody>
</table>

Although we are able to match the trend in recovery with $S_{wi}$ (5.1), the quantitative match is poor in some cases. Maximum recovery is predicted to occur at lower $S_{wi}$ and the variation in recovery with $S_{wi}$ is predicted to be less than what is observed experimentally. Recovery and residual oil saturation, as a function of the Amott-Harvey water-oil index $I_{w-o}$, is shown in Figure 5.4. Again, the trend and maximum oil recovery are well predicted, though the predicted results are somewhat shifted towards more oil-wet conditions.

Our initial hypothesis that the distribution of contact angles in pores contacted by oil is independent of initial water saturation and brine salinity (in terms of $\text{Ca}^{2+}$ content) does not seem to be entirely supported when comparing predicted and experimental trends in Amott wettability indices. In Table 5.2 the wettability indices corresponding to Figure 3.1 are tabulated. These experiments were all performed with high salinity brines. It is clear that as initial water saturation increases the rock exhibits more water-wet behaviour than what can be attributed to just increasing $S_{wi}$. 

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This observation is further supported by Figure 5.5, where more experimental data points are included. A fixed distribution of contact angles will result in a linear increase in water index with $S_{w,r}$, which is not seen experimentally. Physically, this can be explained using the pore-level scenario suggested by Kovscek et al. [1993]. Initially a water film covers the rock, preventing direct contact by the oil. At a certain capillary pressure this film will rupture, allowing the rock to become more oil-wet. As $S_{w,r}$ increases the maximum capillary pressure during primary oil flooding is reduced, preventing some of the pores attaining oil-wet characteristics. It would seem that for $S_{w,r}$ greater than 0.18 a significant fraction of the pores remain water-wet. To see if the quantitative match would improve, this trend was incorporated into the predictions, Figure 5.5.

![Figure 5.4: Recovery and residual oil saturation as a function of Amott wettability index $I_{w-o}$ for (a-b) 3 pore volumes injected and (c-d) 20 pore volumes injected. Predictions are shifted towards more oil-wet conditions compared to experimental data.](image)
Figure 5.5: Influence of initial water saturation on Amott water (a) and oil (b) indices. From the experimental water indices it is clear that variation in wettability can not only be attributed to variation in $S_{wi}$.

After primary oil flooding we assigned a target volume fraction of oil-filled pores and throats that would become oil-wet. The largest oil-filled pores were made oil-wet with an intrinsic contact angle randomly distributed between $90^\circ$ and $118^\circ$. Though this contradicts the pore-level scenario suggested by Kovscek et al. [1993], that suggested that the largest oil-filled pores would remain water-wet, it is consistent with the approach used by other network modelling studies [McDougall and Sorbie, 1995; Oren and Bakke, 2003] that have investigated the experimental data by Jadhunandan and Morrow [1995]. Oil-filled throats connected to oil-wet
pores were made oil-wet with the same distribution of contact angles with a probability equal to the target oil-wet fraction. Progressively smaller oil-filled pores were made oil-wet until the target fraction was reached. The remaining oil-filled pores and throats were assigned intrinsic contact angles uniformly between 50° and 60°. We varied the upper bound on the oil-wet contact angle distribution along with the oil-wet fraction to better match the experimental Amott wettability indices for $S_{wi} > 0.18$, the results are shown in Table 5.2 and Figure 5.5. The upper bound of the contact angle distribution was reduced from 118 degrees at $S_{wi} = 0.18$ to 109 degrees at $S_{wi} = 0.31$, while the lower bound was kept at 90 degrees. The oil-wet fraction was reduced from 1 to 0.87. This did indeed widen the range of wetting conditions observed, Figure 5.4. However, maximum recovery still occurs at initial water saturations lower than those observed experimentally, 5.1 (c).

Figure 5.6: Effect from differences in saturation history when determining Amott water $I_w$, oil $I_o$, and combined $I_{wo}$ wettability indices. The additional forced displacement when allowing an infinite number of pore volumes to be injected will result in both lower water and oil indices, resulting in less variation in estimated wetting state.

Øren and Bakke [2003] also used a pore-scale network model, similar to the one presented in this work, to predict recoveries while matching the trend in $S_{wi}$ and Amott wettability indices. Whereas we predicted maximum oil recovery to occur at weakly oil-wet conditions, they were able to reproduce the findings by Jadhunandan
and Morrow [1995] that the maximum occurs at weakly water-wet conditions. When
determining the final residual saturation after each flooding cycle, we considered it
most realistic that this would be the saturation achieved after 20 pore volumes
injected (PVI), as determined by the Buckley-Leverett analysis, following secondary
oil flooding and tertiary water flooding. Though not explicitly stated, it is assumed
that Øren and Bakke used secondary water and oil flooding cycles to determine the
wetting state, allowing each cycle to continue until only a final trapped saturation
remained, in effect allowing an infinite number of pore volumes to be injected. This
will result in additional spontaneous and forced displacement, compared to our
approach.

Table 5.3: Matched Amott wettability indices for different experimental core
samples.

<table>
<thead>
<tr>
<th>$S_{wi}$</th>
<th>Exp. Data</th>
<th>Infinite PVI</th>
<th>$r_{min}$ correlation</th>
<th>$S_{wc} = 0.22$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$I_w$</td>
<td>$I_o$</td>
<td>$I_w$</td>
<td>$I_o$</td>
</tr>
<tr>
<td>0.079</td>
<td>0.00</td>
<td>0.47</td>
<td>0.00</td>
<td>0.47</td>
</tr>
<tr>
<td>0.113</td>
<td>0.00</td>
<td>0.37</td>
<td>0.01</td>
<td>0.38</td>
</tr>
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<td>0.20</td>
<td>0.01</td>
<td>0.21</td>
</tr>
<tr>
<td>0.159</td>
<td>0.05</td>
<td>0.15</td>
<td>0.05</td>
<td>0.15</td>
</tr>
<tr>
<td>0.181</td>
<td>0.02</td>
<td>0.20</td>
<td>0.03</td>
<td>0.21</td>
</tr>
<tr>
<td>0.188</td>
<td>0.05</td>
<td>0.13</td>
<td>0.05</td>
<td>0.12</td>
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<td>0.227</td>
<td>0.08</td>
<td>0.04</td>
<td>0.08</td>
<td>0.03</td>
</tr>
<tr>
<td>0.240</td>
<td>0.20</td>
<td>0.07</td>
<td>0.20</td>
<td>0.08</td>
</tr>
<tr>
<td>0.250</td>
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<td>0.02</td>
<td>0.13</td>
<td>0.02</td>
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<tr>
<td>0.250</td>
<td>0.34</td>
<td>0.03</td>
<td>0.34</td>
<td>0.03</td>
</tr>
<tr>
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<td>0.26</td>
<td>0.04</td>
<td>0.27</td>
<td>0.04</td>
</tr>
<tr>
<td>0.311</td>
<td>0.34</td>
<td>0.00</td>
<td>0.35</td>
<td>0.01</td>
</tr>
<tr>
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<td>0.00</td>
<td>0.42</td>
<td>0.01</td>
</tr>
<tr>
<td>0.320</td>
<td>0.59</td>
<td>0.00</td>
<td>0.57</td>
<td>0.00</td>
</tr>
</tbody>
</table>

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Figure 5.7: Recovery and residual oil saturation as a function of Amott wettability index $I_{w-o}$ for (a-b) 3 pore volumes injected and (c-d) 20 pore volumes injected. For all cases, the flooding cycles were terminated once the absolute residual saturations were reached, in effect allowing an infinite number of pore volumes to be injected.

To investigate the influence from these differences in saturation history, we reran our variable wettability cases, but used the secondary flooding cycles to determine the Amott wetting indices while allowing infinite pore volumes to be injected. From Figure 5.6 it is clear that this will result in less variation in the combined Amott wettability index $I_{w-o}$ but without changing the overall predicted wetting state (water or oil-wet). Maximum recovery is still predicted to occur at weakly oil-wet conditions, as evident from Figure 5.7 (infinite PVI case), where the wetting states of 14 experimental core samples were matched (Table 5.3). The water index was matched by varying the oil-wet fraction during secondary water flooding while the oil index was matched by adjusting the upper bound of the oil-wet contact angle distribution, keeping the lower bound at a constant intrinsic contact angle of 80 degrees. As predicted, a larger variation in the oil-wet fraction was needed to match
the experimental data. For the $S_{wi} = 0.311$ an oil-wet fraction of 0.83 was needed, compared to a fraction of 0.87 used when terminating the flooding cycle after 20 PVI.

For all cases investigated so far the larger pores have been made preferentially oil-wet. In Figure 5.7 we investigate the effect from letting the smaller pores become preferentially oil-wet ($r_{min}$ correlation). Once again the wetting states of 14 experimental core samples were matched (Table 5.3) while determining the Amott indices from the secondary flooding cycles, allowing an infinite number of PVI. There is very little difference in the results when compared to letting the larger pores become preferentially oil-wet. The reason for this is that recovery efficiency is dominated by the remaining water-filled elements following primary oil flooding with the oil-wet fraction of the invaded elements generally being quite high. Maximum recovery is predicted to occur at an oil-wet fraction of about 0.97.

In the network model we assumed a constant connate water saturation of 7.9 percent. Experimentally these low saturations could only be obtained by flooding the cores with nitrogen gas. When only flooding with brine the lowest $S_{wi}$ obtained was 22 percent. This, combined with the fact that all the waterfloods were conducted on different core samples, makes it difficult to estimate accurately the true connate water saturation. What is clear is that this has significant impact on the predicted recoveries since the difference between $S_{wi}$ and $S_{wc}$ will add an additional water-wet component to the system, as already discussed for the fixed wettability cases. To quantify the effect we again matched the wetting states of 14 experimental core samples (Table 5.3) while keeping $S_{wc} = 0.22$ for cases where $S_{wi} > 0.22$, and $S_{wc} = S_{wi}$ for the rest. The wetting states were determined from the secondary oil flooding and tertiary water flooding cycles, allowing an infinite number of PVI. Predicted recoveries are shown in Figure 5.7, and there now is close agreement with the experimental results, especially at 3 pore volumes injected. These results are however not contradictory, but suggests that there is less of a correlation between maximum recovery and wetting state, than between maximum recovery and total amount of water-wet pore space during water flooding. From Figure 5.8 it would seem that maximum recovery occurs when about 10 percent of the effective pore space ($1 - S_{wc}$) is water-wet. The deviation seen at higher water-wet fractions is due to differences in how the water-wet elements are distributed on the pore-scale.
Figure 5.8: Relationship between oil recovery and the amount of effective pore space \((1 - Swc)\) that is water-wet when commencing water flooding \((Swi)\). The deviation between the cases at higher water-wet fractions is due to differences in how the water-wet elements are distributed on the pore-scale.

When \(Swi > Swc\) the remaining water-filled elements will mostly be found in throats whereas if \(Swi = Swc\) the water-wet elements are distributed in a mix of the smaller pores and throats. The pore-scale explanation for this trend is consistent with the behaviour illustrated in Figure 5.2. Maximum recovery will occur when the water relative permeability is low, something that occurs when there is a large number of separate water clusters. This can be the result of either \(Swi > Swc\) or the oil-wet fraction being less than 1. The relative permeability and fractional water flow when oil recovery is maximized is shown in Figure 5.9 for the infinite PVI case and when \(Swc = 0.22\), corresponding to \(Swi = 0.18\) and 0.25 for the two cases respectively. The water relative permeabilities are both very low and similar in shape, resulting in high oil recovery.
Figure 5.9: Relative permeability ($k_r$) and fractional water flow ($f_w$) when oil recovery is maximized. This will occur at $S_{wi} = 0.18$ for the infinite PVI case and $S_{wi} = 0.25$ when $S_{wc} = 0.22$. The water relative permeability is very similar in both cases, resulting in similar recoveries.

The calculated Amott water-oil index will also be significantly influenced by the choice of wettability hysteresis model (difference between advancing and receding contact angle). The Morrow [1975] model used, as illustrated in Figure 3.6, was developed using an ideal system. We will however not investigate this any further as it does not affect the overall understanding of the problem.

5.1.1 Field-scale implications

Due to capillary rise effects, initial water saturations might be considerably higher than the connate water saturation in the region above the oil-water contact, commonly referred to as the oil-water transition zone. When estimating reserves using finite difference reservoir simulation, relative permeability curves are needed for this zone, referred to as scanning curves ($S_{wi} > S_{wc}$). Empirical interpolation techniques are typically used for this [Killough, 1976; Carlson, 1981]. These models generally assume that the scanning curves lie between the bounding primary oil flooding and water flooding curves ($S_{wi} = S_{wc}$). However, from the last section it is clear that this is rarely the case. In a previous paper we compared field-scale oil recovery predictions when using different techniques to generate the scanning curves
[Jackson et al., 2003]. Using pore-scale network modelling to generate the curves resulted in significantly higher prediction of overall recovery factor than when using empirical interpolation techniques. This is because in mixed-wet reservoirs maximum oil recovery is achieved when a significant portion of the pore space remain water-wet, something that is not captured by the currently used empirical models.

5.2 Mixed-wet intergranular carbonate

In the petroleum industry multiphase flow experiments are routinely performed on cores from hydrocarbon bearing reservoirs. Capillary pressure data are not usually available from steady-state measurements but rather found from centrifuge or mercury intrusion experiments. In both cases only pressures from the forced displacements are typically available. In this section we will use mercury-air capillary pressures to modify the network and then predict relative permeability. Though only available for the primary flooding cycle, this data has the benefit of not being influenced by wettability characterization issues as the mercury-air contact angle is generally assumed to be fixed at 140 degrees with an interfacial tension of 0.48 N/m.

The capillary pressure response of the network model was matched to experimental data for two samples of an intergranular carbonate using the same procedure that was described for the sand pack, and the results are shown in Figure 5.10. Both carbonate samples consisted of compacted, poorly sorted, peloidal grainstone. Since no spontaneous displacement data were available, the pore body size distribution was determined by maintaining the pore body to throat radius aspect ratio from the original Berea network. Since mercury will enter both micro and clay bound porosity, this method will not help in determining the connate water saturation. A realistic threshold radius is thus needed to determine what fraction of the pore space is accessible, effectively determining the minimum throat radius. Since no clay bound porosity is found in the samples a choice of about 0.1 µm would seem to be a realistic value in this case, resulting in connate water saturation of about 2 percent (Table 5.4). From the mercury intrusion data it is clear that the samples are fairly similar. The absolute permeability was predicted to be 1.60 and 1.28 mD for samples 1 and 2, compared to experimental values of 1.40 and 0.92 mD respectively.
Note that this is more than three orders of magnitude lower than the original network permeability, indicating that we have significantly altered the pore size distribution. These values are also tabulated in Table 5.5. No further parameters relating to the network were tuned for the subsequent flow predictions. Experimental primary oilflooding relative permeability data (only available for sample 1) will give some validation of the network modification process since the flow response is less affected by wettability, with the assumption that the rock is strongly water-wet. The predictions are in fairly good agreement with experimental data (Figure 5.11) suggesting that the modified network is representative of the rock. Fluid parameters used are given in Table 5.4.

Figure 5.10: Comparison between experimental and matched mercury-air capillary pressure for two samples of intergranular carbonates.
Table 5.4: Fluid and rock properties used in predictions for mixed-wet intergranular carbonates.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface tension, $\sigma$ ($10^{-3}$ N/m)</td>
<td>29.9</td>
</tr>
<tr>
<td>Water viscosity, $\mu_w$ ($10^{-3}$ Pa/s)</td>
<td>0.927</td>
</tr>
<tr>
<td>Oil viscosity, $\mu_o$ ($10^{-3}$ Pa/s)</td>
<td>6.17</td>
</tr>
<tr>
<td>Porosity, Sample 1</td>
<td>0.264</td>
</tr>
<tr>
<td>Porosity, Sample 2</td>
<td>0.241</td>
</tr>
<tr>
<td>Initial Water Saturation, $S_{wi}$, Sample 1</td>
<td>0.181</td>
</tr>
<tr>
<td>Initial Water Saturation, $S_{wi}$, Sample 2</td>
<td>0.220</td>
</tr>
<tr>
<td>Connate Water Saturation, $S_{wc}$</td>
<td>0.021</td>
</tr>
<tr>
<td>Water-wet contact angles, $\theta_i$ (deg)</td>
<td>25 – 65</td>
</tr>
<tr>
<td>Oil-wet contact angles, $\theta_i$ (deg)</td>
<td>80 – 82</td>
</tr>
<tr>
<td>Oil-wet fraction by pore volume, Sample 1 and 2</td>
<td>0.68</td>
</tr>
<tr>
<td>Oil-wet fraction by pore volume, Sample 2 (less oil-wet)</td>
<td>0.65</td>
</tr>
</tbody>
</table>

Table 5.5: Experimental and predicted values for mixed-wet intergranular carbonates for absolute permeability and mean residual oil saturation following water flooding with associated standard deviation (sd).

<table>
<thead>
<tr>
<th>Sample</th>
<th>Experimental</th>
<th>Predicted</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$K$ (mD)</td>
<td>$S_{or}$</td>
</tr>
<tr>
<td>1</td>
<td>1.40</td>
<td>0.30</td>
</tr>
<tr>
<td>2</td>
<td>0.92</td>
<td>0.42</td>
</tr>
<tr>
<td>2 (less oil-wet)</td>
<td>0.92</td>
<td>0.42</td>
</tr>
</tbody>
</table>

Table 5.6: Experimental and predicted values for mixed-wet intergranular carbonates for Amott wettability indices with associated standard deviation (sd).

<table>
<thead>
<tr>
<th>Sample</th>
<th>Experimental</th>
<th>Predicted</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$I_w$</td>
<td>$I_o$</td>
</tr>
<tr>
<td>1</td>
<td>0.50</td>
<td>0.00</td>
</tr>
<tr>
<td>2</td>
<td>0.74</td>
<td>0.00</td>
</tr>
<tr>
<td>2 (less oil-wet)</td>
<td>0.74</td>
<td>0.00</td>
</tr>
</tbody>
</table>
Water flooding adds the additional complexity of wettability characterization. The Amott water index is broadly controlled by adjusting the oil-wet fraction, whereas the residual oil saturation and oil index is more affected by the distribution of intrinsic contact angles in the oil-wet pores. A distribution towards strongly oil-wet conditions will result in low residual oil saturation as oil layers remain stable, allowing oil to escape even at low saturation. Conversely, a distribution towards more neutral conditions will result in more residual oil, as well as a lower oil index since a higher proportion of the pores will have receding contact angles less than 90°. The distribution of contact angles in the water-wet fraction has less influence on the predicted results, though a distribution towards more strongly water-wet conditions will result in poorer oil connectivity as snap-off events become more dominant. A flowchart of the outlined methodology is shown in Figure 5.12.

Using Cryo-scanning electron microscopy (Cryo-SEM) it is possible to visualize the distribution of oil and water at the pore-scale. Based on these studies there is some justification for suggesting that the pore size and geometry is important in determining which pores become oil-wet in carbonates [Fassi-Fihri et al., 1991]. Hence, we assume that the smallest oil-filled pores following primary oil flooding become oil-wet [Kovscek et al., 1993].
Figure 5.12: Flowchart for relative permeability predictions.
Both carbonate samples were from an oil-water transition zone. Sample 2 was taken lower in the zone than sample 1 and thus had a higher initial water saturation, 22 percent compared to 18 percent. It also exhibits more water-wet characteristics, higher residual oil and lower Amott water index (Table 5.5 and 5.6), than sample 1. This is a very similar scenario to what was investigated in the last section, where the influence of initial water saturation on wettability and production characteristics was discussed. However, rather than predicting oil recoveries we will now directly investigate the influence on relative permeability. Experimental centrifuge data from sample 1 was used to characterise the wettability, as shown in Figure 5.13 (a). Though the absolute capillary pressures were not that well matched, which is not surprising considering the uncertainties in both the wettability hysteresis model and the experimental centrifuge data, both residual oil saturation and Amott wettability indices were well matched as evident from Table 5.5 and 5.6. This same wetting condition was subsequently used for sample 2. The higher initial water saturation did indeed make the predicted wetting condition more water-wet, as shown in Figure 5.13 (b), but the experimental values were somewhat under-predicted. This is, however, consistent with the conclusions from the last section where we noted that the higher initial water saturation would probably reduce the pore space fraction becoming oil-wet due to the lower capillary pressure reached during primary oil-flooding. Reducing the oil-wet fraction from 0.68 to 0.65, while keeping the same distributions of contact angles, significantly improved the match with Amott wettability indices and residual oil saturation, as shown in Figure 5.13 (c) and tabulated in Table 5.5 and 5.6.

The predictions of relative permeability are shown in Figure 5.14. While the predictions for sample 2, Figure 5.14 (c), are excellent, both the water and oil relative permeability for sample 1 are not that well predicted, Figure 5.14 (a), with both being under-predicted. The most obvious reason for this would be that the network used, originally constructed from a Berea sandstone, is in fact not representative of the carbonate samples. This is supported by investigating the back scattered electron (BSE) images shown in Figure 5.15. The grain size distribution is clearly much more heterogeneous than in a Berea sandstone with the images shown not covering a representative elementary volume (REV). The network used for the predictions consists of about 12,300 pores, roughly equivalent to a $23^3$ regular...
network, something that, from visual inspection of the BSE images, is unlikely to be larger than the REV of these carbonate samples. However, since the steady state flow experiments were conducted on much larger samples, and the original network is much larger than the REV of a Berea sandstone, the effects are not observed in the experimental or predicted results. The higher level of heterogeneity in the carbonates will result in not just under-estimation of the correlation length, but also in a too low average connection number and too low size contrasts between pore bodies and throats. The fact that the network does not capture the essential topological features of these carbonate samples, does significantly reduce the confidence one can attach to the predictions. However, if network topology and connectivity were the main reasons for the poor predictions, one would also expect this to influence the primary oil flooding results, which is not the case. Also, samples 1 and 2 would appear to be morphologically very similar, evident from both the mercury intrusion experiments as well as the BSE images, and water flood predictions of sample 2 are considerably better. These predictions were performed with a distribution of intrinsic contact angles in the oil-wet part between 80 and 82 degrees, corresponding to advancing contact angles between 116 and 120 degrees. This distribution was found by following the methodology illustrated in Figure 5.12, but it would seem to be rather narrow and low when compared to distributions found in similar carbonates. A final possible reason for the discrepancy in water flooding predictions can be the influence of viscous forces. Although both samples were found to contain negligible vuggy porosity, the range of pore sizes is large. Our assumption of complete capillary dominance might therefore not be valid in the larger pores, something that would affect the filling sequence of the network. To conclude this section, we have shown promising relative permeability predictions of two intergranular carbonate samples. However, it is uncertain whether a network originally constructed to represent a sandstone can sufficiently capture the essential topological features of these heterogeneous carbonate samples. It is possible that the predictions can be improved by using information directly obtained from the BSE images, like for example the size aspect ratio between pore bodies and throats.
Figure 5.13: Comparison between experimental and predicted water-oil capillary pressure for secondary water and oil flooding cycles. (a) Sample 1 was used to characterise the wettability. (b) Using the same wetting condition for sample 2 as was found from sample 1 results in too oil-wet conditions. (c) Reducing the oil-wet fraction for sample 2 improves predictions.
Figure 5.14: Comparison between experimental and predicted water flooding relative permeability for sample 1 (a), sample 2 (b) and sample 2 with a lower oil-wet fraction (c).
Figure 5.15: Back scattered electron (BSE) images of samples 1 (a) and 2 (b). These images suggest that the carbonate samples have a much more heterogeneous grain size distribution than would be expected in a Berea sandstone, raising doubt whether the network used in fact representative of the carbonate samples.
5.3 Mixed-wet reservoir sandstone

This dataset was based on a consolidated sandstone, taken from an oil-bearing reservoir. The same procedure of using primary mercury intrusion experiment to modify the network while applying a threshold to determine likely connate water saturation was used. A choice of 1 µm would seem to be a realistic value in this case, resulting in $S_{wc} = 0.11$. The absolute permeability was predicted to be 814 mD which compares well to the experimental value of 750 mD. Mercury intrusion and steady state flow experiments are not conducted on the same cores, hence the connate water saturation might be significantly different. The non-accessible porosity is subsequently adjusted such that $S_{wc}$ in the network model is consistent with experimental data.

![Graph](image.png)

Figure 5.16: Comparison between experimental and matched mercury-air capillary pressure for a reservoir sandstone. Mercury will enter both micro and clay bound porosity. This porosity is not explicitly included in the network model and as a result capillary pressures corresponding to $S_{wc} < 0.11$ will not be matched.

Though the Cryo-SEM studies found that pore size and geometry was important in determining which pores become oil-wet in carbonates, this is not necessarily the case for sandstones [Fassi-Fihri et al., 1991; Durand and Rosenberg, 1998]. It was found that the presence of clay minerals, in particular kaolinite, was far
more likely to make a pore oil-wet than its size. The distribution of these clay minerals might very well not be related to pore size. In this section we will therefore test three approaches to assigning wettability. In addition to the previous approach, where the smallest pores become oil-wet, we will also make the largest pores oil-wet. Finally we will assign oil-wet elements in spatially correlated patches. This is done by randomly selecting some oil-invaded pore regardless of size. All oil-invaded pores within a defined correlation length are then made oil-wet. Oil-filled throats connected to oil-wet pores are also made oil-wet. This process continues until a defined oil-wet fraction is achieved.

Following aging the sandstone exhibited mixed-wet characteristics with an Amott water index of 0.55, indicating that about half the pore space had become oil-wet. No oil index was measured. Fluid and rock properties used in the predictions are given in Table 5.7. In Figure 5.17 the water distribution in sections of the network model at $S_{w} = 0.5$ is shown for the different wettability characterization schemes, with the corresponding relative permeability curves shown in Figure 5.18. The saturation shown is towards the end of the spontaneous displacement and most of the remaining oil-filled elements are thus either trapped or oil-wet. In both cases where oil-wet elements are correlated to their inscribed radius (indicated as $r_{\text{min}}$ and $r_{\text{max}}$) there is little continuity in completely water-filled elements. As water repeatedly has to flow through layers in order to connect from inlet to outlet, the water relative permeability will stay very low until water-filled elements start to connect across the model. This behaviour is very similar to that described in the previous section when $S_{oi} > S_{wc}$. In the case where the smallest pores become oil-wet, the oil relative permeability is reduced very quickly as the larger pores, which are also the most conductive, are filled by water early in the displacement. Spatially correlating the oil-wet elements, with a correlation length of about 7 pores, creates more continuity through the oil-wet pores, making it more likely for water to be able to flow from inlet to outlet in completely water-filled elements. The result is a more gradual increase in water relative permeability, consistent with the experimental data. There will necessarily be more statistical variation between the different realizations when using a spatial correlation approach, as evident from the larger error bars in Figure 5.18 when compared to previous figures. All the predicted Amott water indices are
consistent with the experimental values, Table 5.8. There is more variation in the predicted oil indices, as there were no experimental data to compare against.

Table 5.7: Fluid and rock properties used in predictions for a mixed-wet reservoir sandstone.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface tension, $\sigma$ (10⁻³ N/m)</td>
<td>30.0</td>
</tr>
<tr>
<td>Water viscosity, $\mu_w$ (10⁻³ Pa/s)</td>
<td>1.05</td>
</tr>
<tr>
<td>Oil viscosity, $\mu_o$ (10⁻³ Pa/s)</td>
<td>1.39</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.27</td>
</tr>
<tr>
<td>Connate water saturation</td>
<td>0.34</td>
</tr>
<tr>
<td>Water-wet contact angles, $\theta_i$ (deg)</td>
<td>0 – 60</td>
</tr>
<tr>
<td>Oil-wet fraction by pore volume</td>
<td></td>
</tr>
<tr>
<td>$r_{min}$ correlation</td>
<td>0.53</td>
</tr>
<tr>
<td>$r_{max}$ correlation</td>
<td>0.63</td>
</tr>
<tr>
<td>spatial correlation</td>
<td>0.43</td>
</tr>
<tr>
<td>Oil-wet contact angles, $\theta_i$ (deg)</td>
<td></td>
</tr>
<tr>
<td>$r_{min}$ correlation</td>
<td>70 – 110</td>
</tr>
<tr>
<td>$r_{max}$ correlation</td>
<td>140 – 180</td>
</tr>
<tr>
<td>spatial correlation</td>
<td>100 – 160</td>
</tr>
</tbody>
</table>

Table 5.8: Predicted Amott wettability indices for a mixed-wet reservoir sandstone.

<table>
<thead>
<tr>
<th></th>
<th>Water</th>
<th></th>
<th>Oil</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Amott Index</td>
<td>Standard deviation</td>
<td>Amott Index</td>
<td>Standard deviation</td>
</tr>
<tr>
<td>Experimental</td>
<td>0.55</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>$r_{max}$ correlation</td>
<td>0.51</td>
<td>0.01</td>
<td>0.46</td>
<td>0.01</td>
</tr>
<tr>
<td>$r_{min}$ correlation</td>
<td>0.54</td>
<td>0.01</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Spatial correlation</td>
<td>0.56</td>
<td>0.08</td>
<td>0.32</td>
<td>0.08</td>
</tr>
</tbody>
</table>
Figure 5.17: Distribution of water-filled elements during water flooding at \( S_w = 0.5 \) with oil-wet elements correlated by (a) maximum pore radius, (b) minimum pore radius or (c) spatial correlation. The saturation shown is towards the end of spontaneous displacement. Since water-wet elements are generally filled first, phase connectivity during water flooding is improved if there is spatial correlation in the oil-wet elements.
Figure 5.18: Comparison between experimental and predicted relative permeability for a reservoir sandstone. The experimental wetting state is fairly well predicted in all cases and the only difference between the cases is how wettability is characterized on the pore-scale. (a) The larger pores become preferentially oil-wet. (b) The smaller pores become preferentially oil-wet. (c) The oil-wet pores are spatially correlated.
5.4 Oil-wet reservoir sandstone

The final sandstone dataset had steady-state relative permeabilities measured on two core samples with experimental permeabilities of 248 and 328 mD. Since no mercury injection data were available, primary oil flooding capillary pressure had to be used for the network modification process, Figure 5.19. This was a centrifuge experiment performed on a different core sample from those used for relative permeability measurements, hence the difference in connate water saturation. Uncertainties in interfacial tension and contact angles meant that no reliable estimate of absolute permeability could be made. Rather than being strongly water-wet during primary oil flooding, the core exhibited mixed-wet characteristics with Amott water and oil indices of 0.33 and 0. Though this is consistent with a uniform distribution of receding contact angles between 10 and 40 degrees, there still is quite a large degree of uncertainty in the exact wetting state.

Following wettability alteration the core exhibited mainly oil-wet characteristics with Amott water and oil indices of 0.00 and 0.14. The low residual oil saturation is also an indication of an oil-wet system, a result of oil being able to escape through layers. The comparison between experimental and predicted relative permeability is good, Figure 5.19 (b). The predictions were made with $S_{oil} = 0.03$ and intrinsic contact angles distributed at random uniformly between 70 and 122 degrees.

The statistical fluctuations between realizations are less than for mixed-wet samples as all pores contacted by oil are assumed to be oil-wet. The predicted Amott indices of 0.00 and 0.15, with standard deviations of 0 and 0.01, for water and oil respectively, are also in good agreement with experimental values. Fluid and rock properties are given in Table 5.9.
Figure 5.19: Comparison between predicted and experimental properties for an oil-wet reservoir sandstone. (a) Centrifuge primary oil flooding capillary pressures were used to modify the network. (b) Predicted water flooding relative permeability are compared to experimental steady-state data. The low residual oil saturation is a good indication oil-wet characteristics.
Table 5.9: Fluid and rock properties used in predictions for an oil-wet reservoir sandstone.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface tension, $\sigma$ (10$^{-3}$ N/m)</td>
<td>51.8</td>
</tr>
<tr>
<td>Water viscosity, $\mu_w$ (10$^{-3}$ Pa/s)</td>
<td>1.00</td>
</tr>
<tr>
<td>Oil viscosity, $\mu_o$ (10$^{-3}$ Pa/s)</td>
<td>0.29</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.15</td>
</tr>
<tr>
<td>Connate water saturation</td>
<td>0.00</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.03</td>
</tr>
<tr>
<td>Contact angles during primary oil flooding, $\theta_r$ (deg)</td>
<td>10 – 40</td>
</tr>
<tr>
<td>Contact angles during water flooding, $\theta_i$ (deg)</td>
<td>70 – 122</td>
</tr>
</tbody>
</table>
Chapter 6

Conclusions

The aim of this work is not simply to match experiments, but to use easily acquired data to predict difficult to measure properties such as relative permeability. The confidence one can attach to these predictions is directly related to the three main components of pore-scale network modelling that we have focused on in this work – the geometric properties of the network such as topology and pore size distribution, the pore-scale physics, and the wettability characterization.

A state of the art pore-scale network model was developed, that combined topologically disordered networks that represent real systems with detailed displacement mechanisms for any sequence of water and oil flooding for any wettability. Though most of the implemented pore-scale physics has already been described in the literature, a new correlation for oil layer conductance was proposed that is more accurate than previously published work. The correlation was validated by an extensive series of finite element computations.

The implementation of the pore-scale network model was validated using experimental data from water-wet Berea sandstone and a network topology specifically generated to represent this sandstone. The predictions of relative permeability were not only in excellent agreement with experimental data but also agreed well with those presented by other authors [Piri and Blunt, 2002; Øren and Bakke, 2003]. The other water-wet dataset used, a sand-pack, was also very well predicted, further increasing our confidence in the presented pore-scale network model.

By developing a methodology combining realistic network topology with network properties tuned to experimental data such as mercury injection capillary pressure, we successfully predicted flow properties for several datasets including a
sand pack, a reservoir carbonate and two reservoir sandstones while using a network initially developed to represent Berea sandstone. During primary oil flooding relative permeability is controlled by the network geometry and the pore-scale displacement processes and wettability is unambiguous. Predictions of both absolute permeability and primary oil flooding relative permeability were very good, suggesting this methodology is sufficient to predict single and multiphase properties for a wide range of porous media.

During water flooding relative permeability is strongly affected by wettability. The trend in oil recovery from a series of mixed-wet Berea sandstone cores [Jadhunandan and Morrow, 1995] was well predicted by closely reproducing the experimental conditions like $S_{wi}$ and saturation history. The focus of this work is not so much on obtaining a quantitative match with the experiments, but rather on understanding the pore-scale processes that produce these surprising experimental recovery trends. However, by modifying our assumptions about the experimental conditions, a quantitative match was obtained.

Wettability characterization for mixed-wet systems is perhaps the most uncertain part of what has been investigated in this work. Though theoretical models have been suggested in the literature [Kovscek et al., 1993], these do not always satisfactorily describe what is observed experimentally, both in terms of observed transport properties and from pore-scale imaging [Fassi-Fihri et al., 1991; Durand and Beccat, 1998]. In the case of the mixed-wet sandstone samples we suggest that good predictions require the oil-wet pores to be spatially correlated. This ensured that the predicted relative permeability was in better agreement with experimental data than when correlating the oil-wet pores based on size only.

6.1 Applications and future direction

With the outlined methodology of first tuning a realistic network and subsequently predicting the flow performance, constrained by commonly available experimental data, we have shown how pore-scale network modelling can become a very useful tool in analyzing multiphase flow in porous media. By predicting experimental measurements we gain useful insight into pore-scale processes that might not be immediately obvious from just examining the data. By constraining predictions to a defined set of measurements, the predictions will also serve as quality control to the
experiments. For this work we have only used a single network constructed from Berea sandstone. To improve confidence in predictions from a wider range of rocks it would be preferable to have a library of networks representing different rock types. The network that most closely matches the geological structure of the sample of interest would then be chosen for modelling studies.

An even more promising application of predictive pore-scale network modelling is where experimental data is not available or difficult to obtain. Available experimental data can be used to anchor the model to a specific core condition. In the reservoir these conditions might, however, vary considerably. Assessing the impact these variations have on relative permeability can be done more reliably using network modelling than extrapolation from experimental data, particularly for situations where there are wettability variations in the reservoir, or three-phase flow [Piri and Blunt, 2002]. In a previous paper [Jackson et al., 2003] we used network modelling to generate relative permeability curves for a transition zone near the oil-water contact. These were subsequently used in a full-field reservoir simulation model and the predicted oil recovery was significantly different from that obtained using more traditional interpolation techniques.
Bibliography


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Hazlett, R. D., S. Y. Chen, and W. E. Soll, Wettability and rate effects on immiscible displacement: Lattice Boltzmann simulation in microtomographic images of


Lindquist, W. B., S. M. Lee, D. A. Coker, K. W. Jones, and P. Spanne, Medial axis analysis of void structure in three-dimensional tomographic images of porous


Appendix A

Description of Data Input File

The pore-scale network model is written in C++ and uses a keyword based input file. Most keywords are optional and there is no necessary order to them. Comments in the data file are indicated by ‘%’, resulting in the rest of the line being discarded. All keywords should be terminated by ‘#’. The input data file can be supplied as an argument to the executable.

C:\path_to_executable\poreflow.exe default.dat

A.1 Required keywords

A.1.1 NETWORK

This specifies the files containing data such as inscribed radii, volumes and the connection list defining the network topology.

1. Are the files in binary format? Binary files take up less disk space and load substantially quicker than ASCII files. However, binary files can not be interchanged between different computer platforms (e.g. Windows and Solaris).

2. The network data are located in four files when using ASCII format (filename_node1.dat, filename_node2.dat, filename_link1.dat, filename_link2.dat) and two files when using binary format (filename_node.bin and filename_link.bin). Only the prefix filename is to be specified.
A.1.2 SAT_TARGET

Each line represents a separate flooding cycle (e.g. primary oil flooding, secondary water flooding, etc).

1. Final water saturation target after the flooding cycle (fraction). The actual value might not actually be reached due to trapping or water retained in corners.

2. The cycle can also be terminated when a capillary pressure (Pa) is reached.

3. Target water saturation interval (fraction) between reporting results. The state of the model will be evaluated at the first possible configuration after the incremental target has been reached.

4. Target capillary pressure interval (Pa) between reporting results.

5. Should relative permeability be calculated? If this is not of primary interest it can be very time saving to set this option to false ('F') as most of the CPU time is spent solving the pressure field, required for relative permeability calculations.

6. Calculate resistivity index? CPU time required for this is the same as for relative permeability calculations.

<table>
<thead>
<tr>
<th>SAT_TARGET</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00 66380.0 0.02 5000.0 F F</td>
</tr>
<tr>
<td>1.00 -1.0E21 0.02 10000.0 T T</td>
</tr>
<tr>
<td>0.00 1.0E21 0.05 5000.0 T T</td>
</tr>
</tbody>
</table>

A.1.3 EQUIL_CON_ANG

Once invaded by oil the wettability of a pore element will typically change. Advancing and receding contact angles are defined in terms of an intrinsic contact angle, either distributed according to a truncated Weibull distribution

\[
\theta_i = (\theta_{i,\text{max}} - \theta_{i,\text{min}})(-\delta \ln[x(1 - e^{-\frac{1}{\delta}}) + e^{-\frac{1}{\delta}}])^{1/\gamma} + \theta_{i,\text{min}},
\]

(A.1)

where \(\delta\) and \(\gamma\) are parameters defining the shape of the distribution and \(x\) is a random number between 0 and 1, or alternatively distributed uniformly by setting \(\delta\) and \(\gamma\) to less than 0 in the input file.
1. What model should be used for determining receding and advancing contact angles? Model 1 sets $\theta_i = \theta_r = \theta_a$. Model 2 separates $\theta_r$ and $\theta_a$ by a constant angle, with $\theta_a(\theta_i = 0^\circ) = 0^\circ$ and $\theta_r(\theta_i = 180^\circ) = 180^\circ$. With a separation angle of $25.2^\circ$ this corresponds to the Class II model defined by Morrow [1975]. Model 3 corresponds to the Class III model defined by Morrow [1975] and is illustrated in Figure 3.6.

2. Minimum intrinsic contact angle (degrees)

3. Maximum intrinsic contact angle (degrees)

4. $\delta$ exponent (set this to a negative number for uniform distribution).

5. $\gamma$ exponent (set this to a negative number for uniform distribution).

6. How are the contact angles distributed on the pore-scale? ‘rMax’ associates the larger pores (in terms of inscribed radius) with the larger angles, ‘rMin’ associates the larger pores with the smaller angles and ‘rand’ distributes the angles randomly. Throats are assigned the angle of either connecting pore based on equal probability.

7. The separation angle for intrinsic contact angle model 2.

```
EQUIL_CON_ANG
2    30.0    60.0    -1.0    -1.0    rand    25.2
```

A.2 Keywords controlling the reporting of results
The remaining keywords are all optional. The default parameters are those given as example in each section, unless otherwise specified.

A.2.1 TITLE

All output files are prefixed by the indicated title (e.g. title_draincycle_1.out). If this keyword is omitted the title is taken to be the same as the name of the input data file.

```
TITLE
default
```

A.2.2 RES_FORMAT

There is a choice between three formats (‘excel’, ‘matlab’ or ‘std’) for the results files containing capillary pressure, relative permeability, etc. The excel
format will create files with extension .csv, the matlab format will create files with extension .m and the standard format will create files with extension .out.

RES_FORMAT
std
#

A.2.3 WRITE_NET

Using this keyword it is possible to write the network that was used for the simulation to file. Omitting this keyword will result in no network files being written.

1. Should the files be written in binary format (true ‘T’ or false ‘F’)?

2. The filename along with the relative path to be used. The extensions, _node1.dat, _node.bin, etc., will be automatically added to the filename.

WRITE_NET T ../data/sandstone_s8
#

A.2.4 OUTPUT

Using this keyword it is possible to create output files containing the properties of individual network elements in terms of radii, volumes, connection numbers, etc. (title_pores.out and title_throats.out) and files containing the distribution of saturations in the network at every reporting interval (title_pores_Sw.out and title_throats_Sw.out). Both sets of files can become very space consuming. The file format used is the same as that used by the geostatistical package GSLIB [Deutsch and Journel, 1998]. The data are stored in columns. The first row is some arbitrary file header, followed by the number of data columns and the titles of each column.

1. Create files with the properties of individual network elements (true ‘T’ or false ‘F’)?

2. Create files with the water saturation of all pores and throats at every reporting interval (true ‘T’ or false ‘F’)?

OUTPUT F F
#
A.2.5 FILLING_LIST

Output files indicating the sequence that pores and throats got filled during the simulation can be created. The resulting files are formatted for easy entry into matlab for post-processing, with the filenames being poreLocation.m, throatConnection.m, fill_draincycle_1.m and fill_imbcycle_2.m.

1. Create filling list for oil flooding cycles (true ‘T’ or false ‘F’)?
2. Create filling list for water flooding cycles (true ‘T’ or false ‘F’)?
3. Create files with pore location and throat connection data (true ‘T’ or false ‘F’)?

<table>
<thead>
<tr>
<th>FILLING_LIST</th>
<th>F</th>
<th>F</th>
<th>F</th>
</tr>
</thead>
</table>

A.3 Convergence related keywords

A.3.1 SOLVER_TUNE

The pressure solver used for relative permeability calculations is an algebraic multigrid solver [Ruge and Stueben, 1987].

1. The performance of the solver can be tuned by varying the solution tolerance. A lower tolerance will result in an increased number of required solver iterations.

2. Memory allocation for the solver can be adjusted by the memory scaling factor. For large models it might be necessary to increase the factor above the default value.

3. Performance related information about the solver is written to the file fort.11. A value of 0 produces minimal information whereas a value of 3 will produce substantial information about tolerance, memory requirements, etc.

4. Setting this flag to true (‘T’) will output solver information to screen rather than to file.

5. In some cases it might be necessary to discard conductances below a certain threshold to ensure solver convergence. This option should be used with great caution. 
care and only when problems are observed (typically when solving for the oil
pressure in cycles greater than the secondary).

<table>
<thead>
<tr>
<th>SOLVER TUNE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0E-15    5    0    F   0.0E-30</td>
</tr>
</tbody>
</table>

A.3.2 SAT_COVERGENCE

This keyword controls the accuracy at which the incremental water saturation target is reached. It is generally not feasible to calculate water saturation after each filling event, as that would be computationally very expensive. When starting a new saturation step, an approximate number of required filling events is estimated. This estimate is however quite uncertain as the water saturation does not vary linearly with the number of filling events. The actual number of filling events performed before recalculating water saturation should therefore be a relatively small fraction of the initial estimate. Subsequently an updated estimate of the required number of filling events is made, using information from the previous step. Still, only a fraction of the estimated filling events should be performed before recalculating water saturation, as the estimate remains fairly uncertain.

1. Minimum number of filling events between calculating water saturation.
2. Fraction applied to the initial estimate of required number of filling events.
3. Fraction applied to subsequent estimates of required number of filling events.
4. Maximum increase factor in required number of filling events estimates.
5. Only solve for relative permeability when a stable capillary configuration is reached (true ‘T’ or false ‘F’)?

<table>
<thead>
<tr>
<th>SAT_COVERGENCE</th>
</tr>
</thead>
<tbody>
<tr>
<td>10    0.1    0.8    2.0    F</td>
</tr>
</tbody>
</table>

A.3.3 SAT_COMPRESS

This keyword will change the target saturation interval, specified by entry 3 in SAT_TARGET, once relative permeability of the defending fluid drops below a specified threshold. If this keyword is omitted, the originally specified interval target will be used.

1. Relative permeability threshold.
2. New target saturation interval between the reporting of results.

3. Apply to oil flooding cycle (true ‘T’ or false ‘F’)?

4. Apply to water flooding cycle (true ‘T’ or false ‘F’)?

<table>
<thead>
<tr>
<th>SAT_COMPRESS</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1 0.005 T F</td>
</tr>
</tbody>
</table>

# A.3.4 RELPERM_DEF

1. Use flow rate at residual saturation (‘residual’) to calculate relative permeability, rather than that at single phase conditions (‘single’)? Using residual saturations will normalize all relative permeabilities between 0 and 1.

2. Maintain the conditions for trapping as defined in keyword TRAPPING (true ‘T’ or false ‘F’)? If set to false, the defending fluid only has to be connected to one face to be considered as not trapped, even when injecting from a single face of the network.

<table>
<thead>
<tr>
<th>RELPERM_DEF</th>
</tr>
</thead>
<tbody>
<tr>
<td>single T</td>
</tr>
</tbody>
</table>

# A.4 Keywords specifying fluid and rock properties

## A.4.1 INIT_CON_ANG

The initial receding contact angles $\theta_r$, used in elements that have never been invaded by oil, are distributed either uniformly or according to a truncated weibull distribution.

1. Minimum initial receding contact angle (degrees).

2. Maximum initial receding contact angle (degrees).

3. $\delta$ exponent (set to a negative number for a uniform distribution).

4. $\gamma$ exponent (set to a negative number for a uniform distribution).

<table>
<thead>
<tr>
<th>INIT_CON_ANG</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0 0.0 0.2 3.0</td>
</tr>
</tbody>
</table>

#
A.4.2 FRAC_CON_ANG

Not all oil-invaded elements need necessarily attain oil-wet characteristics in mixed-wet systems. This effect can be modelled by defining two separate distributions of intrinsic contact angles. This wettability alteration will be applied after primary oil-flooding and will replace the contact angles defined by EQUIL_CON_ANG in those elements selected to belong to this second distribution. Only a single distribution, as defined by EQUIL_CON_ANG, will exist if this keyword is omitted. The first line of data defines the second distribution.

1. The fraction of oil-invaded elements following primary oil flooding whose contact angles should be altered.
2. Should the fraction be pore volume based (‘T’) or a quantitative split between pores (‘F’).
3. Minimum intrinsic contact angle (degrees).
4. Maximum intrinsic contact angle (degrees).
5. $\delta$ exponent (set to a negative number for a uniform distribution).
6. $\gamma$ exponent (set to a negative number for a uniform distribution).

The second line defines how this second distribution is distributed on the pore-scale. Four approaches are possible. The first approach assumes that the second distribution is spatially correlated. This approach is selected by the keyword ‘corr’ followed by the diameter (in terms of pores) of the correlated regions. One can also select to make the largest (‘rMax’) or smallest (‘rMin’) pores belong to the second distribution. The final approach is randomly selecting the pores (‘rand’). In the last three approaches the connecting throats will be assigned the same contact angle as the pore with a probability equal to the altered fraction (as defined by the first entry in line 1).

1. How should the second distribution be distributed on the pore-scale (‘corr’, ‘rMax’, ‘rMin’ or ‘rand’)?
2. Correlation diameter when using the spatially correlated approach.
A.4.3 FLUID

The fluid description is very simple with no pressure dependent properties.

1. Interfacial tension (mN·m⁻¹)
2. Water viscosity (cp)
3. Oil viscosity (cp)
4. Water resistivity (Ohm·m)
5. Oil resistivity (Ohm·m)
6. Water gravity (kg·m⁻³)
7. Oil gravity (kg·m⁻³)

A.4.4 GRAV_CONST

Define the gravitational constant $g$ ($z = 0$ is at the bottom of the model).

1. Gravitational component in the $x$ direction (m/s²).
2. Component in $y$ direction.
3. Component in $z$ direction.

A.4.5 PRS_DIFF

It is possible to include gravity effects when solving the pressure field. How much influence it will have depends on both the fluid density and the pressure difference imposed across the model.

1. Inlet pressure (Pa).
2. Outlet pressure (Pa).
3. Should gravity effects be included when solving the pressure field (true ‘T’ or false ‘F’)?

<table>
<thead>
<tr>
<th>PRS_DIFF</th>
<th>1.0</th>
<th>0.0</th>
<th>F</th>
</tr>
</thead>
</table>

A.5 Keywords for various network modelling options

A.5.1 RAND_SEED

This is the seed to the random number generator, which should be a large positive integer. If the keyword is omitted the computer clock will be used as seed.

<table>
<thead>
<tr>
<th>RAND_SEED</th>
<th>54356457</th>
</tr>
</thead>
</table>

A.5.2 CALC_BOX

Most of the elements close to the injection faces will be filled by the injecting fluid, resulting in most of the pressure loss occurring in this region when solving the pressure field for the displaced fluid. To avoid these boundary effects it is normal to only use a fraction of the network (away from the injecting faces) when calculating saturation and relative permeabilities.

1. Dimensionless location for lower boundary.

2. Dimensionless location for higher boundary.

<table>
<thead>
<tr>
<th>CALC_BOX</th>
<th>0.50</th>
<th>1.00</th>
</tr>
</thead>
</table>

A.5.3 PRS_BDRS

To avoid boundary effects only a section of the network is used for calculating relative permeability and water saturation, as defined by the CALC_BOX keyword. When computing relative permeability it is possible to solve the pressure field in the entire network, using the average pressure at the section boundaries for relative permeability,

\[ k_{rp} = \frac{q_{mp} \Delta P_{rp}}{q_{sp} \Delta P_{mp}} \] (A.2)
where $\Delta P_{sp}$ and $\Delta P_{mp}$ are the single and multiphase pressure drops for phase $p$ across the selected section. Alternatively the pressure field can be solved only within the selected section by applying constant pressures at the section boundaries, with relative permeability given by (3.40).

1. Solve the pressure field in the entire network (true ‘T’ or false ‘F’)?
2. Record the average pressure at cross-sectional planes within the selected section of the network (true ‘T’ or false ‘F’)? This is just for reporting purposes and the pressures will be written to the results files.
3. The number of cross-sectional pressure planes where the average pressure is to be recorded.

<table>
<thead>
<tr>
<th>PRS_BDRS</th>
<th>F</th>
<th>F</th>
<th>0</th>
</tr>
</thead>
</table>

**A.5.4 TRAPPING**

This keyword controls some aspects of the trapping routine. If fluid is injected from only one face of the model, the defending fluid must be connected to both the inlet and outlet to be considered as not trapped. If injecting from both faces, the defending fluid only has to be connected to one face to be considered as not trapped.

1. Inject fluid from inlet face?
2. Inject fluid from outlet face?
3. Allow drainage of dangling ends (pores with only one connecting throat) through wetting layers.
4. The water conductance ($m^4\cdot Pa^{-1}\cdot s^{-1}$) of circular elements completely filled with oil.

<table>
<thead>
<tr>
<th>TRAPPING</th>
<th>T</th>
<th>F</th>
<th>T</th>
<th>0.0E-30</th>
</tr>
</thead>
</table>

**A.5.5 POINT_SOURCE**

Rather than inject fluid from the face of the network, it is possible to inject from any interior pore. If this keyword is included it will take precedence over the TRAPPING keyword, and no fluid will be injected from any network face.
1. Pore index to inject from. This will have to be greater than 0 and less than the total number of pores.

**A.5.6 PORE_FILL_ALG**

During spontaneous invasion, the capillary entry pressure for pore bodies will depend on the number $n$ of adjacent oil-filled throats (cooperative pore body filling). Several different models have been proposed in the literature. The default models is the one proposed by Blunt [1998] and is described in Chapter 3.3.2 (‘blunt2’),

$$P_c = \frac{2\sigma \cos \theta_a}{r} - \sigma \sum_{i=1}^{n} A_i x_i , \quad (A.3)$$

where $A_i$ are arbitrary numbers and $x_i$ are random numbers between zero and one. Another model proposed by Blunt [1997a] is given by (‘blunt1’)

$$P_c = \frac{2\sigma \cos \theta_a}{r + \sum_{i=1}^{n} A_i x_i} . \quad (A.4)$$

Also implemented is the model proposed by Øren et al. [1998], given by (‘oren1’)

$$P_c = \frac{2\sigma \cos \theta_a}{r + \sum_{i=1}^{n} A_i r_i x_i} , \quad (A.5)$$

where $r_i$ is the radius of connecting throat $i$. A similar model correcting for non-circular pore shapes is given by (‘oren2’)

$$P_c = \frac{(1 + 2\sqrt{\pi G}) \sigma \cos \theta_a}{r + \sum_{i=1}^{n} A_i r_i x_i} . \quad (A.6)$$

1. Model to be used for cooperative pore body filling (‘blunt1’, ‘blunt2’, ‘oren1’ or ‘oren2’).
A.5.7 PORE_FILL_WGT

The weights $A_i$, used in the models for pore body filling, will clearly have an impact on the filling sequence during spontaneous invasion. These are specific to the chosen model, specified by the keyword PORE_FILL_ALG. Typical values for $A_1 – A_6$ for the models proposed by Øren et al. [1998] are 0.0, 0.5, 1.0, 2.0, 5.0 and 10.0. The approach for calculating the weights for the default model (‘blunt2’) by Blunt [1998] is given in Chapter 3.3.2.

1. Weight for an $I_1$ event, $A_1$.
2. Weight for an $I_2$ event, $A_2$.
3. Weight for an $I_3$ event, $A_3$.
5. Weight for an $I_5$ event, $A_5$.
6. Weight for an $I_6$ event, $A_6$, and up.

```
PORE_FILL_WGT
0    15000    15000    15000    15000    15000
#
```

A.6 Keywords for tuning the network properties

If any of the keywords in this section are omitted, the original properties of the network will be retained.

A.6.1 MODIFY_PORO

All pore and throat volumes can be adjusted by a constant factor such that the target porosity is reached. We assume that the total porosity, $\phi_t = \phi_n + \phi_c$, is made up of the net porosity $\phi_n$ and the micro and clay bound porosity $\phi_c$.

1. Target net porosity, $\phi_n$.
2. Target micro and clay bound porosity, $\phi_c$. 
A.6.2 MODIFY_RAD_DIST

This keyword is used for modifying the pore size distribution, useful when tuning a network to become representative of a given type of porous medium. The first line of data refers to throats and the second to pores. The various options for pores are identical to those for throats.

1. There are 6 approaches available for how the pore/throat size distribution should be modified. Setting the index to ‘−1’ will bundle the throats together with the pores or vice versa. So if the first line of data is set to ‘−1’ the second line will apply to pores and throats, rather than just pores. Setting the index to ‘0’ will result in nothing being done. The pore/throat size distribution can be read from file by setting the index to ‘1’. Setting the index to ‘2’ will result in the pore/throat radius being determined by the radii of connecting pores or throats. When setting the index to ‘3’, each pore/throat radius will be multiplied by a constant factor. The shape of the pore/throat size distribution can also be stretched or compressed by setting the index to ‘4’. Finally, by setting the index to ‘5’ the radii are randomly distributed, either uniformly or according to a truncated weibull distribution. For options 1 to 5 additional parameters are needed.

A.6.2.1 READ FROM FILE (OPTION ‘1’)

2. The file containing the target distribution. The file should contain two columns. The first column is the pore/throat diameter in micrometers. This should be monotonically decreasing. The second column should be the corresponding fraction of pore/throat space occupied, going from 0 to 1.

3. If the target distribution is derived from mercury injection data it might be necessary to apply a lower cut-off to exclude effects from mercury entering the micro porosity. Micro porosity (and clays) should be accounted for with the MODIFY_PORO keyword. No cut-off will be applied if a negative value is specified.
4. It might also be necessary to apply a higher cut-off.

A.6.2.2 ASPECT RATIO (OPTION ‘2’)  
The average connecting radius will be multiplied by a user defined aspect ratio, $\alpha$, distributed uniformly or according to a truncated weibull distribution. The radius of a pore body is then given by

$$r_p = \max \left( \alpha \frac{\sum_i r_i}{n}, \max(r_i) \right), \quad (A.7)$$

while the throat radius is given by

$$r_t = \min \left( \alpha \frac{\sum_i r_i}{n}, \min(r_i) \right). \quad (A.8)$$

2. Minimum aspect ratio. If minimum and maximum aspect ratios are set to a negative number the original ratios of the network will be used.

3. Maximum aspect ratio.

4. $\delta$ exponent (set to a negative number for a uniform distribution).

5. $\gamma$ exponent (set to a negative number for a uniform distribution).

A.6.2.3 MULTIPLICATION FACTOR (OPTION ‘3’)  
2. Multiplication factor.

A.6.2.4 STRETCH OR COMPRESS DISTRIBUTION (OPTION ‘4’)  
The original pore/throat size distribution will be either stretched or compressed along the size axis according to the function

$$r = \frac{r_o^a}{\bar{r}_o^{a-1}}, \quad (A.9)$$

where $r_o$ is the original radius and $\bar{r}_o$ is the pore volume based average radius.

2. The exponent $a$ determines if the distribution is stretched ($a > 1$) or compressed ($a < 1$).
3. Should the function be applied to pores or throats with radii greater than the volume based average (true ‘T’ or false ‘F’)?

4. Should the function be applied to pores or throats with radii less than the volume based average (true ‘T’ or false ‘F’)?

A.6.2.5 NEW RANDOM DISTRIBUTION (OPTION ‘5’)

2. Minimum radius.

3. Maximum radius.

4. \( \delta \) exponent (set to a negative number for a uniform distribution).

5. \( \gamma \) exponent (set to a negative number for a uniform distribution).

The third line of data contains some additional parameters.

1. Should the average throat length to radius ratio be maintained from the original network? If this is set to true (‘T’) all throat lengths will be scaled along with pore locations and absolute model size.

2. Should the new pore and throat size distributions be written to file (true ‘T’ or false ‘F’)? The files will be named RadDist_pores.csv and RadDist_throats.csv.

3. How many data points should there be in the distributions written to file?

```
MODIFY_RAD_DIST
1   ./hg_final.txt  -1.0  -1.0
2   -1.0  -3.0   0.2   3.0
T T  50
```

A.6.3 MODIFY_G_DIST

In the same way that pore and throat size distributions can be modified, so can the various shape factors. Again, the first line of data refers to throats and the second to pores, and the various options for pores are identical to those for throats. Square \((G = 1/16)\) and circular \((G = 1/4\pi)\) elements will not be modified. For triangular elements the maximum shape factor is \(\sqrt{3}/36\) which represents an equilateral triangle.

1. There are 5 approaches available for how the shape factor distribution should be modified. Setting the index to ‘-1’ will bundle the throats together with the pores or vice versa. So if the first line of data is set to ‘-1’ the second line will
apply to pores and throats, rather than just pores. Setting the index to ‘0’ will result in nothing being done. The shape factor distribution can be read from file by setting the index to ‘1’. When setting the index to ‘3’, each pore or throat shape factor will be multiplied by a constant factor. The shape of the shape factor distribution can also be stretched or compressed by setting the index to ‘4’. Finally, by setting the index to ‘5’ the shape factors are randomly distributed, either uniformly or according to a truncated weibull distribution.

For options 1 to 5 additional parameters are needed, but these are identical to those described for MODIFY_RAD_DIST and will not be repeated here.

When applying (A.9) to shape factors, \( \bar{G}_o \) refers to the median rather than the volume based average. If the distributions are read from file, the second column refers to the quantitative fraction of pores or throats.

The third line contains some additional parameters.

1. Should the new pore and throat shape factor distributions be written to file (true ‘T’ or false ‘F’)? The files will be named ShapeFactDist_pores.csv and ShapeFactDist_throats.csv.

2. How many data points should there be in the distributions written to file?

```
<table>
<thead>
<tr>
<th>MODIFY_G_DIST</th>
<th>-1</th>
<th>5</th>
<th>0.001</th>
<th>0.04811</th>
<th>-1.0</th>
<th>-1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>F</td>
<td>50</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>#</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
```

A.6.4 MODIFY_CONN_NUM

The average coordination number of the network is very important for fluid connectivity and hence relative permeability. For a given network this can be reduced by removing throats.

1. Target coordination number. This should be less than the original (can be found from the .prt file).

2. Which throats should be removed? Four different options are available. Lowest volume (‘volume’), smallest shape factor (‘shape’), smallest radius (‘radius’) or selected at random (‘rand’).
A.6.5 MODIFY_MOD_SIZE

By changing the absolute size of the network the absolute permeability will also change. All lengths will be scaled (pore positions, radii, volumes and lengths). In most cases it is however best to let the model size be scaled through the keyword MODIFY_RAD_DIST where the length to radius ratio is maintained from the original network.

1. Fractional change to the absolute size of the model.

A.7 Examples of input data files

A.7.1 Water-wet Berea sandstone

This is the data file used for Chapter 4.2.

<table>
<thead>
<tr>
<th>SAT_TARGET</th>
<th>%finalSat</th>
<th>maxPc</th>
<th>maxDeltaSw</th>
<th>maxDeltaPc</th>
<th>calcKr</th>
<th>calcI</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.00</td>
<td>1.0E21</td>
<td>0.02</td>
<td>500000.0</td>
<td>T</td>
<td>F</td>
</tr>
<tr>
<td></td>
<td>1.00</td>
<td>-1.0E21</td>
<td>0.02</td>
<td>500000.0</td>
<td>T</td>
<td>F</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>INIT_CON_ANG</th>
<th>% min</th>
<th>max</th>
<th>delta</th>
<th>gamma</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.0</td>
<td>0.0</td>
<td>-0.2</td>
<td>-3.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EQUIL_CON_ANG</th>
<th>% model</th>
<th>min</th>
<th>max</th>
<th>delta</th>
<th>gamma</th>
<th>scheme</th>
<th>m2_separation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>3</td>
<td>50.0</td>
<td>60.0</td>
<td>-1.0</td>
<td>-1.0</td>
<td>rand</td>
<td>25.2</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>RES_FORMAT</th>
<th>matlab</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>REL_PERM_DEF</th>
<th>% kr_def</th>
<th>trpCond</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>single</td>
<td>F</td>
</tr>
</tbody>
</table>
SAT_COMPRESS
% kr_thres maxDeltaSw OilFlood WatFlood
  0.1  0.001 T T
#

TRAPPING
% Inject fluid from allow drainage water cond in
% entry exit of dangling ends filled circ elem
  T F T 0.0E-30
#

SOLVER_TUNE
% min memory scaling solver verbose conductance
% tolerance factor output solver cut-off
  1.0E-30 8 0 F 0.0
#

PRS_BDRS
% calc kr using record press num press
% avg press profiles profiles
  F F 20
#

PORE_FILL_ALG
  blunt2
#

PORE_FILL_WGT
  0.0 18904 18904 18904 18904 18904
#

FLUID
% interfacial water oil water oil water oil
% tension viscosity viscosity resist. resist. density density
% (mN/m) (cp) (cp) (Ohm.m) (Ohm.m) (kg/m3) (kg/m3)
  30.0 1.05 1.39 1.2 1000.0 1000.0 1000.0
#

CALC_BOX
  0.5 1.0
#

NETWORK
% bin filename
  T ../Data/Berea
#

SAT_COVERGENCE
% minNumFillings initStepSize nextStepSize maxIncr stable
  10 0.1 0.8 2.0 F
#

A.7.2 Water-wet sand pack

This is the data file used for Chapter 4.3.

RAND_SEED
  9512367
#
SAT_TARGET
%finalSat  maxPc  maxDeltaSw  maxDeltaPc  calcKr  calcI
 0.00  16000.0  0.3  100000.0  F  F
 1.00 -1.0E21  0.3  100000.0  F  F
 0.00  16000.0  0.02  1000.0  T  F
 1.00 -1.0E21  0.02  1000.0  T  F
#
SAT_COMPRESS
% kr_thres  maxDeltaSw  OilFlood  WatFlood
 0.1  0.005  F  T
#
INIT_CON_ANG
% min  max  delta  gamma
 0.0  0.0  0.2  3.0
#
EQUIL_CON_ANG
% model  min  max  delta  gamma  scheme  m2_separation
 3  30.0  40.0 -1.0 -1.0  rand  25.2
#
RES_FORMAT
matlab
#
TRAPPING
% Inject fluid from  allow drainage  water cond in
% entry  exit  of dangling ends  filled circ elem
  T  F  T  0.0E-30
#
RELPERM_DEF
% kr_def  trpCond
residual  F
#
SOLVER_TUNE
%  min  memory scaling  solver  verbose  conductance
%  tolerance  factor  output  solver  cut-off
  1.0E-30  7  0  F  0.0
#
PRS_BDRS
% calc kr using  record press  num press
%  avg press  profiles  profiles
  F  F  20
#
FORE_FILL_ALG
   blunt2
#
FORE_FILL_WGT
  0 7473 7473 7473 7473 7473
#
FLUID
% interfacial water oil water oil water oil
% tension viscosity viscosity resist. resist. density density
% (mN/m) (cp) (cp) (Ohm.m) (Ohm.m) (kg/m3) (kg/m3)
  70.25  0.97  0.018  1.2  1000.0  1000.0  1.22
#

CALC_BOX
  0.50  1.00
#

NETWORK
% bin   filename
    T   ../../../Data/dury_final
#

SAT_COVERAGE
% minNumFillings initStepSize nextStepSize maxIncr stable
   10    0.1    0.8     2.0      F
#

A.7.3 Mixed-wet Berea sandstone

This is the data file used for Chapter 5.1 for the variable wettability case and $S_{wf} = 0.24$.

RAND_SEED
  6844625
#

SAT_TARGET
% finalSat maxPc maxDeltaSw maxDeltaPc calcKr calcI
  0.24   1.0E21  0.20  500000.0   F    F
  0.90  -1.0E21  0.015  500000.0   T    F
  0.14   1.0E21  0.015  500000.0   T    F
  0.91  -1.0E21  0.015  500000.0   T    F
#

INIT_CON_ANG
% min   max   delta  gamma
  0.00   0.00   0.2    3.0
#

EQUIL_CON_ANG
% model  min   max   delta  gamma scheme m2_separation
    3    50.0  60.0  -1.0   -1.0    rand      25.2
#

FRAC_CON_ANG
% fraction volBased min   max   delta  gamma
  0.94    T    90.0  112.0  -10.0  -1.0
% method
    rMax
#

RES_FORMAT
  matlab
#
A.7.4 Mixed-wet carbonate

This is the data file used for Chapter 5.2 for sample 2 with a lower oil-wet fraction.
EQUIL_CON_ANG
% model  min   max   delta  gamma scheme m2_separation
3   25.0  65.0   -1.0   -1.0    rand     25.2
#

FRAC_CON_ANG
% fraction  volBased  min   max   delta    gamma
0.65        T    80.0    82.0   -1.0     -1.0
% method
rmin
#

RES_FORMAT
matlab
#

TRAPPING
% Inject fluid from entry exit allow drainage water cond in
% of dangling ends filled circ elem
T     F                T               0.0E-30
#

SOLVER_TUNE
% min    memory scaling   solver    verbose   conductance
% tolerance    factor        output    solver     cut-off
1.0E-40       7             0         F        0.0E-40
#

PRS_BDRS
% calc kr using record press num press
% avg press profiles profiles
F                F             20
#

PORE_FILL_ALG
blunt2
#

PORE_FILL_WGT
0  844113  844113  844113  844113  844113
#

FLUID
% interfacial  water    oil    water    oil    water    oil
% tension  viscosity  viscosity resist. resist. density  density
% (mN/m) (cp)       (cp)     (Ohm.m) (Ohm.m)  (kg/m3)  (kg/m3)
29.9       0.927     6.17        1.2   1000.0   829.3   1094.6
#

PRS_DIFF
% prsIn  prsOut  gravity
1.0    0.0      T
#

CALC_BOX
0.50  1.00
#
A.7.5 Mixed-wet sandstone

This is the data file used for Chapter 5.3 when using spatially correlated mixed-wetting.

**SAT_TARGET**

<table>
<thead>
<tr>
<th>finalSat</th>
<th>maxPc</th>
<th>maxDeltaSw</th>
<th>maxDeltaPc</th>
<th>calcKr</th>
<th>calcI</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000</td>
<td>1.0E21</td>
<td>0.20</td>
<td>500000.0</td>
<td>F</td>
<td>F</td>
</tr>
<tr>
<td>1.000</td>
<td>-1.0E21</td>
<td>0.01</td>
<td>500000.0</td>
<td>T</td>
<td>F</td>
</tr>
<tr>
<td>0.000</td>
<td>1.0E21</td>
<td>0.20</td>
<td>500000.0</td>
<td>F</td>
<td>F</td>
</tr>
</tbody>
</table>

**INIT_CON_ANG**

<table>
<thead>
<tr>
<th>min</th>
<th>max</th>
<th>delta</th>
<th>gamma</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>0.2</td>
<td>3.0</td>
</tr>
</tbody>
</table>

**EQUIL_CON_ANG**

<table>
<thead>
<tr>
<th>model</th>
<th>min</th>
<th>max</th>
<th>delta</th>
<th>gamma</th>
<th>scheme</th>
<th>m2_separation</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0.0</td>
<td>60.0</td>
<td>-1.0</td>
<td>-1.0</td>
<td>rand</td>
<td>25.2</td>
</tr>
</tbody>
</table>

**FRAC_CON_ANG**

<table>
<thead>
<tr>
<th>fraction</th>
<th>volBased</th>
<th>min</th>
<th>max</th>
<th>delta</th>
<th>gamma</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.43</td>
<td>T</td>
<td>100.0</td>
<td>160.0</td>
<td>-1.0</td>
<td>-1.0</td>
</tr>
</tbody>
</table>

**RES_FORMAT**

matlab

**TRAPPING**

<table>
<thead>
<tr>
<th>Inject fluid from</th>
<th>allow drainage</th>
<th>water cond in</th>
<th>entry</th>
<th>exit</th>
<th>of dangling ends</th>
<th>filled circ elem</th>
</tr>
</thead>
<tbody>
<tr>
<td>T</td>
<td>F</td>
<td>T</td>
<td>0.0E-30</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**SOLVER_TUNE**

<table>
<thead>
<tr>
<th>min</th>
<th>memory scaling</th>
<th>solver</th>
<th>verbose</th>
<th>conductance</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0E-40</td>
<td>7</td>
<td>0</td>
<td>F</td>
<td>0.0E-40</td>
</tr>
</tbody>
</table>

**PRS_BDRS**

<table>
<thead>
<tr>
<th>calc kr using</th>
<th>record press</th>
<th>num press</th>
</tr>
</thead>
<tbody>
<tr>
<td>F</td>
<td>F</td>
<td>20</td>
</tr>
</tbody>
</table>
A.7.6 Oil-wet sandstone

This is the data file used for Chapter 5.4.
TRAPPING
% Inject fluid from allow drainage water cond in
% entry exit of dangling ends filled circ elem
T F T 0.0E-30
#

SOLVER_TUNE
% min memory scaling solver verbose conductance
% tolerance factor output solver cut-off
1.0E-40 8 0 F 0.0E-40
#

PRS_BDRS
% calc kr using record press num press
% avg press profiles profiles
F F 20
#

PORE_FILL_ALG
  blunt2
#

PORE_FILL_WGT
  0 24837 24837 24837 24837 24837
#

FLUID
% interfacial water oil water oil water oil
% tension viscosity viscosity resist. resist. density density
% (mN/m) (cp) (cp) (Ohm.m) (Ohm.m) (kg/m3) (kg/m3)
30.0 1.0 0.289 1.2 1000.0 1000.0 800.0
#

PRS_DIFF
% prsIn prsOut gravity
10.0 0.0 T
#

CALC_BOX
  0.5 1.0
#

NETWORK
% bin filename
  T ..../..../Data/Statoil_sst_40avg
#

MODIFY_PORO
% phi_eff phi_clay
  0.153 0.0
Pore-Scale Modeling of Three-Phase Flow

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Abstract

We present a three-dimensional network model to simulate two- and three-phase capillary dominated processes at the pore level. The displacement mechanisms incorporated in the model are based on the physics of multi-phase flow observed in micromodel experiments. All the important features of immiscible fluid flow at the pore-scale, such as wetting layers, spreading layers of the intermediate-wet phase, hysteresis and wettability alteration are implemented in the model. Wettability alteration allows any values for the advancing and receding oil/water, gas/water and gas/oil contact angles to be assigned. Multiple phases can be present in each pore or throat (element), in wetting and spreading layers, as well as occupying the center of the pore space. In all, some thirty different generic fluid configurations for two- and three-phase flow are analyzed. Double displacement and layer reformation are implemented as well as direct two-phase displacements and layer collapse events. Every element has a circular, square or triangular cross-section. A random network that represents the pore space in Berea sandstone is used in this study. The model computes relative permeabilities, saturation paths, and capillary pressures for any displacement sequence. A methodology to track a given three-phase saturation path is presented that enables us to compare predicted and measured relative permeabilities on a point-by-point basis. A new and robust displacement based clustering algorithm is presented. We predict measured relative permeabilities for two-phase flow in a water-wet system. We then successfully predict the steady-state oil, water and gas three-phase relative permeabilities measured by Oak [1]. We then study gas injection into media of different wettability and interpret the results in terms of pore-scale displacement processes.
The list of publications as a result of this research is as follows:


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Chapter 1

Introduction

The simultaneous flow of three phases - oil, water and gas - in porous media is of great interest in many areas of science and technology such as petroleum reservoir and environmental engineering. Three fluid flow occurs in enhanced oil recovery schemes such as tertiary gas injection into oil and water, gas cap expansion, solution gas drive, gravity drainage, water flooding with different initial oil and gas saturations, steam injection, thermal flooding, depressurization below the bubble point, and water alternative gas (WAG) injection. In an environmental context three-phase flow occurs when a non-aqueous phase liquid (NAPL), leaking from an underground storage tank for instance, migrates through the unsaturated zone and may coexist with water and air (gaseous phase).

In order to understand fluid flow in porous media, one needs to know the constitutive relationships between macroscopic properties of the system such as relative permeabilities, capillary pressures, and fluid saturations. These relationships are used in macroscopic partial differential equations to describe the transport of fluid. The determination of constitutive relationships is complicated as they are dependent on the fluids’ properties, the pore space, and the saturation history.

Experimental measurements of three-phase relative permeabilities and capillary pressures have been the subject of several studies [1–30], but they are extremely difficult to perform and at low saturation the results are very uncertain [16, 23, 31, 32]. Two independent fluid saturations are required to define a three-phase system and there is an infinite number of possible fluid arrangements making a comprehensive suite of experimental measurements for all three-phase displacements impossible. This is why numerical simulations of three-phase flow almost always rely on available empirical correlations to predict relative permeability and capillary pressure from measured two-phase properties [4, 20, 22, 33–54]. These models may
give predictions that vary as much as an order of magnitude from each other, or from direct measurements, since they have little or no physical basis [43, 53, 55].

It is important to have a reliable physically-based tool that can provide plausible estimates of macroscopic properties. Any theoretical or numerical approach to this problem not only needs a detailed understanding of the multiphase displacement mechanisms at the pore level but also an accurate and realistic characterization of the structure of the porous medium [56]. During the last two decades our knowledge of the physics of two- and three-phase flow at the pore level has considerably increased through experimental investigation of displacements in core samples and micromodels [57–71]. To describe the geometry of the pore space several authors have developed different statistical [72–74] and process based [75–77] techniques. In addition the pore space can be imaged directly using micro CT tomography [78, 79]. An example of a three-dimensional pore space image of a sandstone is shown in Fig. (1.1). It is possible to simulate multi-phase flow directly on a three-dimensional pore-space image by solving Navier Stokes equations or by using Lattice-Boltzman techniques [80–83]. However, for capillary controlled flow with multiple phases, these methods become cumbersome and computationally expensive.

An attractive alternative approach is to describe the pore space as a network of pores connected by throats with some idealized geometry (see Fig.(1.2)) [77, 84]. Then a series of displacement steps in each pore or throat are combined to simulate multiphase flow. Fatt [85–87] initiated this approach by using a regular two-dimensional network to find capillary pressure and relative permeability. Since then, the capabilities of network models have improved enormously and have been applied to describe many different processes. Table 1.1 lists some of the recent applications of network modeling. Recent advances in pore-scale modeling have been reviewed by Celia & Reeves [88] and Blunt [89].

For a random close packing of spheres Bryant and co-workers were able to predict permeability, elastic and electrical properties and relative permeability [105, 109, 240]. Øren et al. extended this approach by reconstructing a variety of sandstones and generating topologically equivalent networks from them. Using these networks several authors have been able to predict relative permeability and oil recovery for a variety of systems [75–77, 116, 125, 130, 134].

In this work we extend this predictive approach to three-phase flow. Before reviewing previous three-phase network models in detail, we review the fundamentals of contact angles, spreading coefficient and wettability alteration as well as spreading and wetting layers.
### Table 1.1: Network and percolation type modeling references

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1. Non-Aqueous Phase Liquid

2. Solution Gas Drive
Figure 1.1: The void space of a sandstone produced by process based simulation [75–77]
Figure 1.2: The Berea network used in this work. The network is a disordered lattice of pores connected by throats. The network topology, the radii of the pores and throats, their shapes and their volumes are all determined from a three-dimensional representation of the pore space of the system of interest (see Fig.(1.1)). This network will be used to predict two- and three-phase relative permeabilities (see Table (4.2) for dimensions and statistics of the network).
Chapter 2

Physics of Three-Phase Flow at the Pore-Level

2.1 Spreading Coefficients and Interfacial Tensions

The ability of oil to spread on water in the presence of gas is described by the spreading coefficient which is a representation of the force balance where the three phases meet. If the interfacial tensions are found by contacting pairs of pure fluids in the absence of the third, the coefficient is called initial and is defined by [241]:

$$C^i_s = \sigma_{gw} - \sigma_{go} - \sigma_{ow}$$  \hspace{1cm} (2.1)

where $\sigma$ is an interfacial tension between two phases labeled $o$, $w$, and $g$ to stand for oil, water, and gas respectively. However, when three phases are present simultaneously, the interfacial tensions are different from those in two-phase systems. For instance, the gas/water interfacial tension may be significantly lower than its two-phase value because oil may cover the interface by a thin film of molecular thickness [242]. The other two-phase interfacial tensions may also vary when the third phase is present. If the three phases remain long enough in contact, thermodynamic equilibrium will be reached when liquids become mutually saturated. In these circumstances the spreading coefficient is named equilibrium and is given by Eq. (2.2), which is either negative or zero [241].

$$C^{eq}_s = \sigma^{eq}_{gw} - \sigma^{eq}_{go} - \sigma^{eq}_{ow}$$  \hspace{1cm} (2.2)

Three-phase systems may be divided into one of the following cases (see Fig. 21...
Figure 2.1: Different three-phase systems: (a) Non-spreading, $C_i^s < 0$ and $C_{eq}^s < 0$, (b) Partially spreading, $C_i^s > 0$ and $C_{eq}^s < 0$, (c) Spreading, $C_i^s > 0$ and $C_{eq}^s \approx 0$.

(2.1)): (a) Non-spreading, $C_i^s < 0$ and $C_{eq}^s < 0$: a blob of oil will remain stationary on water, for example $CS_2$ on water [241]. (b) Partially spreading, $C_i^s > 0$ and $C_{eq}^s < 0$: where a quick initial spreading happens and then when the water surface is covered by a thin oil film, oil retracts to a lens. An example is benzene on water. (c) Spreading, $C_i^s > 0$ and $C_{eq}^s \approx 0$: in this case, oil spreads on water and excess oil makes the film thicker and thicker. When the thickness of the oil film is larger
than the range of intermolecular forces the equilibrium spreading coefficient becomes zero. Soltrol, a mixture of hydrocarbons, is an example of this case [70].

In the rest of the work, we will drop the superscript $eq$ and always assume that we are dealing with interfacial tensions at equilibrium.

### 2.2 Three-Phase Contact Angles

The contact angle is defined as the angle between the two-phase line and the solid surface measured through the denser phase. In a three phase system a horizontal force balance can be written for each of the three pairs of fluids, i.e. oil-water, gas-water, and gas-oil, residing on a solid to obtain Young’s equation (see Fig. (2.2)):

\[
\begin{align*}
\sigma_{os} &= \sigma_{ws} + \sigma_{ow} \cos \theta_{ow} \quad (2.3) \\
\sigma_{gs} &= \sigma_{ws} + \sigma_{gw} \cos \theta_{gw} \quad (2.4) \\
\sigma_{gs} &= \sigma_{os} + \sigma_{go} \cos \theta_{go} \quad (2.5)
\end{align*}
\]

Figure 2.2: Horizontal force balance in three two-phase systems: (a) oil/water/solid, (b) gas/water/solid, and (c) gas/oil/solid.
A constraint on the three-phase contact angles and interfacial tensions can be derived by manipulation of Eqs.(2.3)-(2.5):

\[ \sigma_{gw} \cos \theta_{gw} = \sigma_{go} \cos \theta_{go} + \sigma_{ow} \cos \theta_{ow} \]  

(2.6)

Eq. (2.6) was derived first by Bartell & Osterhoff [243] in the context of solid/oil/water systems and rediscovered by Zhou & Blunt [242] in contaminant hydrology. This constraint has many implications for three-phase processes. For instance consider a three-phase strongly oil-wet system, i.e. \( \theta_{ow} \approx \pi \). At ambient conditions, typical interfacial tensions for water/n-alkane systems are \( \sigma_{go} = 20 \text{ mN/m} \) and \( \sigma_{ow} = 50 \text{ mN/m} \) [241]. This means \( \sigma_{gw} \cos \theta_{gw} < 0 \) which in turn implies \( \theta_{gw} > \frac{\pi}{2} \). The analysis above for oil-wet systems indicates that gas is not the most non-wetting phase in the presence of water.

Blunt [244] showed in a \( n \) phase system there are \( \frac{n(n-1)}{2} \) contact angles, \( \frac{(n-1)(n-2)}{2} \) constraints and \( (n - 1) \) independent contact angles. In three-phase systems, only two of the contact angles need to be defined independently.

Van Dijke et al. [149] presented a linear relationship to find gas/oil and gas/water contact angles from the oil/water contact angle and interfacial tensions which also satisfies the constraint given by Eq. (2.6):

\[ \cos \theta_{go} = \frac{1}{2\sigma_{go}} \{ C_s \cos \theta_{ow} + C_s + 2\sigma_{go} \} \]  

(2.7)

\[ \cos \theta_{gw} = \frac{1}{2\sigma_{gw}} \{ (C_s + 2\sigma_{ow}) \cos \theta_{ow} + C_s + 2\sigma_{go} \} \]  

(2.8)

### 2.3 Wettability Alteration and Contact Angle Hysteresis

Wettability is the ability of one fluid to spread on a solid and form a wetting film [143]. Based on the oil/water contact angle, porous media with different wettability can be categorized into three main groups: water-wet, neutrally-wet and oil-wet corresponding to oil/water contact angles being less than, very close to and larger than \( \frac{\pi}{2} \) respectively.

While most clean rock surfaces in contact with refined oils are water-wet, few, if any oil reservoirs are completely water-wet. This is because of direct contact of crude oil with the solid surface which changes its wettability by adsorption of the polar components of the crude or the presence of naturally oil-wet minerals within the
rock. This makes any values of oil/water and consequently gas/water and gas/oil contact angles possible [245–249]. Kovscek et al. [247] developed a model where the wettability of the rock surface is assumed to be altered by the direct contact of oil. Before a porous medium is invaded by oil it is assumed to be full of water and water-wet. Once it is invaded by oil, a thin film of water prevents oil touching the solid surface directly. But at a threshold capillary pressure, this film can collapse and allows oil to contact the solid surface and change its wettability. Regions of the pore space not contacted by oil remain water-wet.

The contact angle also depends on the direction of displacement. This difference between *advancing*, i.e. wetting phase displacing the non-wetting one, and *receding*, i.e. non-wetting phase displacing the wetting one, contact angles may be as large as $50^\circ$ - $90^\circ$ [241, 250, 251] depending on surface roughness, surface heterogeneity, swelling, rearrangement or alteration of the surface by solvent [241].

To accommodate any type of displacement process, we assign eight contact angles to each pore and throat: $\theta_{PD}^{ow}$ (oil displacing water in an element that has not changed its wettability before), $\theta_{PD}^{gw}$ (gas displacing water in an element that has not changed its wettability before), and six contact angles when the wettability has been altered: $\theta_{ow}^{a}$ (water displacing oil), $\theta_{ow}^{r}$ (oil displacing water), $\theta_{gw}^{a}$ (water displacing gas), $\theta_{gw}^{r}$ (gas displacing water), $\theta_{go}^{a}$ (oil displacing gas), $\theta_{go}^{r}$ (gas displacing oil).

There is an ambiguity in defining a third contact angle from Eq. (2.6) if advancing and receding values are different. For instance, imagine water is being injected into oil and gas where the appropriate gas/water and oil/water contact angles to be used are $\theta_{gw}^{a}$ and $\theta_{ow}^{a}$ respectively. Now if one uses Eq. (2.6) to find the third contact angle, $\theta_{go}$, it is not clear that the calculated value is the advancing or receding gas/oil contact angle. This problem is also evident when one uses Eqs. (2.7) and (2.8), where it is not known, for example, which oil/water contact angle, i.e. advancing or receding, should be used to calculate receding gas/oil contact angle needed, for example, in gas injection into oil and water.

In this work, we first decide on the values of two of the contact angles and then calculate the third one using Eq. (2.6). We use $\theta_{ow}^{r}$ and $\theta_{go}^{r}$ to calculate a $\theta_{gw}$. We also use $\theta_{ow}^{a}$ and $\theta_{go}^{a}$ to find another value of $\theta_{gw}$. The smaller of two values of $\theta_{gw}$ is considered as receding and the larger one as the advancing value. We always make sure in every single pore and throat, the receding contact angle for each phase is less than or equal to the advancing value, i.e. $\theta_{ij}^r \leq \theta_{ij}^a$. 
2.4 Spreading and Wetting Layers

During primary drainage, oil can occupy centers of the pore space, leaving water as a wetting layer in the corners and crevices of the pore space. During subsequent cycles of water and/or gas injection these water layers are still present and maintain continuity of water.

After gas injection into an element containing oil in the center and water in wetting layers, gas will occupy the center and it is possible that oil will remain in a layer sandwiched between the gas and water. These are called spreading layers; as we discuss later their stability is related to the spreading coefficient, contact angles, corner angles and capillary pressures, and are likely to be present in spreading systems.

Later, we will present detailed analysis of possible pore space configurations in terms of displacement history, contact angles and spreading coefficient. However, to motivate the critique of previous pore-scale models of three-phase flow, we need to emphasize the definition of some key terms.

A spreading system has $C_s = 0$ and oil spontaneously forms layers between water and gas in the pore space. A non-spreading system has $C_{eq}^s < 0$ and while oil layers can also be present [71, 252, 253] they tend to be stable for more restricted range of capillary pressures. Also, we refer to wetting and spreading layers - these layers are typically a few microns in thickness and have a non-negligible hydraulic conductivity and maintain phase continuity. In contrast, films are of molecular thickness (of order a nanometer) and have negligible conductivity and do not contribute to phase continuity - where present films simply modify the apparent, or equilibrium, interfacial tensions, as discussed above.
3.1 Previously Developed Three-Phase Pore-Scale Network Models

Here we present a detailed review of previously developed three-phase network models.

Heiba et al. [135] extended statistical network modeling previously used for two-phase systems [94, 106] to three-phase flow. A Bethe lattice, or Cayley network was used to represent the porous medium. Relative permeabilities were calculated from Stinchcombe’s formula [254] using new series approximations from percolation theory. Only a single phase could occupy a throat. A given fluid was considered to be able to flow only when the site that it occupied was a member of a continuous flow path from the inlet to the outlet. The displacement of one phase by another was controlled by accessibility and local entry capillary pressure. Six groups of displacement were considered: gas into oil, oil into gas, gas into water, water into gas, water into oil, and oil into water. Two spreading systems were investigated where in the first one gas and water were displacing oil while in the second case water and oil were displacing oil and gas. The results showed that the gas and water relative permeabilities were functions of only their own saturations. Oil layers prevented the direct contact of gas and water. Oil isoperms were found to be strongly curved, meaning that the oil relative permeability was not only a function of its own saturation. Extensions of the theory to handle the complications involved by the effects of wettability and phase swelling due to mass transfer were also discussed. It was concluded that three-phase relative permeabilities are generally path functions rather than state functions (function of saturation only) except in particular situa-
tions such as when two phases are separated by the third. This model used rather simple networks and displacement rules.

Soll & Celia [136] developed a computational model of capillary-dominated two- and three-phase movement at the pore level to simulate capillary pressure-saturation relationships in a water-wet system. Regular two- or three-dimensional networks of pores, connected to each other by throats, were used to represent the porous medium. Hysteresis was modeled by using advancing and receding values for the contact angles for each pair of fluids. Every pore was able to accommodate one fluid at a time as well as wetting layers. Viscous forces were considered to be negligible but the effects of gravity were included to modify the local capillary pressures. In order to reproduce their micromodel experiments [65], oil as a spreading phase was allowed to advance ahead of a continuous invasion front. Several pores could be filled simultaneously. This model was the first to incorporate layer flow in three-phase network modeling albeit in a rather ad hoc fashion. The results were compared with capillary pressure-saturation results and fluid distributions from the two- and three-fluid micromodel experiments. The amount of oil layer flow was used as a fitting parameter. Predicted two-phase air/water and oil/water capillary pressures were in good agreement with measured values [65] although the model did not so successfully match three-phase data. The model was not used to calculate relative permeabilities.

Øren et al. [137] described details of the pore level displacement mechanisms taking place during immiscible gas injection into waterflood residual oil (tertiary gas injection) which then were incorporated into a two-dimensional strongly water-wet square network model with rectangular links and spherical pores in order to compute oil recovery in spreading and non-spreading systems. Simulated recoveries compared very well with the measured values from micromodel experiments [62, 63]. The authors described a double drainage mechanism where gas displaces trapped oil that displaces water allowing immobile oil to become connected boosting oil recovery. Oil recovery decreased with decreasing spreading coefficient. In non-spreading systems, the probability of direct gas-water displacement was high and capillary fingering of gas resulted in early gas breakthrough and low oil recovery. In spreading systems, oil reconnection was more effective and direct gas/oil displacement was preferred. It was concluded that a simple invasion percolation algorithm [92, 255] including the spreading layers works well in mimicking the complex three-phase behavior seen in micromodels. In this work, relative permeabilities were not calculated. We will also study the effects of spreading coefficient and the competition between
the displacement of oil and water by gas in this paper.

Pereira et al. [56, 144] developed a dynamic two-dimensional network model for drainage-dominated three-phase flow in strongly water- and oil-wet systems when both capillary and viscous forces were important. The displacement mechanisms in spreading and non-spreading systems were described by generalization of two-phase displacement mechanisms. Both pores and throats were assumed to be lenticular in cross-section allowing wetting and spreading layers to be present. No volumes were allocated to the throats and layers and there was no pressure drop in the pores. Resistance to the flow through the throats was modeled using the mean hydraulic radius concept, i.e. twice the ratio of area open to flow to wetted perimeter. Pressure of a fluid in a throat was an interpolation of pressures of the same fluid in the neighboring pores. Trapping of different fluids was considered only for non-spreading systems. Coalescence and reconnection of trapped clusters was also simulated. Pores could be occupied by two or three bulk fluids at the same time separated by flat interface(s).

The simulated recoveries at gas breakthrough, were compared against the measured values in micromodels [63]. A large difference between the recoveries in oil spreading and non-spreading systems was reported. This was believed to be due to existence of oil layers in the spreading systems and the preference for direct gas/water displacement in non-spreading systems. The highest recovery, i.e. 85%, was that of oil-wet case in both spreading and non-spreading systems. This was due to existence of continuous wetting layers of oil. The oil recovery was much lower for the water-wet case in a non-spreading system, i.e. 14%. This was because there were no spreading layers of oil. Even when layers were present for the spreading system, the oil recovery was much lower, i.e. 40%, in a water-wet medium than for the oil-wet case. Water in water-wet systems played the same role as oil in oil-wet systems, i.e. water recoveries in water-wet spreading and non-spreading systems were high. It was confirmed that the high oil recoveries were due to the presence of wetting or spreading oil layers, despite the fact that the conductance of a layer of water or oil in a throat was only around 1% of the conductance of a throat full of a single phase. In non-spreading systems, direct water displacement by gas was preferred over gas-oil-water double displacement leading to low oil recovery. An order of magnitude reduction in conductivity of the oil layers decreased oil recovery and made the behavior of the spreading system similar to that of a non-spreading system. Also a reduction in initial oil saturation for tertiary gas injection decreased the oil recovery. This was true for both spreading and non-spreading systems in-
indicating that the recovery of the intermediate wetting phase is strong function of saturation history. This was reported to be consistent with experiments by Dria et al. [23] and Oak [1, 21]. It was also concluded that the recovery of the wetting fluid is independent of the saturation history. Relative permeabilities were not calculated in this work.

Paterson et al. [138] developed a water-wet percolation model to study the effects of spatial correlations in the pore size distributions on three-phase relative permeabilities and residual saturations. This was an extension of their previous work on two-phase systems [115]. Fractal maps derived from fractional Brownian and Levy motion (fBm and fLm) were used to assign pore size. A simple site percolation model with trapping was used. Trapping was incorporated based on Hoshen-Kopelman algorithm [256]. In three-phase simulations, direct displacement of oil and water by gas and also double drainage were implemented. The model assigned the same volume to all pores and so the fraction of sites occupied by a phase gave its saturation. All the sites were assumed to have the same conductivity regardless of their radii. The simulation results for correlated properties showed lower residual saturations in comparison to uncorrelated ones. Incorporating bedding by giving a direction to the correlations had a major impact on relative permeability. When the bedding was parallel to the flow direction, the relative permeabilities were greater and residual saturations lower than those when bedding was perpendicular to the flow. This was also the case for two-phase relative permeabilities [115]. The effects of spreading coefficient were also studied. It was shown that the less negative the spreading coefficient, the lower the final residual oil saturation. It was also shown that for more negative spreading coefficients, direct gas to oil and gas to water displacements are preferred over double drainage. This effect was reported to be more significant for correlated systems.

Fenwick & Blunt [141, 142] developed a three-phase network model for strongly water-wet systems. A regular cubic network composed of pores and throats with equilateral triangular or square cross-sections was used. Oil/water and gas/water contact angles were considered to be zero. Two- and three-phase displacement mechanisms including oil layer flow observed in micromodel experiments were incorporated into the model. Double drainage was generalized to allow any of six types of double displacement where one phase displaces a second that displaces a third, as observed by Keller et al. [71]. The model was able to simulate any sequence of oil, water and gas injection. Using a geometrical analysis, a criterion for stability of oil layers was derived which was dependent on oil/water and gas/oil capillary
pressures, contact angles, equilibrium interfacial tensions, and the corner half angle. It was argued that oil layers could be present even for negative spreading coefficient systems. Using a simple calculation [242], it was shown that the layers are of order a micron across or thicker in the corners, roughness, and grooves of the pore space. The work was the first to suggest an expression to estimate conductance of an oil layer which then was used to compute oil relative permeability, i.e. in the computation of relative permeability a finite conductance was assigned to oil layers, and to wetting layers of water. Using a simple argument, it was shown that at low oil saturation the oil relative permeability should vary quadratically with saturation, as observed experimentally [13, 257–259].

It was shown that in three-phase systems relative permeabilities and oil recoveries are strong functions of saturation path. An iterative methodology which couples a physically-based network model with a 1-D three-phase Buckley-Leverett simulator was developed in order to find the correct saturation path for a given process with known initial condition and injection fluid [142]. This enabled the network model to compute the properties for the right displacement sequence. The three-phase relative permeabilities were called self-consistent when the saturation path that was used by the network model to compute them will be exactly produced by the conventional three-phase Buckley-Leverett simulator if the network model relative permeabilities were used in the flow equations to compute the macroscopic flow. Self-consistent relative permeabilities for secondary and tertiary gas injection into different initial oil saturations were presented. The resultant saturation paths compared well qualitatively with experimental data by Grader & O’Meara [13]. The paths in the oil/water vs. gas/oil capillary pressure space were all located in the region where oil layers were stable meaning that oil did not get trapped. Oil relative permeabilities for different initial conditions were reported to be different from each other consistent with several experimental studies [1, 2, 16, 25, 43].

Mani & Mohanty [139, 140] also used a regular cubic network of pores and throats to simulate three-phase flow in water-wet systems. Pores and throats were considered to be spherical and cylindrical respectively. The oil/water capillary pressure was fixed at its original value during the gas invasion processes. The parameters of the network were tuned to match the two-phase mercury-air experimental capillary pressures of Berea sandstone [90].

Both dynamic and quasi-static simulations were carried out. The work had two important features: (I) Dynamic simulation of capillary-controlled gas invasion, where it was assumed each phase pressure was not constant across the network. (II)
Re-injection of the produced fluids at the outlet of the medium into the inlet in order to simulate larger systems. This was used to see whether trapped oil ganglia become reconnected by double drainage to form spanning clusters. The two-phase processes were simulated at low capillary number using traditional quasi-static assumptions. Pressure drops across pores were ignored. The model included fluid flow through wetting and spreading layers. The conductance of the layers were accounted for by assuming that they are equivalent to the conductance of smaller tubes found by reducing the size of the original tube by different factors, e.g. 1.5, 10, and 25. However, for the capillary pressure histories used in this work, no stable oil layers were observed in both spreading and non-spreading systems. Gas invasion was modeled by three displacement mechanisms: direct gas/water, direct gas/oil, and double drainage. For each displacement, a potential was considered which was the difference between the pressures of two involved fluids minus the threshold capillary pressure of the displacement. The displacement with the largest potential was carried out first. Re-injection of fluids was simulated by replacing the fluid distribution in the inlet zone by the fluids in the outlet zone. The process was terminated after steady state was reached at the imposed pressure conditions, i.e. when no further gas invasion was possible at the imposed capillary pressure. The final oil saturation in spreading systems was zero. The capillary pressure curves obtained from dynamic and quasi-static simulations were virtually identical. For non-spreading systems with a low oil/water capillary pressure, drainage of water and oil was reported to occur with similar probability. Displacement of water from the medium created trapped oil clusters that were surrounded by gas. Due to the assumed absence of oil layers in non-spreading systems, oil ganglia could not be displaced by gas at any gas/oil capillary pressure. The water relative permeability was a function of the water saturation alone for both two-phase and three-phase systems, and was not dependent on the saturation history, spreading coefficient and the imposed oil/water capillary pressure, as found by previous authors. Similarly for spreading three-phase systems, it was shown that gas relative permeability is a function of its own saturation only and do not depend on the imposed oil/water capillary pressure. But for non-spreading systems, the three-phase gas relative permeability was different from the two-phase drainage curves and were dependent on the oil/water capillary pressure, spreading coefficient and the saturation history. The three-phase oil relative permeability was a function of the oil saturation, the imposed oil/water capillary pressure, the spreading coefficient and the saturation history in both spreading and non-spreading systems.
Laroche et al. [123, 143] developed a pore network model to predict the effects of wettability heterogeneities with different patterns and spatial distributions on displacement mechanisms, sweep efficiency, and fluid distribution in gas injection into oil and water. A dalmatian type of wettability heterogeneity, i.e. continuous water-wet surfaces enclosing discontinuous regions of oil-wet surfaces or vice-versa, was used. A series of three-phase glass micro-model experiments with different wettabilities were also carried out. Measured oil/water contact angles for the water-wet and oil-wet surfaces were 0° and 105° respectively. n-Dodecane, water, and nitrogen were the three fluids used in the experiments. All the two-phase interfacial tensions, densities, and viscosities were measured. The initial spreading coefficient was reported to be 7.3 mN/m and hence the oil was assumed to be spreading. The capillary number throughout the experiments was reported to be about $10^{-5}$ indicating capillary controlled displacements. A 2-D regular pore and throat network was used to simulate the experiments. All the throats were considered to have triangular cross-section while the pores were assumed to be cylindrical in cross-section. The pore and throat size distributions were similar to those of Berea sandstone. Saturations, conductance, and relative permeabilities were calculated using similar techniques to Fenwick & Blunt [141]. The fluid distributions at the end of two- and three-phase simulations were in good qualitative agreement with those found experimentally.

Hui & Blunt [260, 261] developed a mixed-wet model of three-phase flow for a bundle of capillary tubes. The tubes had different sizes and were equilateral triangle in cross-section. Wettability alteration was modeled by changing the wettability of surfaces that came into contact with oil after primary drainage. This enabled the model to simulate three-phase flow with any combination of oil/water, gas/water, and gas/oil contact angles. In all, some ten fluid configuration were considered. Primary drainage, water flooding, and tertiary gas injection were simulated. Empirical expressions were used to calculate the conductance of corners, layers, and center of each tube using the area open to flow to each fluid. The model was then able to calculate relative permeabilities and capillary pressures as a function of saturation. The effects of wettability, spreading coefficient, and initial oil saturation on relative permeabilities were investigated. Possible configuration changes during each process along with the threshold capillary pressure of each change were presented. The stability of layers in different configurations and their collapsing capillary pressures was discussed. We will extend this approach to study 30 different possible fluid configurations in three-phase flow and will incorporate them in a three-dimensional
random network model.

Lerdahl et al. [146] used the technique developed by Bakke et al. [75] to reconstruct a three-dimensional void space, Fig. (1.1), and then convert it to a pore and throat network, Fig. (1.2), for use in a water-wet network model to study drainage-dominated three-phase flow. Simulated results were compared successfully against the experimental data by Oak [1]. We will use a similar network in our studies and also compare our predictions against Oak’s experiments [1]. In our study, we will compare results on a point-by-point basis using our saturation tracking algorithm and extend the model to mixed-wet systems, to study imbibition- and drainage-dominated processes, following the approach of Hui & Blunt [260, 261].

Lasrsen et al. [147] used a water-wet three-dimensional cubic pore network model based on the work of Fenwick & Blunt [141, 142] to simulate a series of micromodel experiments of WAG (water alternating gas) injection processes. All the pores and throats were assumed to have square cross-sections. The network model was used in an iterative procedure similar to the one used by Fenwick & Blunt [142] to find self-consistent saturation paths. Three WAG injections with different gas/water injection ratios were carried out. Self consistent relative permeabilities and experimental observations were not presented.

Van Dijke et al. [148–150] presented a process-based mixed-wet model of porous media using a bundle of capillary tubes with circular cross-sections to study the saturation dependencies of three-phase capillary pressures and relative permeabilities for spreading and non-spreading systems. The larger pores were considered to be oil-wet and the smaller ones water-wet. It was shown that based on interfacial tensions and contact angles, the three-phase saturation space could be divided up to three different regions with a different intermediate-wet phase. The relative permeability of this phase is a function of two saturations. Also capillary pressure between the most wetting and non-wetting phases is dependent on two saturations. The relative permeabilities of the other two phases were a function of only their own saturation in this region. For water-wet systems, the results agreed those found by previous network modeling studies [260, 261]. The authors extended this approach to determine the functional dependency of relative permeability and capillary pressure for media of arbitrary wettability.

Van Dijke et al. [151, 152] developed a regular three-dimensional three-phase network model for systems with different wettability expanding on other previous studies on bundles of capillary tubes. Every element was allowed to have a different oil/water contact angle and Eqs. (2.7) and (2.8) were used to determine the gas/oil
Chapter 3. Literature Review

and gas/water contact angles [149]. While layers were not incorporated explicitly in saturation or conductance computations, they were allowed to establish continuity of different phases. The model was a cubic array of only throats with a circular cross-section. The coordination number could be changed by removing throats from the network. An extensive series of simulations of three-phase flow was performed. For networks with a high coordination number, the saturation dependencies were qualitatively similar to those predicted for capillary bundles. As the coordination number was reduced, connectivity was impaired and trapping became significant. The authors also compared their network simulations with micromodel experiments of WAG [262, 263] where there were repeated cycles of water and gas flooding. To reproduce the results, they incorporated multiple displacements where a train trapped clusters may displace each other until there is invasion into a connected phase. They suggested that such multiple displacements were significant in WAG flooding. While certainly such displacements were observed in the micromodel experiments, we suggest that in three-dimensional displacements the phases are likely to be better connected and so the movement of trapped ganglia is less significant. We will only consider double displacements in this paper.

The conclusion of this section is that while many three-phase pore-scale displacement mechanisms are well understood, and the generic functionality of relative permeability has been discussed, three-phase network models to date have not addressed the full range of possible configurations in mixed-wet systems and their predictive powers are limited.

The network model described here combines three essential components: (1) a description of the pore space and its connectivity that mimics real systems; (2) a physically-based model of wettability alteration; and (3) a full description of fluid configurations for two- and three-phase flow. This will enable us to predict three-phase relative permeabilities for media of arbitrary wettability using geologically realistic networks.

Comparison of the experimental and predicted relative permeabilities in three-phase systems is only possible if both have identical saturation paths. This is because macroscopic properties in three-phase systems are strongly dependent on saturation history of the system. In this work, we present an algorithm to simulate experimental saturation paths and predict relative permeabilities to compare with measured values.
Chapter 4

Displacement Mechanisms

4.1 Porous Medium

In recent years, several advances have been made in the construction of realistic representations of porous media. Øren, Bakke and co-workers [75–77] have developed random network models based on the pore space geometry of the rock of interest. The model is derived either from a direct three-dimensional image of the pore space obtained from micro CT scanning, or from simulating the geological processes by which the rock was formed, see Fig.(1.1). Many other authors have also developed techniques to derive pore structures from a variety of measurements [74, 79, 105, 109, 128, 160, 240, 264–274]. While such approaches are not routine, and the correct pore-space characterization of carbonates is very much an open question, for simple sandstones there are reliable methods for determining an equivalent network structure that attempts to mimic the properties of the real pore space.

Microscopic observations have shown that clastic sediments, e.g. sandstones and carbonates, are three-dimensional irregular networks of irregularly shaped pores and throats [85]. Inspection of thin sections have shown that the irregular pores and throats can be modeled reasonably well by irregular triangles and high-order polygons [275, 276] as they provide corners where more than one phase can reside and also have a wide range of shape factors that allow capturing many basic features of capillary behavior of the real porous media [276]. As well as triangular cross-section elements, authors have used geometries with circular [151, 152], square [141, 142, 147], star-shape [110, 163, 165–167], and lenticular [56, 144] cross-sections (see Fig.(4.1)) to represent such pores and throats.

The network model in this work reads as input any two or three-dimensional regular or random network comprised of pores connected by throats. Each pore or
throat is assigned a total volume, an inscribed radius and a shape. The inscribed radius is used to assign a capillary entry pressure during multiphase flow. In this model the pore and throats have a scalene triangular, square or circular cross-section. The cross-section has the same shape factor $G$ (ratio of cross-sectional area to perimeter squared) \([276]\) as the real system from which the network is derived:

$$G = \frac{A}{P^2} \tag{4.1}$$

A clay volume is associated with the network. This represents an immobile volume that remains water saturated throughout all displacements. It can be adjusted to match the observed connate water saturation \([75–77]\). Table \((4.1)\) lists all the parameters that the model reads to recognize a network. A Berea network is used for the modeling studies in this work. A network of pores and throats is generated that presents the topology of the void space of the rock of interest (see Fig. \((1.2)\)). The pores and throats have sizes and shapes that reproduce the principal geometric features of the three-dimensional image (see Fig. \((1.2)\)) \([76]\). Table \((4.2)\) lists the network statistics. Fig. \((4.2)\) compares the pore and throat size distributions of the network.
Table 4.1: Network parameters read by the model consistent with the networks generated by Øren, Bakke and co-workers [75–77].

<table>
<thead>
<tr>
<th>No.</th>
<th>Item</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Total number of pores and throats</td>
</tr>
<tr>
<td>2</td>
<td>Length, width and depth of the network</td>
</tr>
<tr>
<td>3</td>
<td>Volume of each pore and throat</td>
</tr>
<tr>
<td>4</td>
<td>X, Y, and Z coordinations of each pore</td>
</tr>
<tr>
<td>5</td>
<td>Inscribed radius of each pore and throat</td>
</tr>
<tr>
<td>6</td>
<td>Number of connecting pore(s) to each pore (1)</td>
</tr>
<tr>
<td>7</td>
<td>Index of connecting pore(s) to each pore</td>
</tr>
<tr>
<td>8</td>
<td>Whether each pore is at the inlet</td>
</tr>
<tr>
<td>9</td>
<td>Whether each pore is at the outlet</td>
</tr>
<tr>
<td>10</td>
<td>Index of the throat connecting two pores</td>
</tr>
<tr>
<td>11</td>
<td>Shape factor of each pore and throat</td>
</tr>
<tr>
<td>12</td>
<td>Clay pore volume</td>
</tr>
<tr>
<td>13</td>
<td>Index of the first and second connecting pores to each throat</td>
</tr>
<tr>
<td>14</td>
<td>Micro-porosity volume in each throat</td>
</tr>
<tr>
<td>15</td>
<td>Spacing (2)</td>
</tr>
<tr>
<td>16</td>
<td>Length of the first and second pore connecting to each throat</td>
</tr>
<tr>
<td>17</td>
<td>Length of each throat</td>
</tr>
</tbody>
</table>

1. Coordination number of each pore

2. Distance between the centers of the two connecting pores

### 4.2 Pore and Throat Cross-Sectional Shapes

- **Triangular Elements**

  An irregular triangle with the corner half angles of $\alpha_1$, $\alpha_2$, and $\alpha_3$ and the convention of $0 \leq \alpha_1 \leq \alpha_2 \leq \alpha_3 \leq \frac{\pi}{2}$, see Fig. (4.3), is considered. The $\alpha_1$ and $\alpha_2$ are two corner half angles associated with the base of the triangle and $r$ is the inscribed radius which is related to the area, $A$, and perimeter, $P$, of the element through [276]:

  \[
  r = \frac{2A}{P} = 2PG
  \]  

(4.2)

Since the cross-section is a composition of six triangles with equal height of $r$ (see Fig. (4.3)), from elementary geometry $A$ is given by:
Chapter 4. Displacement Mechanisms

Figure 4.2: Pore and throat size distributions for the Berea network

\[ A = \frac{r^2}{4G} = r^2 \sum_{i=1}^{3} \cot \alpha_i \]  

(4.3)

Since \( \alpha_3 = \frac{\pi}{2} - \alpha_1 - \alpha_2 \), the shape factor \( G = A/P^2 \) is then given by:

\[ G = \frac{1}{4} \left[ \sum_{i=1}^{3} \cot \alpha_i \right]^{-1} = \frac{1}{4} \tan \alpha_1 \tan \alpha_2 \cot (\alpha_1 + \alpha_2) \]  

(4.4)

The shape factor for irregular triangles ranges from zero corresponding to a slit-like element to \( \frac{\sqrt{3}}{36} \approx 0.048113 \) belonging to equilateral triangles. A given value of \( G \) corresponds to a range of triangles where the limits of the range are denoted by \( \alpha_{2,\text{min}} \) and \( \alpha_{2,\text{max}} \) which in turn correspond to the triangles where \( \alpha_{2,\text{min}} = \alpha_1 = \alpha \) and \( \alpha_{2,\text{max}} = \frac{\pi}{4} - \frac{\alpha_1}{2} \), see Fig. (4.4). The shape factor is related to \( \alpha_{2,\text{min}} \) and \( \alpha_{2,\text{max}} \) by:

\[ G = \frac{1}{4} \left[ \frac{2}{\tan \alpha_{2,\text{min}}} + \tan(2\alpha_{2,\text{min}}) \right] \]  

(4.5)
Table 4.2: Berea network statistics

<table>
<thead>
<tr>
<th>Item</th>
<th>Throats</th>
<th>Pores</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number</td>
<td>26146</td>
<td>12349</td>
<td>38495</td>
</tr>
<tr>
<td>Porosity excl. clay (%)</td>
<td>4.562</td>
<td>13.746</td>
<td>18.309</td>
</tr>
<tr>
<td>Porosity incl. clay (%)</td>
<td>6.238</td>
<td>17.785</td>
<td>24.024</td>
</tr>
<tr>
<td>Average shape factor</td>
<td>0.035</td>
<td>0.033</td>
<td>0.034</td>
</tr>
<tr>
<td>Triangular cross sections (%)</td>
<td>90.729</td>
<td>95.506</td>
<td>92.261</td>
</tr>
<tr>
<td>Rectangular cross sections (%)</td>
<td>7.542</td>
<td>4.324</td>
<td>6.510</td>
</tr>
<tr>
<td>Circular cross sections (%)</td>
<td>1.729</td>
<td>0.170</td>
<td>1.229</td>
</tr>
<tr>
<td>ASCHA (deg.) (1)</td>
<td>15.235</td>
<td>13.744</td>
<td>14.751</td>
</tr>
<tr>
<td>AWCHA (deg.) (2)</td>
<td>48.828</td>
<td>49.215</td>
<td>48.954</td>
</tr>
<tr>
<td>Minimum radius (µm)</td>
<td>0.903</td>
<td>3.623</td>
<td>0.903</td>
</tr>
<tr>
<td>Maximum radius (µm)</td>
<td>56.850</td>
<td>73.539</td>
<td>73.539</td>
</tr>
<tr>
<td>Average radius (µm)</td>
<td>10.970</td>
<td>19.167</td>
<td>13.60</td>
</tr>
<tr>
<td>Connected to the inlet</td>
<td>254</td>
<td>0</td>
<td>254</td>
</tr>
<tr>
<td>Connected to the outlet</td>
<td>267</td>
<td>0</td>
<td>267</td>
</tr>
<tr>
<td>Isolated clusters</td>
<td>-</td>
<td>-</td>
<td>3</td>
</tr>
<tr>
<td>Isolated</td>
<td>3</td>
<td>6</td>
<td>9</td>
</tr>
<tr>
<td>Minimum coordination number</td>
<td>-</td>
<td>1</td>
<td>-</td>
</tr>
<tr>
<td>Maximum coordination number</td>
<td>-</td>
<td>19</td>
<td>-</td>
</tr>
<tr>
<td>Average coordination number</td>
<td>-</td>
<td>4.192</td>
<td>-</td>
</tr>
<tr>
<td>Clay volume (%)</td>
<td>1.676</td>
<td>4.039</td>
<td>5.715</td>
</tr>
<tr>
<td>$K_{abs}$ (cal. box: 0.05-0.95) (mD)</td>
<td>-</td>
<td>-</td>
<td>3054.816</td>
</tr>
<tr>
<td>X dimension (mm)</td>
<td>-</td>
<td>-</td>
<td>3</td>
</tr>
<tr>
<td>Y dimension (mm)</td>
<td>-</td>
<td>-</td>
<td>3</td>
</tr>
<tr>
<td>Z dimension (mm)</td>
<td>-</td>
<td>-</td>
<td>3</td>
</tr>
</tbody>
</table>

1. Average Sharpest Corner Half Angle

2. Average Widest Corner Half Angle

$$G = \frac{2 \sin \alpha_1}{2 \left[ 2 + \frac{\sin(2\alpha_1)}{\sin(2\alpha_{2, max})} \right]^{-2}} = \frac{\sin(2\alpha_{2, max}) \cos(2\alpha_{2, max})}{4[1 + \cos(2\alpha_{2, max})]^2}$$ \hspace{1cm} (4.6)

For a given $G$ the value of $\alpha_2$ is selected randomly ($\alpha_{2, min} \leq \alpha_2 \leq \alpha_{2, max}$). Then Eq. (4.4) is used to find the corresponding value of $\alpha_1$. And finally $\alpha_3 = \frac{\pi}{2} - \alpha_1 - \alpha_2$.

- **Rectangular and Circular Elements**

The shape factor for rectangular cross-section elements with all corner half angles being equal to $\frac{\pi}{4}$ is $\frac{1}{16}$ while for circular cross-section elements $G = \frac{1}{4\pi}$.


Chapter 4. Displacement Mechanisms

4.3 Pressure Difference Across an Interface

To find the pressure difference across an interface, we use the Young-Laplace equation:

$$P_i - P_j = \sigma_{ij} \left( \frac{1}{r_1} + \frac{1}{r_2} \right) \quad (ij = ow, gw, go) \quad (4.7)$$

where ow, gw, and go stand for oil/water, gas/water, and gas/oil respectively, $r_1$ and $r_2$ are the principal radii of curvature, and $P_i$ and $P_j$ are pressures of the phases on either sides of the interface.

There are two types of interface (see Fig.(4.5)), (I): Main Terminal Menisci (MTM) [276], which is the invading meniscus at the pore/throat junction separating wetting and non-wetting fluids. The shape of such a meniscus is assumed to be spherical meaning that the two radii of curvature are the same ($r_1 = r_2 = r$). The pressure difference across an MTM is then given by (see Fig.(4.6)):

$$P_i - P_j = \frac{2\sigma_{ij}}{r} = \frac{2\sigma_{ij} \cos \theta}{R} \quad (4.8)$$

where $R$ is the radius of the capillary pore. In the case of non-circular cross-section capillaries, $R$ would be the inscribed radius. (II): Arc Menisci (AM), which is the interface at a corner of a non-circular element. It is assumed that the curvature of the interface is negligible in the plane perpendicular to that of the paper meaning that the principal radii of curvature would be $r_1 = r$ and $r_2 = \infty$ [241, 276]. The pressure difference across such an interface is given by:

$$P_i - P_j = \frac{\sigma_{ij}}{r} \quad (4.9)$$
Figure 4.4: Distribution of shape factor vs. the second largest corner half angle in irregular triangles

### 4.4 Displacement Mechanisms

#### 4.4.1 Drainage

Drainage in a capillary element is referred to an event where a wetting phase is displaced by a non-wetting phase with a positive capillary pressure. Drainage occurs by a piston-like mechanism (see Fig. (4.7)-(a)). Imagine a capillary element filled by a wetting phase with a non-wetting phase having access at one end of it where it forms an MTM. The capillary pressure, $P_{c,ij}$, is simply the pressure difference across the interface:

$$ P_{c,ij} = P_i - P_j \quad (ij = ow, gw, go) \quad (4.10) $$

An increase in $P_{c,ij}$ results in the MTM hinging at the entrance of the element which may remove a small amount of the wetting phase. If the increase in the capillary pressure continues, at some threshold capillary pressure the MTM enters the element with a fixed drainage curvature and receding contact angle [276]. While the MTM displaces the wetting phase from the center of the element may allow – in
non-circular elements and only if the receding contact angle is less than $(\frac{\pi}{2} - \alpha)$ – the residual of the displaced phase to remain at the corners creating new AM’s. If the effects of gravity are ignored then the curvature of the AM’s will be exactly the same as that of the invading MTM meaning that the volume of the wetting fluid that is left at the corners depends on the curvature of the invading MTM or, in other words, on the threshold capillary pressure of the displacement which in turn is a function of cross-sectional shape of the element [276]. The threshold capillary pressure is found using the theory that was originally suggested by Mayer and Stowe [277], developed by Princen [278–280] and applied independently by Lenormand et al. [57] (MS-P).

The MS-P theory is based on equating the curvature of AM’s left at the corners by the displacement to that of the invading MTM. The method has been applied by several authors to derive expressions to compute threshold capillary pressures of piston-like displacement in elements with circular and different angular cross-sections such as those by Legait [281] for capillary tubes with variable square cross-sections and different contact angles, by Mason & Morrow [276] for water-wet irregular tri-
angles which was later extend by Morrow [282] to include the effects of contact angle and contact angle hysteresis in equilateral triangles, and by Van Dijke & Sorbie [283] for three-phase threshold capillary pressures in elements with non-circular cross-section and different wettability. Here we present the generalization of the model by Ma et al. [284] to regular n-sided (polygon) elements and Øren et al. [76] and Patzek [125] to irregular triangles.

1. Cylindrical Elements

Conservation of energy for the displacement translates to equating the virtual work of the MTM movement to the change in the surface free energy (see Fig.(4.7)-(b)):

\[ P_c A_{\text{eff}} dx = \sigma_{1s} L_{1s} dx - \sigma_{2s} L_{2s} dx \] (4.11)

where \( A_{\text{eff}} \) is the cross-sectional area occupied by the non-wetting phase, \( L_{1s} \) and \( L_{2s} \) are the lengths of phase-1-solid and phase-2-solid interfaces in the cross-sectional plane. For cylindrical tubes, \( A_{\text{eff}} \) is equal to the cross-sectional area, and lengths \( L_{1s} \) and \( L_{2s} \) are the same and equal to the perimeter of the tube. If Young’s equation is written as:

\[ \sigma_{1s} - \sigma_{2s} = \sigma_{12} \cos \theta \] (4.12)

then Eq. (4.11) can be reordered as:

\[ \frac{P_c}{\sigma_{12}} = \frac{L \cos \theta}{A} = \frac{P_{\text{eff}}}{A_{\text{eff}}} = \frac{2 \cos \theta}{R} \] (4.13)

where \( P_{\text{eff}} \) is the effective perimeter.

\[ P_{\text{eff}} = L \cos \theta \] (4.14)

2. Regular n-Sided Elements

Similar to the cylindrical elements conservation of energy can be written for tubes with angular cross-sections. The only difference is that AM’s may be left at the corners by the displacement (see Fig.(4.7)-(c)). Equating the displacement work to the surface free energy change gives:
Figure 4.7: Effective perimeter and area for tubes with cylindrical and regular angular cross-section [284]

\[ P_{e}A_{eff}dx = (L_{12}\sigma_{12} + L_{1s}\sigma_{1s} - L_{1s}\sigma_{2s})dx \]  

(4.15)

where \( L_{12} \) is the length of the AM between wetting and non-wetting phases.
Using Young’s equation (see Eq. (4.12)), Eq. (4.15) can be rewritten as follows:

\[
\frac{P_c}{\sigma_{12}} = \frac{1}{r_d} = \frac{L_{12} + L_{1s} \cos \theta}{A_{eff}} = \frac{P_{eff}}{A_{eff}}
\] (4.16)

where

\[P_{eff} = L_{12} + L_{1s} \cos \theta\] (4.17)

In a piston-like drainage, the general relationship between normalized curvature of the MTM, \(C_{n,d}\), contact angle and corner half angle is given by:

\[
\left[\frac{\cos^2 \theta_1}{\tan \alpha} - \frac{\sin 2\theta_1}{2} - \left(\frac{\pi}{2} - \alpha - \theta_1\right)\right]\frac{1}{C_{n,d}^2} - \frac{\cos \theta_1}{\tan \alpha} \frac{2}{C_{n,d}} + \frac{1}{\tan \alpha} = 0
\] (4.18)

where

\[C_{n,d} = \frac{R}{r_d}\] (4.19)

The solution is:

\[C_{n,d} = \cos \theta_1 + \sqrt{\frac{\tan \alpha}{2} [\sin 2\theta_1 + \pi - 2\alpha - 2\theta_1]}\]

\[\theta_1 < \frac{\pi}{2} - \alpha\] (4.20)

where \(\theta_1\) is given in Tables (4.3), (4.4), (4.5), and (4.6) for different conditions when Eq. (4.20) is used. The threshold capillary pressure is related to the normalized curvature by:

\[P_{c,d} = \frac{\sigma_{12}C_{n,d}}{R}\] (4.21)

If the \(\theta_1\) is larger than \(\frac{\pi}{2} - \alpha\) then the displacement won’t leave any AM’s at the corners and the normalized curvature of drainage is given by:

\[C_{n,d} = 2 \cos \theta_1\]

\[\frac{\pi}{2} - \alpha < \theta_1 < \frac{\pi}{2}\] (4.22)
3. Irregular Triangular Elements

For an angular cross-section element, the conservation of energy equations are the same as those of the n-sided regular tubes, i.e. Eqs. (4.15), (4.16), and (4.17). For a piston-like drainage, the effective area is given by:

\[
A_{\text{eff}} = A - r_d^2 \sum_{i=1}^{n} \left[ \frac{\cos \theta_2 \cos (\theta_2 + \alpha_i)}{\sin \alpha_i} - \left( \frac{\pi}{2} - (\theta_2 + \alpha_i) \right) \right] = \frac{R^2}{4G} - r_d^2 S_1 \tag{4.23}
\]

where \( n \) is the number of corners that do have an AM formed by the displacement and \( \theta_2 \) is the angle that the AM’s left at the corners by the displacement make with the wall towards the corner rather than the center which is not necessarily the contact angle. Tables (4.3), (4.4), (4.5), and (4.6) give the \( \theta_2 \) for different circumstances.

\[
L_{1s} = \frac{R}{2G} - 2r_d \sum_{i=1}^{n} \frac{\cos (\theta_2 + \alpha_i)}{\sin \alpha_i} = \frac{R}{2G} - 2r_d S_2 \tag{4.24}
\]

\[
L_{12} = 2r_d \sum_{i=1}^{n} \left( \frac{\pi}{2} - \theta_2 - \alpha_i \right) = r_d S_3 \tag{4.25}
\]

From Eqs. (4.16), (4.23), (4.24), and (4.25):

\[
r_d = \frac{R \cos \theta_1 \left[ -1 \pm \sqrt{1 + (4GD / \cos^2 \theta_2)} \right]}{4GD} \tag{4.26}
\]

where

\[
D = S_1 - 2S_2 \cos \theta_2 + S_3 \tag{4.27}
\]

From two roots given by Eq. (4.26) the \( r_d \) which is smaller than \( R \) is the valid one. The threshold capillary pressure is:

\[
P_c = \frac{\sigma}{r_d} = \frac{\sigma (1 + 2\sqrt{\pi G}) \cos \theta_1}{R} F_d(\theta_2, G, E) \tag{4.28}
\]

where
\[ F_d(\theta_2, G, E) = \frac{1 + \sqrt{1 - \left(4G \cos^2 \theta_2 \right)}}{1 + 2\sqrt{\pi G}} \]  \hfill (4.29)

\[ E = \sum_{i=1}^{3} \cos \theta_2 \frac{\cos(\theta_2 + \alpha_i)}{\sin \alpha_i} - \left[ \frac{\pi}{2} - \theta_2 - \alpha_i \right] \]  \hfill (4.30)

The \( F_d \) depends on the corner half angles and is not universal for a given \( G \). When AM’s are present at all corners, \( E \) will be dependent on only \( \theta_2 \) and \( F_d \) is universal for a given \( G \) and is given by:

\[ E = -\pi + 3\theta_2 - 3 \sin \theta_2 \cos \theta_2 + \frac{\cos^2 \theta_2}{4G} \]  \hfill (4.31)

One should note that \( F_d(\theta_2 = 0, G, E) = 1 \) regardless of number of present AM’s at the corners.

### 4.4.2 Imbibition

An event in which a non-wetting phase is displaced by a wetting phase at a positive capillary pressure is called imbibition (see Fig. (4.7)-(a)) and may be carried out with advancing contact angle by three different types of displacement mechanism: (I) piston-like, (II) snap-off, and (III) pore-body filling.

#### (I) Piston-like Mechanism (Displacement by MTM)

An MTM might be present at one end of the element filled by the non-wetting phase which might be either an old one created by drainage or a new one formed by the wetting phase arriving at the entrance of the element by an invasion percolation process [92, 255]. If there is contact angle hysteresis then when the capillary pressure drops, the MTM hinges from the receding contact angle towards the advancing value while it stays pinned at its position. If the capillary pressure is lowered enough, the advancing contact angle is reached and it is only then that the MTM invades the element with the imbibition curvature that would be different from that of drainage. If there is no contact angle hysteresis, with a small reduction in the capillary pressure the MTM enters the tube with the same curvature at which drainage took place. While the capillary pressure is reduced, the AM’s left at the corners – if there are any – adjust their contact angles to have curvatures the same as that of the invading MTM. This is while they stay pinned at their positions acquired at the end of the
Table 4.3: Threshold capillary pressures for piston-like and pore-body filling displacements with layers of the invading phase contributing to the displacement - oil to water, gas to water and gas to oil

<table>
<thead>
<tr>
<th>Item</th>
<th>Cross-section</th>
<th>Contact Angle Range</th>
<th>Equation(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Triangular</td>
<td>$\theta_{ij} &lt; \frac{\pi}{2} - \alpha_1$</td>
<td>(4.28)-(4.30)</td>
</tr>
<tr>
<td>2</td>
<td>Triangular</td>
<td>$\theta_{ij} &lt; \theta_{extreme} &amp; \theta_{ij} \geq \frac{\pi}{2} - \alpha_1$</td>
<td>(4.13)</td>
</tr>
<tr>
<td>3</td>
<td>Triangular</td>
<td>$\theta_{ij} \geq \theta_{extreme} &amp; \theta_{ij} \geq \frac{\pi}{2} - \alpha_1$</td>
<td>(4.34)-(4.40),(4.46),(4.64)-(4.66)</td>
</tr>
<tr>
<td>4</td>
<td>Square</td>
<td>$\theta_{ij} &lt; \frac{\pi}{4}$</td>
<td>(4.20)-(4.21)</td>
</tr>
<tr>
<td>5</td>
<td>Square</td>
<td>$\theta_{ij} &lt; \theta_{extreme} &amp; \theta_{ij} \geq \frac{\pi}{4}$</td>
<td>(4.13)</td>
</tr>
<tr>
<td>6</td>
<td>Square</td>
<td>$\theta_{ij} \geq \theta_{extreme} &amp; \theta_{ij} \geq \frac{\pi}{4}$</td>
<td>(4.34)-(4.40),(4.43),(4.64)-(4.66)</td>
</tr>
<tr>
<td>7</td>
<td>Circular</td>
<td>$0 \leq \theta_{ij} \leq \pi$</td>
<td>(4.13)</td>
</tr>
</tbody>
</table>

1. $\theta_1$ is the contact angle that interface moved with last time
2. $\alpha_1$ is the half angle of the sharpest corner
3. $\theta_{ij} = \theta_{ij}^{r}, ij = ow, go, gw - \theta_{ow} = \theta_{ow}^{PD}$ and $\theta_{gw} = \theta_{gw}^{PD}$ for displacement of water by gas and oil during primary drainage respectively
4. $\theta_{extreme} = \pi - \theta_3$, where $\theta_3$ is calculated using Eqs. (4.47) and (4.44) for elements with triangular and square cross-sections respectively
5. It can be either $\pi - \theta_1$ or $\theta_1$ based on the type of interface that $\theta_1$ belongs to

The threshold capillary pressure under which the piston-like imbibition may take place can be found again using the MS-P theory but the difference with the case where the theory was applied to find threshold capillary pressure of the drainage is that the three-phase contact line is fixed in the imbibition and the hinging contact angle.
Table 4.4: Threshold capillary pressures for piston-like and pore-body filling displacements with layers of the invading phase contributing to the displacement - water to oil, water to gas, and oil to gas

<table>
<thead>
<tr>
<th>Item</th>
<th>Cross-section</th>
<th>Contact Angle Range</th>
<th>Equation(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Triangular</td>
<td>$\theta_{ij} &gt; \frac{\pi}{2} + \alpha_1$</td>
<td>(4.28)-(4.30)</td>
</tr>
<tr>
<td>2</td>
<td>Triangular</td>
<td>$\theta_{ij} \geq \theta_{extreme}$ &amp; $\theta_{ij} \leq \frac{\pi}{2} + \alpha_1$</td>
<td>(4.13)</td>
</tr>
<tr>
<td>3</td>
<td>Triangular</td>
<td>$\theta_{ij} &lt; \theta_{extreme}$ &amp; $\theta_{ij} \leq \frac{\pi}{2} + \alpha_1$</td>
<td>(4.34)-(4.40),(4.46),(4.64)-(4.66)</td>
</tr>
<tr>
<td>4</td>
<td>Square</td>
<td>$\theta_{ij} &gt; \frac{3\pi}{4}$</td>
<td>(4.45)</td>
</tr>
<tr>
<td>5</td>
<td>Square</td>
<td>$\theta_{ij} \geq \theta_{extreme}$ &amp; $\theta_{ij} \leq \frac{3\pi}{4}$</td>
<td>(4.13)</td>
</tr>
<tr>
<td>6</td>
<td>Square</td>
<td>$\theta_{ij} &lt; \theta_{extreme}$</td>
<td>(4.34)-(4.40),(4.43),(4.64)-(4.66)</td>
</tr>
<tr>
<td>7</td>
<td>Circular</td>
<td>$0 \leq \theta_{ij} \leq \pi$</td>
<td>(4.13)</td>
</tr>
</tbody>
</table>

1. $\theta_1$ is the contact angle that interface moved with last time
2. $\alpha_1$ is the half angle of the sharpest corner
3. $\theta_{ij} = \theta_{ij}^e, ij = ow, go, gw$
4. $\theta_{extreme} = \theta_3$, where $\theta_3$ is calculated using Eqs. (4.47) and (4.44) for elements with triangular and square cross-sections respectively
5. It can be either $\pi - \theta_1$ or $\theta_1$ based on the type of interface that $\theta_1$ belongs to

1. **Cylindrical Elements**

The threshold capillary pressure is found using Eq. (4.13) with the advancing contact angle.

2. **Regular n-Sided Elements**

Eq. (4.16) with $r_d$ replaced by the imbibition radius $r_i$ gives the radius corresponding to the threshold capillary pressure of imbibition. The effective area
Table 4.5: Threshold capillary pressures for piston-like and pore-body filling displacements with no layers of the invading phase contributing to the displacement - oil to water, gas to water and gas to oil

<table>
<thead>
<tr>
<th>Cross-section</th>
<th>Contact Angle Range</th>
<th>Equation(s)</th>
<th>$\theta_1$</th>
<th>$\theta_2$</th>
<th>$\theta$</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triangular</td>
<td>$\theta_{ij} &lt; \frac{\pi}{2} - \alpha_1$</td>
<td>(4.28)-(4.30)</td>
<td>$\theta_{ij}$</td>
<td>$\theta_{ij}$</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Triangular</td>
<td>$\theta_{ij} \geq \frac{\pi}{2} - \alpha_1$</td>
<td>(4.13)</td>
<td>—</td>
<td>—</td>
<td>$\theta_{ij}$</td>
<td>—</td>
</tr>
<tr>
<td>Square</td>
<td>$\theta_{ij} &lt; \frac{\pi}{4}$</td>
<td>(4.20)-(4.21)</td>
<td>—</td>
<td>$\theta_{ij}$</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Square</td>
<td>$\theta_{ij} \geq \frac{\pi}{4}$</td>
<td>(4.13)</td>
<td>—</td>
<td>—</td>
<td>$\theta_{ij}$</td>
<td>—</td>
</tr>
</tbody>
</table>

1. $\theta_1$ is the contact angle that interface moved with last time

Table 4.6: Threshold capillary pressures for piston-like and pore-body filling displacements with no layers of the invading phase contributing to the displacement - water to oil, water to gas, and oil to gas

<table>
<thead>
<tr>
<th>Cross-section</th>
<th>Contact Angle Range</th>
<th>Equation(s)</th>
<th>$\theta_1$</th>
<th>$\theta_2$</th>
<th>$\theta$</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triangular</td>
<td>$\theta_{ij} &gt; \frac{\pi}{2} + \alpha_1$</td>
<td>(4.28)-(4.30)</td>
<td>$\theta_{ij}$</td>
<td>$\pi - \theta_{ij}$</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Triangular</td>
<td>$\theta_{ij} \leq \frac{\pi}{2} + \alpha_1$</td>
<td>(4.13)</td>
<td>—</td>
<td>—</td>
<td>$\theta_{ij}$</td>
<td>—</td>
</tr>
<tr>
<td>Square</td>
<td>$\theta_{ij} &gt; \frac{3\pi}{4}$</td>
<td>(4.45)</td>
<td>—</td>
<td>$\theta_{ij}$</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Square</td>
<td>$\theta_{ij} \leq \frac{3\pi}{4}$</td>
<td>(4.13)</td>
<td>—</td>
<td>—</td>
<td>$\theta_{ij}$</td>
<td>—</td>
</tr>
</tbody>
</table>

1. $\theta_1$ is the contact angle that interface moved with last time

and perimeter are given by:

$$A_{eff} = \frac{1}{2} \frac{R^2}{\tan \alpha} - \frac{1}{2} r_i b \sin(\alpha + \beta) + \frac{r_i^2 \beta}{2}$$  \hspace{1cm} (4.32)

$$P_{eff} = \left[ \frac{R}{\tan \alpha} - b \right] \cos \theta_2 + r_i \beta$$  \hspace{1cm} (4.33)

where $\theta_2$ is the contact angle of the displacement. The meniscus-apex distance $b$, see Fig. (4.8), can be calculated by (see Appendix (A)):

$$b = r_{\text{extreme}} \frac{\cos(\alpha + \theta_1)}{\sin \alpha}$$  \hspace{1cm} (4.34)

if the AM has not moved yet. The $\theta_1$ is the contact angle that the interface moved with previous time. The $r_{\text{extreme}}$ is:
Figure 4.8: Imbibition by invasion of an MTM - conditions of the AM’s at the corners [284]

\[ r_{\text{extreme}} = \frac{\sigma}{P_{c,\text{extreme}}} \]  
(4.35)

where \( P_{c,\text{extreme}} \) belongs to the last move of the interface.

If the AM has moved:

\[ b = r_i \frac{\cos(\theta_2 + \alpha)}{\sin \alpha} \]  
(4.36)

The angle \( \beta \), see Fig. (4.8), is given by:

\[ \beta = \sin^{-1} \left[ \frac{b \sin \alpha}{r_i} \right] \]  
(4.37)

if the AM has not moved yet. If the AM has moved:

\[ \beta = \frac{\pi}{2} - \theta_2 - \alpha \]  
(4.38)

The hinging contact angle is:

\[ \theta^h = \cos^{-1} \left[ \frac{r_{\text{extreme}}}{r_i} \cos(\theta_1 + \alpha_i) \right] - \alpha_i \]  
(4.39)

if the AM has not moved yet. If the AM has moved:

\[ \theta^h = \theta_2 \]  
(4.40)
In contrast to the drainage case, there is not an analytical solution to find \( r_i \). The \( r_i \) is found by an iterative procedure which solves Eq. (4.16) (with \( r_d \) replaced by the imbibition radius \( r_i \)) together with Eqs. (4.34)-(4.40) simultaneously, and then the threshold capillary pressure of imbibition will be:

\[
P_c = \frac{\sigma}{r_i}
\]

(4.41)

For advancing contact angles less than \( \frac{\pi}{2} \), the capillary pressure is always positive but it may also be positive for angles much larger \( \frac{\pi}{2} \) depending on the effective perimeter, \( P_{\text{eff}} \). The maximum advancing contact angle, \( \theta_3 \), at which imbibition (defined as \( P_c > 0 \)) may take place is when \( P_{\text{eff}} = 0 \). This happens when the AM’s are flat and have a hinging contact angle of \( \frac{\pi}{2} - \alpha \). It is given by:

\[
\theta_3 = \cos^{-1} \left[ \frac{-\cos(\alpha + \theta_1) \sin \alpha}{C_{n,r} \cos \alpha - \cos(\alpha + \theta_1)} \right]
\]

(4.42)

where the \( C_{n,r} \) is the curvature at which the saturation of the wetting phase started to increase and \( C_{n,r} \geq C_{n,d} \).

For elements with square cross section, the \( r_i \) and \( \theta_3 \) may be written as follows:

\[
\begin{align*}
    r_i &= \frac{A_{\text{eff}}}{P_{\text{eff}}} = \frac{R^2 - b \cos \theta^h + r_i^2(\frac{\pi}{2} - \theta^h - \alpha)}{2r_i \beta + 2[R - b] \cos \theta_2} \\
    \theta_3 &= \cos^{-1} \left[ \frac{-r_{\text{extreme}} \beta}{R - b} \right]
\end{align*}
\]

(4.43)

(4.44)

If the advancing contact angle is larger than \( \theta_3 \) then the capillary pressure is negative and the displacement is defined as drainage. For the threshold capillary pressures: (I) if \( \theta_2 < \frac{\pi}{2} + \alpha \) then Eq. (4.13) is used with \( \theta \) replaced by the advancing contact angle (II) but if \( \theta_2 > \frac{\pi}{2} + \alpha \) then it is given by:

\[
P_c = \frac{\sigma}{R} \left[ \cos \theta_2 - \sqrt{\frac{\tan \alpha}{2}} \left( -\sin 2\theta_2 + 2\theta_2 - 2\alpha - \pi \right) \right]
\]

(4.45)

3. **Irregular Triangular Elements**

The procedure is similar to that of the n-sided elements described above with expressions for \( r_i \) and \( \theta_3 \) replaced by the following:
where \( n \) is the number of contributing corners and \( A \) is the summation of corner areas (only those corners that do not have a contributing AM).

\[
\theta_3 = \cos^{-1}\left[\frac{-2r_{extreme}\sum_{i=1}^{n} \beta_i}{R - 2\sum_{i=1}^{3} b_i}\right]
\]

(4.47)

or

\[
\theta_3 = \cos^{-1}\left[\frac{-4G\sum_{i=1}^{3} \cos(\theta_1 + \beta_i)}{(RP_{c,extreme}/\sigma) - \cos \theta_1 + 12G \sin \theta_1}\right]
\]

(4.48)

For drainage: (I) if \( \theta_2 < \frac{\pi}{2} + \alpha \) then the threshold capillary pressure is given by Eq. (4.13) with \( \theta \) being the advancing contact angle (II) but if \( \theta_2 > \frac{\pi}{2} + \alpha \) then Eqs. (4.28)-(4.30) are used.

**(II) Snap-off Mechanism (Displacement by AM’s)**

Snap-off corresponds to an imbibition event where the non-wetting phase in the center of a pore or throat is displaced by the AM’s of the wetting phase residing in the corners or layers. This occurs only if there is no MTM present at the entrance of the element. The AM’s will be present at the corners only if the contact angle by which the element is drained be less than \( \frac{\pi}{2} - \alpha \) otherwise imbibition is possible only by invasion of an MTM.

If there is no contact angle hysteresis, when the pertinent capillary pressure is reduced, the AM’s grow and move smoothly towards the center of the element and meet to refill the element with the wetting phase.

But if there is contact angle hysteresis, when the relevant capillary pressure decreases, the invading phase starts swelling and consequently contributing AM’s - starting from the sharpest corner - may hinge and eventually move - when the hinging contact angle reaches the advancing value - towards the center to meet the other moving or pinned AM’s. When AM’s meet, the center of the element is filled spontaneously by the wetting phase. Depending on the magnitude of the advancing contact angle, snap-off can be spontaneous or forced. When it occurs at a positive threshold capillary pressure (\( \theta^a \leq \frac{\pi}{2} - \alpha_1 \)), it is an imbibition event, while it is forced (drainage) when the threshold capillary pressure is negative (\( \theta^a > \frac{\pi}{2} - \alpha_1 \)).
Snap-off is not favored over a piston-like or pore-body filling event when there is a neighboring element with the invading phase in the center that is able to carry out the displacement. The threshold capillary pressures of snap-off events in angular elements with different cross-sectional shape are given next.

1. **Regular n-Sided Elements**

For spontaneous snap-off the AM’s meet each other when they reach halfway along the sides of the element. By equating the half length of one side of the element to the meniscus-apex distance of the moving AM’s, the threshold capillary pressure is found:

\[ P_c = \frac{\sigma}{R} \left[ \cos \theta_2 - \sin \theta_2 \tan \alpha \right] \quad \theta_2 \leq \frac{\pi}{2} - \alpha \]  

(4.49)

But when the snap-off is forced, the threshold capillary pressure is a function of the curvature of the AM when it starts to move. This is because when the AM starts to move it can be unstable and may fill the element by the wetting phase immediately. The threshold capillary pressures are:

\[ P_c = \frac{\sigma}{r_{\text{extreme}}} \frac{\cos(\theta_2 + \alpha)}{\cos(\theta_1 + \alpha)} \quad \theta_2 \leq \pi - \alpha \]  

(4.50)

\[ P_c = \frac{\sigma}{r_{\text{extreme}}} \frac{-1}{\cos(\theta_1 + \alpha)} \quad \theta_2 \geq \pi - \alpha \]  

(4.51)

2. **Irregular Triangular Elements**

If the snap-off is spontaneous then depending on how large is the advancing contact angle and whether AM’s are present at all corners, different scenarios, on which moving AM meets which moving or pinned AM, are imaginable. These scenarios have different threshold capillary pressures. The event with the highest capillary pressure is most favorable. They are as follows:

\[ P_c = \frac{\sigma}{R} \left[ \cos \theta_2 - \frac{2 \sin \theta_2}{\cot \alpha_1 + \cot \alpha_2} \right] \]  

(4.52)

if the moving AM’s at corners 1 and 2 meet. If the moving AM at the corner 1 meets pinned AM at the corner 2:

\[ P_c = \frac{\sigma (\cot \alpha_1 \cos \theta_2 - \sin \theta_2)}{R (\cot \alpha_1 + \cot \alpha_2) - b_2} \]  

(4.53)
Chapter 4. Displacement Mechanisms

\[ P_c = \frac{\sigma}{R} \left[ \cos \theta_2 - \frac{2 \sin \theta_2}{\cot \alpha_1 + \cot \alpha_3} \right] \]  
(4.54)

if the moving AM’s at corners 1 and 3 meet. If the moving AM at the corner 1 meets pinned AM at the corner 3:

\[ P_c = \frac{\sigma (\cot \alpha_1 \cos \theta_2 - \sin \theta_2)}{R (\cot \alpha_1 + \cot \alpha_3) - b_3} \]  
(4.55)

\[ P_c = \frac{\sigma}{R} \left[ \cos \theta_2 - \frac{2 \sin \theta_2}{\cot \alpha_2 + \cot \alpha_3} \right] \]  
(4.56)

if the moving AM’s at corners 2 and 3 meet. If the moving AM at the corner 2 meets pinned AM at the corner 3:

\[ P_c = \frac{\sigma (\cot \alpha_2 \cos \theta_2 - \sin \theta_2)}{R (\cot \alpha_2 + \cot \alpha_3) - b_3} \]  
(4.57)

If only one corner has a contributing AM, we assume that the element is filled when the AM moves and meets a noncontributing AM at one of the other corners.

\[ P_c = \frac{\sigma (\cot \alpha_1 \cos \theta_2 - \sin \theta_2)}{R (\cot \alpha_1 + \cot \alpha_3)} \]  
(4.58)

\[ P_c = \frac{\sigma (\cot \alpha_1 \cos \theta_2 - \sin \theta_2)}{R (\cot \alpha_1 + \cot \alpha_2)} \]  
(4.59)

if only corner 1 has a contributing AM and it meets a noncontributing AM at corners 3 or 2 respectively.

\[ P_c = \frac{\sigma (\cot \alpha_2 \cos \theta_2 - \sin \theta_2)}{R (\cot \alpha_2 + \cot \alpha_3)} \]  
(4.60)

\[ P_c = \frac{\sigma (\cot \alpha_2 \cos \theta_2 - \sin \theta_2)}{R (\cot \alpha_2 + \cot \alpha_1)} \]  
(4.61)

if only corner 2 has a contributing AM and it meets a noncontributing AM at corners 3 or 1 respectively.

\[ P_c = \frac{\sigma (\cot \alpha_3 \cos \theta_2 - \sin \theta_2)}{R (\cot \alpha_2 + \cot \alpha_3)} \]  
(4.62)
\[ P_c = \frac{\sigma (\cot \alpha_3 \cos \theta_2 - \sin \theta_2)}{R (\cot \alpha_1 + \cot \alpha_3)} \]  

(4.63)

if only corner 3 has a contributing AM and it meets a noncontributing AM at corners 2 or 1 respectively.

If the contact angle is the same at all corners then Eqs. (4.58) and (4.59) give the highest capillary pressure when only corner 1 has a contributing AM.

When the snap-off is forced, as soon as the hinging contact angle of the AM at the sharpest corner becomes as large as the advancing value, it starts moving towards the center of the element while the other AM’s are pinned. This means that the absolute value of the curvature decreases. The AM is not stable and spontaneously fills the element. The threshold capillary pressure for this case are given by Eqs. (4.50) and (4.51) where \( \alpha \) is corner half angle of the sharpest corner if AM’s are present at more than one corner.

The equations to compute the threshold capillary pressures for snap-off in two- and three-phase systems with different wettability conditions are tabulated in Tables (4.7), and (4.8).

<table>
<thead>
<tr>
<th>Cross-section</th>
<th>Contact Angle Range</th>
<th>Equation(s)</th>
<th>( \theta_1 )</th>
<th>( \theta_2 )</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triangular</td>
<td>( \theta_{ij} \geq \frac{\pi}{2} + \alpha_1 )</td>
<td>(4.52)-(4.63)</td>
<td>—</td>
<td>( \pi - \theta_{ij} )</td>
<td>( \theta_{ij} ) Min ( P_{c, ij} )</td>
</tr>
<tr>
<td>Triangular</td>
<td>( \theta_{ij} \geq \alpha_1 &amp; \theta_{ij} \leq \frac{\pi}{2} + \alpha_1 )</td>
<td>(4.50) (2)</td>
<td>( \pi - \theta_{ij} )</td>
<td>—</td>
<td></td>
</tr>
<tr>
<td>Triangular</td>
<td>( \theta_{ij} &lt; \alpha_1 )</td>
<td>(4.51) (2)</td>
<td>—</td>
<td>—</td>
<td></td>
</tr>
<tr>
<td>Square</td>
<td>( \theta_{ij} &gt; \frac{3\pi}{4} )</td>
<td>(4.49)</td>
<td>—</td>
<td>( \pi - \theta_{ij} )</td>
<td>—</td>
</tr>
<tr>
<td>Square</td>
<td>( \theta_{ij} \geq \frac{\pi}{4} &amp; \theta_{ij} \leq \frac{3\pi}{4} )</td>
<td>(4.50) (2)</td>
<td>( \pi - \theta_{ij} )</td>
<td>—</td>
<td></td>
</tr>
<tr>
<td>Square</td>
<td>( \theta_{ij} &lt; \frac{\pi}{4} )</td>
<td>(4.51) (2)</td>
<td>—</td>
<td>—</td>
<td></td>
</tr>
</tbody>
</table>

1. \( \theta_1 \) is the contact angle that interface moved with last time
2. It can be either \( \pi - \theta_1 \) or \( \theta_1 \) based on the type of interface that \( \theta_1 \) belongs to

(III) Pore-body Filling Mechanism

This refers to the displacement of one phase in the center of a pore by movement from the center of adjoining throats(s). For drainage - the displacement of a wetting phase by non-wetting phase - the threshold capillary pressure is given by similar
Table 4.8: Threshold capillary pressures for snap-off displacements - water to oil, water to gas, and oil to gas

<table>
<thead>
<tr>
<th>Cross-section</th>
<th>Contact Angle Range</th>
<th>Equation(s)</th>
<th>( \theta_1 )</th>
<th>( \theta_2 )</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triangular</td>
<td>( \theta_{ij} \leq \frac{\pi}{2} - \alpha_1 )</td>
<td>(4.52)-(4.63)</td>
<td>( \theta_{ij} )</td>
<td>Max ( P_{c,ij} )</td>
<td>—</td>
</tr>
<tr>
<td>Triangular</td>
<td>( \theta_{ij} \leq \pi - \alpha_1 ) &amp; ( \theta_{ij} &gt; \frac{\pi}{2} - \alpha_1 )</td>
<td>(4.50) (2)</td>
<td>( \theta_{ij} )</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Triangular</td>
<td>( \theta_{ij} &gt; \pi - \alpha_1 )</td>
<td>(4.51) (2)</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Square</td>
<td>( \theta_{ij} \leq \frac{\pi}{4} )</td>
<td>(4.49)</td>
<td>—</td>
<td>( \theta_{ij} )</td>
<td>—</td>
</tr>
<tr>
<td>Square</td>
<td>( \theta_{ij} &gt; \frac{\pi}{4} ) &amp; ( \theta_{ij} \leq \frac{3\pi}{4} )</td>
<td>(4.50) (2)</td>
<td>( \theta_{ij} )</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Square</td>
<td>( \theta_{ij} &gt; \frac{3\pi}{4} )</td>
<td>(4.51) (2)</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
</tbody>
</table>

1. \( \theta_1 \) is the contact angle that interface moved with last time
2. It can be either \( \pi - \theta_1 \) or \( \theta_1 \) based on the type of interface that \( \theta_1 \) belongs to

expressions for piston-like advance. For imbibition - the displacement of a non-wetting phase by a wetting phase - the displacement is controlled by the largest radius of curvature. The threshold capillary pressure depends on inscribed radius of the pore-body and the number of neighboring throats that either do not hold the invading phase in the center or can not contribute to the displacement as they might be trapped. For a pore with coordination number \( m \) - number of throats connected to each pore - \( (m - 1) \) pore-body filling events are possible and are called \( I_n \), where \( n \) is the order of filling and \( 1 \leq n \leq m - 1 \) (see Fig. (4.9)). For instance, imagine an oil filled water-wet circular cross-section pore with 8 throats connected to it. If two of the throats contain oil in the center, two gas, one trapped water, and only three continuous water, then for the water invasion of the pore: \( n = 2 + 2 + 1 = 5 \). One should note that when \( n = 1 \), the displacement is a piston-like event with the corresponding threshold capillary pressures (see sections (4.4.1) and (4.4.2)) [57, 76]. Blunt [285] and Øren et al. [76] have proposed different empirical models to compute threshold capillary pressure of the pore-body filling as follows:

\[
P_c = \frac{2\sigma \cos \theta}{R_p} - \sigma \sum_{i=1}^{n} e_i x_i \]  
(4.64)

\[
P_c = \frac{2\sigma \cos \theta}{R_p + \sum_{i=1}^{n} e_i R_{t,i} x_i} \]  
(4.65)

\[
P_c = \frac{\sigma(1 + 2\sqrt{\pi G}) \cos \theta}{R_p + \sum_{i=1}^{n} e_i R_{t,i} x_i} \]  
(4.66)
Figure 4.9: Different pore-body filling events for imbibition in a pore with coordination number 4. For $I_n$, $n$ means number of neighboring throats that either do not hold the invading phase in the center or cannot contribute to the displacement as they might be trapped.

where $n$ indicates the order of the filling and is the number of throats that do not take part in the invasion of the bore body, $R_{t,i}$ are the inscribed radii of the such throats, $x_i$ are random numbers, $R_p$ is the inscribed radius of the pore, and $e_i$ are
predefined arbitrary parameters. Eqs. (4.64)- (4.66) show that pore-body filing is favored when \( n \) is small.

The \( e_1 = 0 \) and \( e_2 - e_n = 0.015 \, \mu m^{-1} \) to be used in Eq. (4.64) [285]. The \( e_1 = 0, e_2 = 0.5, e_3 = 1, e_4 = 2, e_5 = 5, \) and \( e_6 = 10 \) to be used in Eqs. (4.65) and (4.66). In this work, we use Eq. (4.66).

The equations to compute threshold capillary pressures for piston-like and pore-body filling displacements in two- and three-phase systems with different wettability conditions are listed in Tables (4.3), (4.4), (4.5), and (4.6).

4.5 Layer Collapse and Formation

Piston-like and snap-off displacements – if the pertinent contact angles, capillary pressures, and corner half angles permit – allow the displaced phase to remain as layer(s) sandwiched between fluids in the corner(s) and center of the element. The formation of layers in an element is also possible by displacement from fluids residing in the layers or center of the neighboring elements. The layers may spontaneously collapse by an increase in pressure of the fluids on either side of the layer. When a layer collapse event takes place, one of the two AM’s bounding the layer will hinge and/or move towards the other one. However, there are cases where both AM’s contribute into the layer collapse event, e.g. oil layer collapse event by water at a corner in a strongly oil-wet element (see chapter (5) for example configurations).

Based on whether the fluids residing on two sides of the layer are the same, layers may be categorized into two main groups; (I): Identical fluids, (II): Different fluids. The displacement history to form such layers in systems with different wettability and spreading coefficient will be discussed later. Here, the stability of the layers, i.e. the threshold capillary pressure for layer collapse and formation events, in each category is discussed [260, 261]:

4.5.1 Identical Fluids on Two Sides of a Layer

Fig. (4.10) illustrates this case. Since fluids residing on both sides of the layer are identical, when the capillary pressure of the fluid pair changes both bounding AM’s contribute to the stability of the layer. The layer stays stable until two AM’s touch each other at point \( C \) when the layer collapses immediately and the corner is filled completely by phase-2. This is the concept that is used to find the threshold capillary pressure of collapse (or formation) of such a layer and is given by (see Appendix (A) for derivation):
4.5.2 Different Fluids on Two Sides of a Layer

Since the layer is surrounded by two different fluids, a change in the pressure of either fluids can result in layer collapse. In other words, the AM’s bounding the layer act independently. Depending on the magnitude of the angle that each AM makes with the wall, two main groups of collapse scenario are imaginable:

1. $\theta_1 \leq \theta_2$

Fig.(4.11) illustrates the case. The stability of the layer depends on the ratio of the curvature of the two AM’s bounding the layer:

$$\frac{r_1}{r_2} = \frac{\sigma_1 P_{c,2}}{\sigma_2 P_{c,1}}$$

(4.69)
where $\sigma_1$ and $\sigma_2$ are the interfacial tensions of the bounding interfaces of the layer and $P_{c,1}$ and $P_{c,2}$ are pertinent capillary pressures. The layer is stable until three-phase contact points meet each other (see Fig. (4.11)-(b)). This means that the layer collapses when the meniscus-apex distance, $b$, for two AM’s become equal. Using Eq. (4.34) for meniscus-apex distance of each AM gives:

$$r_1 \frac{\cos(\theta_1 + \alpha)}{\sin \alpha} = r_2 \frac{\cos(\theta_2 + \alpha)}{\sin \alpha}$$

(4.70)
\[ R_c = \frac{r_1}{r_2} = \frac{\cos(\theta_2 + \alpha)}{\cos(\theta_1 + \alpha)} \] (4.71)

Then the two threshold capillary pressures of the layer collapse corresponding to the invasions by two surrounding fluids can be found by:

\[ P_c = \frac{\sigma_1 P_{c,2}}{\sigma_2 R_c} \] (4.72)

\[ P_c = \frac{\sigma_2 P_{c,1} R_c}{\sigma_1} \] (4.73)

2. \( \theta_1 > \theta_2 \)

Fig. (4.12) illustrates the case. The layer is stable until two AM’s meet at their centers. The ratio of curvature of two AM’s at the collapsing point is found by equating the center-apex distance of one of the AM’s to that of the other one (see Appendix (A) for derivation of center-apex distance for an AM):

\[ -r_1 \left[ 1 - \frac{\cos \theta_1}{\sin \alpha} \right] = -r_2 \left[ 1 - \frac{\cos \theta_2}{\sin \alpha} \right] \] (4.74)

Reordering Eq. (4.74) gives:

\[ R_c = \frac{r_1}{r_2} = \frac{\sin \alpha - \cos \theta_2}{\sin \alpha - \cos \theta_1} \] (4.75)

The two threshold capillary pressures are then found from Eqs. (4.72) and (4.73).

One should not that if the curvature of any of the AM’s is negative (see Fig. (4.13)-(a)), the threshold capillary pressures are found using the same procedure as above.

As we will show the relevant fluid configurations later, it is also possible to have a second layer sandwiched between the fluids residing in the center of the element and the first layer (see Fig. (4.13)-(b)). The stability analysis for the second layer is also the same as that of the first layer.
Figure 4.12: A layer sandwiched between different fluids residing in the corner and center ($\theta_1 > \theta_2$) (a) the layer before collapse (b) position of the AM's at the moment of collapse
Figure 4.13: A layer sandwiched between different fluids (a) one of the AM’s has negative curvature (b) a second layer sandwiched between fluids in the center and the first layer
Chapter 5

Two- and Three-Phase Fluid Generic Configurations

Different oil/water, gas/water and gas/oil contact angles and interfacial tensions make it theoretically possible to accommodate fluids in the corners of the pore space with different configurations. Figs. (5.1) and (5.2) illustrate all the possible generic one-, two- or three-phase configurations for a single corner of an angular pore or throat with any values of two and three phase contact angles - the whole pore or throat is composed of no (circle), three (triangular) or four (square) corners. In all three phase configurations, the constraint among the three-phase contact angles given by Eq. 2.6 is satisfied. The configurations are equally applicable for any other angular pore or throat with any number of corners. Altered wettability surfaces are shown by thicker lines. A configuration can accommodate one, two or three fluids. A fluid located in corner, layer or center of a configuration is called a phase location. For example, configuration group $F$ has three phase locations, water in a corner, an oil layer and gas in the center. For single phase configurations - group A - only one phase location, i.e. water in the center, is considered. Every phase location has a flag associated with it indicating whether the fluid that it accommodates is continuous or trapped. If it is trapped then the trapped cluster number that the phase location belongs to is also attached to it. A cluster of phase locations is trapped when it does not stretch to the inlet and/or outlet, if it does then it is considered continuous. We shall discuss the details of how the phase locations are assigned to the clusters and how their continuity are determined later in this paper.

For elements with a circular cross-section, only one phase may occupy the pore or throat. For square and triangular cross-sections, the phase in the middle of the element must be the same for each corner, but different corners may have different
Table 5.1: The range of contact angles for which each configuration in Figs. (5.1) and (5.2) can exist.

<table>
<thead>
<tr>
<th>Configuration</th>
<th>$\theta_{ow}$</th>
<th>$\theta_{gw}$</th>
<th>$\theta_{go}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A-1, A-2</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
</tr>
<tr>
<td>B-1, B-2</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
</tr>
<tr>
<td>C-1, C-2</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
</tr>
<tr>
<td>C-3, C-4</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
</tr>
<tr>
<td>D-1, D-2</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
</tr>
<tr>
<td>E-1, E-2</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
</tr>
<tr>
<td>F-1, F-2</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
</tr>
<tr>
<td>F-3, F-4</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
</tr>
<tr>
<td>G-1, G-2</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
</tr>
<tr>
<td>G-3, G-4</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
</tr>
<tr>
<td>H-1, H-2</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
</tr>
<tr>
<td>I-1, I-2</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
</tr>
<tr>
<td>J-1, J-2</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
<td>$\leq \frac{\pi}{2} - \alpha$</td>
</tr>
<tr>
<td>K-1, K-2</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
<td>$\geq \frac{\pi}{2} + \alpha$</td>
</tr>
</tbody>
</table>

configurations, depending on the corner angle. However, in a single pore or throat, the contact angles in each corner are the same. Table (5.1) lists the range of contact angles for which each configuration in Figs. (5.1) and (5.2) may exist. A capillary pressure between any two phases, i.e. $P_{cij}$, is defined as $P_i - P_j$. The radius of curvature $r$ of the interface between two phases $i$ and $j$ in Figs. (5.1) and (5.2) is related to the capillary pressure by Eq. (4.9).

One should note that when Eq. (4.9) is applied to calculate the radius of curvature for an interface, $P_i$ and $P_j$ may be different from the inlet or outlet pressures, i.e. global absolute pressures, of the two phases if that phase is trapped. In such cases, the absolute pressures of the trapped clusters are used.

## 5.1 Definitions

A displacement is defined as a change (see later for details) in generic configuration groups (indicated by letters in Figs. (5.1) and (5.2)) in an element by an eligible displacing phase which is the phase residing in a phase location that is topologically capable of doing the change(s). Based on the type of displacement, i.e. piston-like, snap-off or layer collapse and formation, this can be a configuration change in one or all corners of the element. For every configuration changes, there might be different
Figure 5.1: One- and two-phase configurations for a single corner
Figure 5.2: Three phase configurations for a single corner
ways to carry out the displacement. In such a case each one is treated as a separate displacement. For instance, imagine configuration group change $F$ to $C$ due to oil layer collapse (see later for details). The change could be carried out either by invasion of water in the corner or gas in the center which corresponds to a decrease in $P_{c,ow}$ or an increase in $P_{c,go}$ respectively. These two ways are treated as two separate displacements. A displacement occurs at a threshold capillary pressure. The network model simulates a sequence of displacements induced by imposed changes in phase pressures.

For every displacement, there are two phase locations associated with it. One accommodates the displacing fluid of the displacement, i.e. displacing phase location, and the other one accommodates the displaced fluid, i.e. displaced phase location. For example, consider configuration group change $B$ to $C$ by an invasion of gas residing in the center of a neighboring pore into oil in the center of a throat. The displacing and displaced phase locations for this displacement are the gas center in the pore and the oil center in the throat, respectively.

A process is defined as a consecutive sequence of displacements that involve a change in the same capillary pressure in the same direction. The change in capillary pressure, $P_{c,ij}$, is due to injection of either phase $i$ or $j$. For instance, primary drainage is a process involving an increase in oil/water capillary pressure. Water flooding is a different process involving a decrease in oil/water capillary pressure.

Because of contact angle hysteresis, the contact angle can hinge between its receding and advancing values without the contact line moving and is called hinging contact angle. Every interface has two contact angles associated with it: (I): a target contact angle, which is the contact angle that the new AM’s will have just after a displacement in that element. The existing (old) AM’s might reach this value just before displacement. This contact angle may be different from one process to another. For example, imagine a configuration group change A to B by oil primary drainage. The new AM’s in configuration group B will have the target contact angle of $\theta_{ow}^{PD}$. The target contact angle during water flooding for an existing oil/water interface in configuration group B is $\theta_{ow}^a$. (II): the furthest contact angle, which is the maximum, or minimum, hinging contact angle that an interface reached during the last process when the pertinent capillary pressure was changing. This may not necessarily be the same as the target contact angle. For instance, imagine a water flooding is being carried out after primary drainage in a strongly oil-wet system with $\theta_{ow}^a = \pi$. When the oil/water capillary pressure decreases the oil/water AM’s start hinging from $\theta_{ow}^{PD}$ towards the target contact angle ($\theta_{ow}^a$). If water flooding
is stopped at some stage then there might be AM’s, particularly in wide corners, that have not reached the advancing value yet. For such AM’s the last hinging contact angle is considered as its furthest contact angle. For the AM’s that reached the target contact angle, the furthest contact angle will be the same as the target contact angle. For the next process, for instance gas injection, the interface may start hinging from this furthest value towards the new target contact angle.

Every AM has a meniscus-apex distance, i.e. $b$ (see Fig. (6.5)), associated with it and is calculated using Eq. (4.34) to be used in area and threshold capillary pressure calculations. $b$ changes whenever the AM moves.

### 5.2 Configuration Changes

Here we presents points that one should consider to record configuration changes:

1. After every configuration group change, there will be some new displacements to be considered. These displacements are added into the *appropriate* lists (see details later). For every new displacement, the appropriate list is determined knowing what phase is displacing and whether the phases occupying the displacing and displaced phase locations are continuous or trapped.

2. Once a configuration group is changed, the type and the number of AM’s in the corner may also change. There are two possibilities: *(I)* the number of AM’s is the same but the type has been changed - fluid on one side of the AM has been replaced by a new fluid. For example, consider configuration group change $B$ to $C$. In this case the furthest contact angle of the AM before the configuration change is given to the AM after the configuration change and then the interface may hinge from its furthest value towards the target contact angle (due to the changes in the pertinent capillary pressure) and ultimately move. This will prevent any volume error of the fluid residing on the other side of the AM - i.e. water in the corner in example above. We may call this case an *old* AM case. *(II)* the number of AM’s in the corner has either increased or decreased. If it has increased by piston-like or snap-off displacement then the *new* AM will have the furthest contact angle the same as the target value and moves according to the changes in the relevant capillary pressure. For example, imagine configuration group change $B$ to $F$ by piston-like invasion of gas. The furthest contact angle of the new gas/oil AM will be $\theta_{go}$. If the number of AM’s has increased by layer formation, see point (4). And finally
if the number of AM’s has decreased (by layer collapse) then it is treated as an old AM case. An example is the gas layer collapse event by water or oil in configuration group $G$ to form an oil/water AM in configuration group $B$.

3. An AM moves once the hinging contact angle becomes as large as the advancing contact angle of the AM (when the related capillary pressure is decreasing) or as small as the receding contact angle of the AM (when the related capillary pressure increasing). Once the AM moves, the new $b$ is calculated. The value of $b$ is updated as long as the AM keeps moving by changes in the pertinent capillary pressure in the same direction as when it started to move.

4. When a new layer formation event is considered, one should note that there are two displacements that may represent such an event and both must be added to the lists. Imagine an AM where a layer is going to be formed around it. The first displacement may displace some of the fluid above the AM to accommodate the layer while the other one displaces some of the fluid below the AM to make space for the layer. For an example, consider a gas layer formation resulting in configuration group change $B$ to $G$. The two displacements may take place only if $\theta_{go} > \frac{\pi}{2} + \alpha$. By the first one, gas may displace some of the water in the corner to open enough space for the layer while forming a new gas/water interface for which the meniscus-apex distance is calculated. Both target and furthest contact angles of the gas/water interface will be $\theta_{gw}^r$. One should note that the gas/oil interface, in the new configuration, is treated as an old AM. $\pi$ minus the furthest contact angle of the oil/water interface before the configuration group change is given as the furthest contact angle of the gas/oil interface. Then the gas/oil interface may start hinging from its furthest value towards $\theta_{go}^r$ if the gas/oil capillary pressure is increased during the process. Also the meniscus-apex distance of the oil/water interface is given to the gas/oil interface. The threshold capillary pressure of the layer formation is calculated using $\theta_{gw}^r$ and the furthest value of the gas/oil interface. But by the second displacement, gas may displace some of the oil in the center to accommodate itself as a layer. A new gas/oil interface is created and so its meniscus-apex distance is calculated. Both target and furthest contact angles of the gas/oil interface will be $\theta_{go}^r$. The gas/water interface is considered as an old AM and the furthest contact angle of the oil/water interface before the configuration change is used as the furthest contact angle of the gas/water interface. Then the gas/water interface may hinge from its furthest
value towards $\theta_{gw}$ if the gas/water capillary pressure is increased during the process. Also the meniscus-apex distance of the oil/water interface is given to the gas/water interface. The threshold capillary pressure of the layer formation is calculated using $\theta_{go}$ and the furthest contact angle of the gas/water interface.

5. Once a displacement changes a configuration group, there might be other displacements that had been considered for the same configuration group change but through other routes. These displacements are not valid anymore and are omitted from the lists.

6. New piston-like displacements are considered only if the configuration group change has replaced the fluid at the center of the element and there is at least one different phase residing in the center of the neighboring elements.

7. New layer formation displacements are added to the lists only when the phase that is expected to form the layer is located in neighboring element(s) in the center or layer.

8. New snap-off displacements are added to the list as soon as a new AM is formed or the type of an old AM has changed. One should note that this is considered only if the fluid in the center of the element is residing on one side of the AM. A new layer collapse event is considered only if a new layer forms.

9. Once a new configuration group is formed, it might allow new displacements in the neighboring elements. For instance, imagine a piston-like displacement by gas changes configuration group $B$ to $C$ in an element. Formation of a gas layer in the corners, as well as displacement of oil and water in the center, of the neighboring elements are considered if topological and contact angle circumstances permit.

10. There are some configurations (see Figs. (5.1) and (5.2)) that have more than one AM. The AM’s and also layers are numbered from the apex downwards.

Configuration changes make it possible to simulate any sequence of different fluid injection in two- and three-phase systems. New configuration(s) to form by a displacement can be determined knowing the $\theta_{ow}$, $\theta_{gw}$, and $\theta_{go}$ of the displacement and the invading fluid. All changes that can happen to each configuration group, i.e. displacements, during different two- and three-phase processes are presented in detail next.
5.2.1 Configuration Group A

An oil layer formation event may change configuration group A to D. Both target and furthest contact angles of both new oil/water interfaces will be $\theta_{ow}^r$. This may happen only when $\theta_{ow}^r \geq \frac{\pi}{2} + \alpha$. Since the interfaces are being freshly created, the meniscus-apex distance ($b$), which is the same for both interfaces, is calculated. The new displacements to add are: oil layer collapse by water in the corner, oil layer collapse by water in the center, and snap-off of water in the center by the oil in the layer. A very similar event by gas, i.e. gas layer formation, may change configuration group A to E. For both gas/water interfaces, target and furthest contact angles would be $\theta_{gw}^r$. For the new interfaces, $b$ is calculated. This may happen only when $\theta_{gw}^r \geq \frac{\pi}{2} + \alpha$. The new displacements to add are: gas layer collapse by water in the corner, gas layer collapse by water in the center, and the snap-off of water in the center by the gas. Piston like displacement of water by oil may change configuration group A to B. Both target and furthest contact angles of the oil/water interface would be $\theta_{ow}^r$. One should note that if oil has not touched the element before, i.e. wettability has not been altered, then $(\theta_{ow})^{PD}$ is used instead. The new displacements to add are: snap-off of oil in the center by the water in the corner, piston-like displacement of oil in the center by the other phases, i.e. gas and/or water, possibly located in the center of the neighboring elements. For the new oil/water interface, $b$ is calculated. A similar displacement by gas may change configuration group A to C. Both target and furthest contact angles of the gas/water interface will be $\theta_{gw}^r$. It should be noted that if the wettability of the element has not been altered before, then $(\theta_{gw})^{PD}$ is used instead. The new displacements to add are: snap-off of gas in the center by water in the corner, piston-like displacement of gas in the center by the other phases, i.e. oil and/or water. For the new gas/water interface, $b$ is calculated. Fig. (5.3)-(a) indicates all the possible configuration changes that might happen to configuration A.

5.2.2 Configuration Group B

A piston-like or snap-off displacement by water may change configuration group B to A. The contact angle at which the displacement is carried out is $\theta_{ow}^a$. This happens only if $\theta_{ow}^a < \frac{\pi}{2} + \alpha$. No new interfaces are created. The new displacements to add are: oil layer formation, gas layer formation, and piston-like displacement of water in the center by oil and/or gas. If $\theta_{ow}^a > \frac{\pi}{2} + \alpha$ then a piston-like or snap-off displacement by water may change configuration group B to D. A new oil/water
interface is formed and so $b$ is calculated. The new displacements to add are: oil layer collapse by water in the corner, oil layer collapse by water in the center, snap-off of water in the center by the oil in the layer, and piston-like displacement of
water in the center by oil and/or gas.

A piston-like displacement by gas may change configuration group $B$ to $C$. The contact angle to carry out the displacement is $\theta_{go}^r$. This may happen only if $\theta_{go}^r > \frac{\pi}{2} - \alpha$. The gas/water interface in the new configuration is not considered as a new interface. It is assigned the $b$ and the furthest contact angle of the oil/water interface before the configuration change. The interface may hinge from its furthest contact angles towards $\theta_{gw}^r$ by an increase in gas/water capillary pressure. The new displacements to add are: snap-off of gas in the center by the water in the corner, and piston-like displacement of gas in the center by water and/or oil. The piston-like displacement by gas may change the configuration group $B$ to $F$ when $\theta_{go}^r \leq \frac{\pi}{2} - \alpha$. A new gas/oil interface is formed for which both target and furthest contact angles will be $\theta_{go}^r$. $b$ is calculated for the gas/oil interface. The new displacements to add are: oil layer collapse by water in the corner, oil layer collapse by gas in the center, snap-off of gas in the center by the oil in the layer, and piston-like displacement of gas in the center by water and/or oil.

A gas layer formation event may change configuration group $B$ to $G$. The new displacements to add are: gas layer collapse by water in the corner, gas layer collapse by oil in the center, and snap-off oil in the center by gas in the layer. Gas layer formation may also change configuration group $B$ to $I$. The contact angle by which the displacement is carried out is $\theta_{gw}^r$. Two new gas/water interfaces are formed and thus the $b$ that is calculated will be the same for both. Target and furthest contact angles are $\theta_{gw}^r$ for the new interfaces. This may happen only when $\theta_{gw}^r \geq \frac{\pi}{2} + \alpha$. The new displacements to add are: the gas layer collapse by water in the corner, the gas layer collapse by water in the second layer, water layer collapse by gas in the first layer, water layer collapse by oil in the center, and snap-off of oil in the center by water in the second layer. Fig. (5.3)-(b) shows the possible configuration changes to configuration $B$.

### 5.2.3 Configuration Group $C$

A piston-like or snap-off displacement by water may change configuration group $C$ to $A$. The contact angle that is used to carry out the displacement is $\theta_{gw}^a$. This occurs only if $\theta_{gw}^a < \frac{\pi}{2} + \alpha$. No new interface is formed. The new displacements to add are: oil layer formation, gas layer formation, and piston-like displacement of water in the center by oil and/or gas. If $\theta_{gw}^a > \frac{\pi}{2} + \alpha$ then a piston-like or snap-off displacement by water may change configuration group $C$ to $E$. A new gas/water interface is created and thus $b$ is calculated. The new displacements to add are: gas
layer collapse by water in the corner, gas layer collapse by water in the center and water and snap-off of water in the center by gas in the layer.

A piston-like displacement by oil could change configuration group $C$ to $B$. The contact angle at which the displacement takes place is $\theta_{go}^a$. This may happen only if $\theta_{go}^a < \frac{\pi}{2} + \alpha$. The oil/water interface is not treated as a new interface. $b$ and the furthest contact angle of the gas/water interface before the configuration change are assigned to the oil/water interface. The oil/water interface may hinge from its furthest value towards $\theta_{ow}^r$ due to an increase in oil/water capillary pressure. The new displacements to add are: snap-off of oil in the center by the water in the corner, and piston-like displacement of oil in the center by water and/or oil. The piston-like displacement by oil could change the configuration group $C$ to $G$ when $\theta_{go}^a \geq \frac{\pi}{2} + \alpha$. A new gas/oil interface is created and so $b$ is calculated. Both target and furthest contact angles will be $\theta_{go}^o$. The new displacements to add are: gas layer collapse by water in the corner, gas layer collapse by oil in the center, snap-off of oil in the center by the gas in the layer, and piston-like displacement of oil in the center by water and/or gas.

Oil layer formation could change configuration group $C$ to $F$. As we described before, two displacement can cause this change. The two contact angles to be used are $\theta_{ow}^r$ and $\theta_{go}^a$. The new displacements to add are: oil layer collapse by water in the corner, oil layer collapse by gas in the center, and snap-off of gas in the center by oil in the layer. Oil layer formation may also change configuration group $C$ to $H$. The contact angle used to carry out the displacement is $\theta_{ow}^r$. The displacement creates two fresh oil/water interfaces and so the same $b$ is calculated for both. Both target and the furthest contact angles are $\theta_{ow}^r$ for the new interfaces. This may occur only if $\theta_{ow}^r \geq \frac{\pi}{2} + \alpha$. The new displacements to add are: oil layer collapse by water in the corner, oil layer collapse by water in the second layer, water layer collapse by oil in the first layer, water layer collapse by gas in the center, and snap-off of gas in the center by water in the second layer. Fig. (5.4)-(a) summarizes the possible configuration changes to configuration group $C$.

### 5.2.4 Configuration Group $D$

An oil layer collapse event by water may change configuration group $D$ to $A$. The new displacements to add are: oil layer formation, and gas layer formation.

A piston-like or snap-off displacement by oil may change configuration group $D$ to $B$. The contact angle at which the displacement is carried out is $\theta_{ow}^r$. An oil/water interface is omitted. The contact angle of the oil/water interface in the
Figure 5.4: Possible configuration changes to configurations (a) C and (b) D.
corner may hinge from its furthest value to $\theta_{ow}^r$. The new displacements to add are: snap-off of oil in the center by water in the corner, two possible gas layer formations and piston-like displacement of oil in the center by gas and/or water.

A piston-like displacement by gas may change configuration group $D$ to $F$. The contact angle used for the displacement is $\theta_{gw}^r$. This may happen only if $\theta_{go}^r < \frac{\pi}{2} - \alpha$. The gas/oil interface is not considered as a new interface. The furthest contact angle and $b$ of the second oil/water interface before the configuration change are assigned to the gas/oil interface. Then the gas/oil interface may hinge from its furthest value towards $\theta_{go}^r$ due to an increase in the gas/oil capillary pressure. The new displacements to add are: snap-off of gas in the center by oil in the layer, oil layer collapse by gas in the center, water layer formation as a second layer, and piston-like displacement of the gas in the center by water and/or oil. If $\theta_{go}^r < \frac{\pi}{2} - \alpha$ then the piston-like displacement may change the configuration $D$ to $C$. The gas/water interface is not treated as a new interface and gets the furthest contact angle and $b$ of the first oil/water interface before the configuration change. The gas/water interface may then hinge from its furthest value towards $\theta_{gw}^r$ due to an increase in gas/water capillary pressure. The new displacements to add are: snap-off of gas in the center by water in the corner, and piston-like displacement of gas in the center by water and/or oil.

A piston-like displacement by gas may convert configuration group $D$ to $H$. The contact angle at which the displacement takes place is $\theta_{gw}^r$ which is considered to be both the furthest and target contact angles for the fresh gas/water interface. $b$ is calculated. This event happens only if $\theta_{gw}^r < \frac{\pi}{2} - \alpha$. The new displacements to add are: water layer collapse by oil in the first layer, water layer collapse by gas in the center, snap-off of gas in the center by water in the second layer, and piston-like displacement of gas in the center by oil and/or water.

A gas layer formation event may change configuration group $D$ to $K$. As mentioned before, two displacements may carry out such a change. The two contact angles to use in the two displacements are $\theta_{gw}^r$ and $\theta_{go}^r$. This may occur only if $\theta_{go}^r \geq \frac{\pi}{2} + \alpha$. The new displacements to add are: gas layer collapse by water in the corner, gas layer collapse by oil in the second layer, and oil layer collapse by gas in the first layer. Gas layer formation may also change configuration group $D$ to $J$. The two contact angles applied in two displacements are $\theta_{gw}^r$ and $\theta_{go}^r$. The event may take place only if $\theta_{go}^r \geq \frac{\pi}{2} - \alpha$ and $\theta_{gw}^r \geq \frac{\pi}{2} + \alpha$. The new displacements to add are: gas layer collapse by water in the center, gas layer collapse by oil in the first layer, oil layer collapse by gas in the second layer, and snap-off of water in the center by gas.
in the second layer. Fig. (5.4)-(b) summarizes the possible configuration changes to configuration group D.

5.2.5 Configuration Group E

Gas layer collapse by water could change configuration group E to A. The new displacements to add are: oil layer formation, and gas layer formation.

A piston-like or snap-off displacement by gas could change configuration group E to C. The contact angle for the displacement is: $\theta_{gw}^r$. A gas/water interface is omitted. The gas/water interface in the corner may hinge from its furthest value towards $\theta_{gw}^r$. The new displacements to add are: snap-off of gas in the center by water in the corner, two possible oil layer formations, and piston-like displacement of gas in the center by oil and/or water.

A piston-like displacement by oil may change configuration group E to I. The contact angle to use when the displacement is carried out is $\theta_{ow}^r$ which is considered as both the furthest and target contact angles for the new oil/water interface. $b$ is calculated. The displacement happens only if $\theta_{ow}^r < \frac{\pi}{2} - \alpha$. The new displacements to add are: water layer collapse by oil in the center, water layer collapse by gas in the first layer, snap-off of oil in the center by water in the second layer, and piston-like displacement of oil in the center by gas and/or water. If $\theta_{ow}^r \geq \frac{\pi}{2} - \alpha$ and $\theta_{go}^a \geq \frac{\pi}{2} + \alpha$ then the piston-like displacement by oil may change configuration group E to G. The contact angles used for the displacement are $\theta_{ow}^r$ and $\theta_{go}^a$. The gas/oil interface is not treated as a new interface. The furthest contact angle and $b$ of the second gas/water interface before the configuration change are given to the gas/oil interface. Then the gas/oil interface can hinge from its furthest value towards $\theta_{go}^a$ due to a decrease in gas/oil capillary pressure. The new displacements to add are: snap-off of oil in the center by gas in the layer, gas layer collapse by oil in the center, water layer formation as a second layer, and piston-like displacement of the oil in the center by water and/or gas. If $\theta_{go}^a < \frac{\pi}{2} + \alpha$ then piston-like displacement may change the configuration E to B. The furthest contact angle and $b$ of the first gas/water interface before the configuration change are assigned to the oil/water interface as is not considered as a new interface. The oil/water interface may then hinge from its furthest value towards $\theta_{ow}^r$ due to an increase in oil/water capillary pressure. The new displacements to add are: snap-off of oil in the center by water in the corner, and piston-like displacement of the oil in the center by water and/or gas.

An oil layer formation event can change configuration group E to K. Two displacements may cause such an event. The two contact angles at which the dis-
Figure 5.5: Possible configuration changes to configurations (a) $E$ and (b) $F$
placements may occur are $\theta_{ow}$ and $\theta_{go}$. This may occur only if $\theta_{go} \geq \frac{\pi}{2} + \alpha$ and $\theta_{ow} \geq \frac{\pi}{2} + \alpha$. The new displacements to add are: oil layer collapse by water in the center, oil layer collapse by gas in the first layer, gas layer collapse by oil in the second layer, and snap-off of water in the center by oil in the second layer. Oil layer formation can also convert configuration group $E$ to $J$. The two contact angles used in these two displacements are $\theta_{ow}$ and $\theta_{go}$. The displacement may occur only if $\theta_{go} \geq \frac{\pi}{2} + \alpha$. The new displacements to add are: oil layer collapse by water in the center, oil layer collapse by gas in the first layer, gas layer collapse by oil in the second layer, and gas layer collapse by oil in the first layer. Fig. (5.5)-(a) indicates the possible configuration changes to configuration group $E$.

### 5.2.6 Configuration Group $F$

An oil layer collapse event may change configuration group $F$ to $C$. The new displacements to add are: oil layer formation, and snap-off of gas in the center by water in the corner.

A piston-like or snap-off displacement by oil may change configuration group $F$ to $B$. The contact angle for the displacement is $\theta_{go}^a$. No fresh interface is formed. The new displacements to add are: snap-off of oil in the center by water in the corner, two gas layer formations, and piston-like displacement of oil in the center by water and/or gas.

A piston-like displacement by water may change configuration group $F$ to $J$. The contact angle used for the displacement is $\theta_{gw}^a$. This may happen only if $\theta_{gw}^a \geq \frac{\pi}{2} + \alpha$. A new gas/water interface is created and thus $b$ is calculated. Both target and furthest contact angles will be $\theta_{gw}^a$. The new displacements to add are: gas layer collapse by oil in the first layer, gas layer collapse by water in the center, snap-off of water in the center by the gas in the layer, and piston-like displacement of water in the center by oil and/or gas. If $\theta_{gw}^a < \frac{\pi}{2} + \alpha$ then piston-like displacement by water may change configuration group $F$ to $D$. The contact angles used for the displacement are $\theta_{gw}^a$ and $\theta_{ow}^a$. This may occur only if $\theta_{ow}^a \geq \frac{\pi}{2} + \alpha$. The second oil/water interface is not considered as a new interface. The furthest contact angle and $b$ of the the gas/oil interface before the configuration change are assigned to the second oil/water interface. The oil/water interface may hinge from its furthest value towards $\theta_{ow}^a$ due to a decrease in oil/water capillary pressure. The new displacements to add are: snap-off of water in the center by oil in the layer, oil layer collapse by water in the center, two gas layer formation events, and piston-like displacement of the water in the center by gas and/or oil. If $\theta_{ow}^a < \frac{\pi}{2} + \alpha$ then the piston-like
displacement may change the configuration $F$ to $A$. No new interface is formed. The new displacements to add are: oil layer formation, gas layer formation, and piston-like displacement of water in the center by oil and/or gas.

A water layer formation event may change configuration group $F$ to $H$. Two displacements may carry out such a change. The two contact angles to use are $\theta_{gw}^a$ and $\theta_{ow}^a$. This may occur only if $\theta_{ow}^a \geq \frac{\pi}{2} + \alpha$ and $\theta_{gw}^a < \frac{\pi}{2} - \alpha$. The new displacements to add are: oil layer collapse by water in the second layer, water layer collapse by oil in the first layer, water layer collapse by gas in the center, and snap-off of gas in the center by water in the second layer. Fig. (5.5)-(b) shows all possible configuration changes to configuration group $F$.

### 5.2.7 Configuration Group $G$

Gas layer collapse by water or oil may change configuration group $G$ to $B$. The new displacements to add are: gas layer formation, and snap-off of oil in the center by water in the corner.

A piston-like or snap-off displacement by gas could change configuration group $G$ to $C$. The contact angle is $\theta_{go}^r$. No new interface is created. The new displacements to add are: snap-off of gas in the center by water in the corner, two oil layer formations, and piston-like displacement of gas in the center by water and/or oil.

A piston-like displacement by water could convert configuration group $G$ to $K$. The contact angle applied is $\theta_{ow}^a$. $b$ is calculated. This may happen only if $\theta_{ow}^a \geq \frac{\pi}{2} + \alpha$. The new displacements to add are: oil layer collapse by gas in the first layer, oil layer collapse by water in the center, snap-off of water in the center by the oil in the layer, and piston-like displacement of water in the center by oil and/or gas. If $\theta_{ow}^a < \frac{\pi}{2} + \alpha$ then the piston-like displacement by water may change configuration group $G$ to $E$. The contact angles used for the displacement are $\theta_{ow}^a$ and $\theta_{gw}^a$. This may take place only if $\theta_{gw}^a \geq \frac{\pi}{2} + \alpha$. The second gas/water interface is not treated as a new interface. The furthest contact angle and $b$ of the gas/oil interface before the configuration change, are assigned to the second gas/water interface. The oil/water interface may then hinge from its furthest value towards $\theta_{gw}^a$, due to a decrease in gas/water capillary pressure. The new displacements to add are: snap-off of water in the center by gas in the layer, gas layer collapse by water in the center, two oil layer formation events, and piston-like displacement of the water in the center by gas and/or oil. If $\theta_{gw}^a < \frac{\pi}{2} + \alpha$ then the piston-like displacement may convert the configuration $G$ to $A$. The new displacements to add are: oil layer formation, gas layer formation, and piston-like displacement of water in the center by oil and/or...
Figure 5.6: Possible configuration changes to configurations (a) $G$ and (b) $H$
Chapter 5. Two- and Three-Phase Fluid Generic Configurations

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gas.

A water layer formation event may convert configuration group $G$ to $I$. Two
displacements may carry out such a change. Two displacement may carry out such
a change which will use $\theta^a_{gw}$ and $\theta^a_{ow}$. This may happen only if $\theta^a_{gw} \geq \frac{\pi}{2} + \alpha$ and
$\theta^a_{ow} < \frac{\pi}{2} - \alpha$. The new displacements to add are: gas layer collapse by water in the
second layer, water layer collapse by gas in the first layer, water layer collapse by
oil in the center, and snap-off of oil in the center by water in the second layer. Fig.
(5.6)-(a) indicates all possible configuration changes to configuration group $G$.

5.2.8 Configuration Group $H$

A water layer collapse event by gas or oil may change configuration group $H$ to $F$.
The new displacements to add are: water layer formation, oil layer collapse by gas
in the center, and snap-off of gas in the center by oil in the layer.

A piston-like or snap-off displacement by water may change configuration group
$H$ to $D$. The contact angle is $\theta^a_{gw}$. No new interface is formed. The new displace-
ments to add are: snap-off of water in the center by oil in the layer, two possible
gas layer formation events, and piston-like displacement of water in the center by
gas and/or oil.

An oil layer collapse event by water may change configuration group $H$ to $C$.
The new displacements to add are: two oil layer formation events, and snap-off of
gas in the center by water in the corner.

A piston-like displacement by oil is assumed to change configuration group $H$
to $B$, as we don’t consider a third layer. The contact angle under which the dis-
placement is carried out is $\theta^a_{og}$. No new interface is formed. The new displacements
to add are: snap-off oil in the center by water in the corner, two possible gas layer
formation events, and piston-like displacement of oil in the center by gas and/or
water. Fig. (5.6)-(b) indicates all possible configuration changes to configuration
group $H$.

5.2.9 Configuration Group $I$

A water layer collapse event by oil or gas can change configuration group $I$ to $G$.
The new displacements to add are: water layer formation, gas layer collapse by oil
in the center, and snap-off of oil in the center by gas in the layer.

A piston-like or snap-off displacement by water may change configuration group
$I$ to $E$. The contact angle at which the displacement is carried out would is $\theta^a_{ow}$. No
new interface is created. The new displacements to add are: snap-off of water in the center by gas in the layer, two possible oil layer formation events, and piston-like displacement of water in the center by gas and/or oil.

A gas layer collapse event by water may change configuration group $I$ to $B$. The new displacements to add are: two gas layer formation events, and snap-off of oil in the corner.

A piston-like displacement by gas is assumed to change configuration group $I$ to $C$ as we don’t consider a third layer. The contact angle which is used to carry out the displacement is $\theta_{rg}$. No new interface is formed. The new displacements to add are: snap-off of gas in the center by water in the corner, two possible oil layer formation events, and piston-like displacement of gas in the center by oil and/or water. Fig. (5.7)-(a) indicates all possible configuration changes to configuration group $I$.

5.2.10 Configuration Group $J$

An oil layer collapse event may change configuration group $J$ to $E$. The new displacements to add are: gas layer collapse by water in the corner and two oil layer formation events.

A gas layer collapse event by oil or water could change configuration group $J$ to $D$. This may happen only if $\theta_{ow}^a \geq \frac{\pi}{2} + \alpha$ (water displacing) or $\theta_{ow}^g \geq \frac{\pi}{2} + \alpha$ (oil displacing). The new displacements to add are: oil layer collapse by water in the center and two gas layer formation events. If the above oil/water contact condition is not satisfied then configuration group $J$ may be converted to configuration group $A$. The new displacements to add are: oil and gas layer formation events.

A piston-like or snap-off displacement by gas may change configuration group $J$ to $F$. The contact is $\theta_{gw}^r$. No new interface is created. The new displacements to add are: oil layer collapse by gas in the center, snap-off of gas in the center by oil in the layer, water layer formation event, and piston-like displacement of gas in the center by water and/or oil.

A piston-like displacement by oil is assumed to change configuration group $J$ to $B$ as we don’t consider a third layer. The contact angle is $\theta_{ow}^r$. No new interface is formed. The new displacements to add are: snap-off of oil in the center by water in the corner, two possible gas layer formation events, and piston-like displacement of oil in the center by gas and/or water. Fig. (5.7)-(b) indicates all possible configuration changes to configuration group $J$. 
Figure 5.7: Possible configuration changes to configurations (a) I, (b) J, and (c) K
5.2.11 Configuration Group $K$

Gas layer collapse by water or oil may change configuration group $K$ to $D$. The new displacements to add are: oil layer collapse by water in the corner and two gas layer formation events.

An oil layer collapse event by water or gas could change configuration group $K$ to $E$. This may happen only if $\theta_{gw}^w \geq \frac{\pi}{2} + \alpha$ (water displacing) or $\theta_{gw}^g \geq \frac{\pi}{2} + \alpha$ (gas displacing). The new displacements to add are: gas layer collapse by water in the center and two oil layer formation events. If the above gas/water contact angle condition is not satisfied then configuration group $K$ may be converted to configuration group $A$. The new displacements to add are: oil and gas layer formation events.

A piston-like or snap-off displacement by oil may change configuration group $K$ to $G$. The contact angle is $\theta_{ow}^r$. No new interface is created. The new displacements to add are: gas layer collapse by oil in the center, snap-off of oil in the center by gas in the layer, water layer formation, and piston-like displacement of oil in the center by water and/or gas.

Piston-like displacement by oil is assumed to change configuration group $K$ to $C$ as we don’t consider a third layer. The contact angle is $\theta_{gw}^r$. No new interface is formed. The new displacements to add are: snap-off of gas in the center by water in the corner, two possible oil layer formation events, and piston-like displacement of gas in the center by oil and/or water. Fig. (5.7)-(c) indicates all possible configuration changes to configuration group $K$. 
Chapter 6

Pore-Scale Network Modeling

6.1 Continuity and Clustering

In pore network modeling of multiphase flow, one of the most important and difficult tasks to be accomplished is the determination of whether or not a phase location is trapped as well as keeping this information updated during different processes in a robust way.

This is vitally important because for every single and multiple displacement to be carried out, continuity of both displacing and displaced phase locations have to be known a priori (see section (6.4) for details). Also when it comes to compute the relative permeabilities, continuity of phase locations must be known as conductances are calculated only for continuous phase locations. (see section (6.6)).

The algorithm used to determine cluster distributions, critical percolation concentration, and percolation probabilities in network modeling was developed by Hoshen & Kopelman [256] which was later extended to irregular networks by Al-Futaisi & Patzek [286].

6.1.1 Hoshen & Kopelman Algorithm

The algorithm presented by Hoshen & Kopelman [256] was a new method applicable in computer based modeling for determination of cluster distributions, critical percolation concentration and percolation probabilities in a finite random lattice. The method was based on a multiple labeling scheme of members of a cluster in the lattice and was concerned with the determination and counting of the clusters of a particular type of occupant which were randomly distributed in a regular lattice of sites. Every site of the lattice was able to hold only one type of occupant and
was connected to its neighbors by bonds. Every site holding the particular type of
occupant, was assigned a cluster label, \( m^\alpha_t \), where \( \alpha \) was the name of the cluster. Such a cluster could have several labels as a directory of natural numbers.

A directory of positive and negative integer numbers was considered where the
positive ones indicated the number of members in each cluster and the negative
ones provided the links between different labels. The directory was updated when
new members were assigned to the existing clusters, new clusters were found or
coalescence occurred. Every new site was assigned a label in one of the following
ways: (I) if there was not any already labeled neighbor with the same occupant,
a new label was used, (II) if there was only one neighbor with the same occupant,
the label of the neighbor was used (III) if there were more than one neighbor with
the same occupant, the smallest label was used. The distinct feature of the multiple
labeling scheme was that a new site could link two or more already labeled cluster
fragments occupied by the same occupant into a bigger cluster without relabeling
them. The algorithm was able to label the sites, find the clusters, and count them
by a single scan of the lattice.

### 6.1.2 Displacement Based Algorithm

In this work, we use a *new* algorithm whose principles are described below. It is
applicable to any two- or three-dimensional regular and random network with any
number of phases, i.e. phase locations, residing in a pore or throat. In contrast,
the original Hoshen-Kopelman algorithm [256] assumed that only a single phase
occupied each element. Our algorithm, as we will discuss in details shortly, is also
different from the extension of Hoshen-Kopelman algorithm by Al-Futaisi & Patzek
[286] since we *do not* – except for the first time – scan the entire network to update
our information regarding the continuity status of different phases residing in every
element.

First, the network at its initial condition is scanned to determine continuity of
all its present phase locations. Flags are assigned to every single phase location
indicating if it is continuous or trapped. If a phase location is trapped then the
cluster number which it belongs to is also attached to it. To scan the network, a
modified *burning* algorithm is used, see Fig. (6.1). The algorithm uses Table (6.1)
that lists the circumstances under which phase locations holding the same phase
in adjacent pores and throats are considered connected. One should note that we
assume that within a single pore or throat all the corners are connected and so are
all the layers holding the same phase. This definition of connectivity is used to
define clusters of each phase. During the scanning process, if a trapped cluster is found then all phase-locations belonging to the cluster are stored under the same cluster number.

![Flow chart used to determine clusters of each phase](image)

Figure 6.1: Flow chart used to determine clusters of each phase

Once the scanning of the network at its initial status is finished, the injection of different phases and thus different displacements may start. Displacements may create new phase locations, form new trapped clusters and make old trapped clusters break, coalesce, or become continuous. This means that the old flags of phase locations may not be valid anymore and must be updated.

We present a series of *displacement-based* rules to update the flags where there will be *no need* to scan the *entire* network to update our information regarding the new continuity status of the phase locations after each displacement event. This
Table 6.1: Criteria for connectivity of phase locations holding the same phase in adjacent pores and throats

<table>
<thead>
<tr>
<th>Phase location(1)</th>
<th>Phase location(2)</th>
<th>Connected?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Corner</td>
<td>Corner</td>
<td>Yes</td>
</tr>
<tr>
<td>Corner</td>
<td>Layer</td>
<td>No</td>
</tr>
<tr>
<td>Corner</td>
<td>Center</td>
<td>No</td>
</tr>
<tr>
<td>Layer</td>
<td>Layer</td>
<td>Yes</td>
</tr>
<tr>
<td>Layer</td>
<td>Center</td>
<td>Yes</td>
</tr>
<tr>
<td>Center</td>
<td>Center</td>
<td>Yes</td>
</tr>
</tbody>
</table>

means that flags will be *always* valid during all processes.

To present the rules, imagine a displacement occurring in a pore or throat. We may call that pore or throat the *target* element which may have several *neighbors*. For a pore, the neighbors are the throats connected to it and for the throats, the pores. Neighbors do not necessarily contain the same fluid as the target element. Every phase location in the target element and its neighbors is considered as a member of a *chain* of phase locations with the same phase and will act as a *head*. If a chain stretches to the inlet and/or outlet, it is *continuous*, otherwise it is a *trapped* cluster.

The rules are itemized as follows:

1. Before the displacement takes place, all the chain heads in the target element and its neighbors are determined (i.e. *separately* in each pore and throat). For instance in a corner of an element with configuration group $F$, see Fig. (5.2), three chain heads, i.e. water corner, oil layer, and gas center, are determined. One should note that in this stage, there is no need to know how far the chains stretch. Same phase locations in an element will be members of a same chain and either of them could be used as the chain head. For example, in a element with triangular cross-section with all the corners having configuration group $G$, all the gas layers are considered as members of a gas chain and obviously should all have the same flags and only one of them is used as a chain head. This is also the case for the water corners. However, phase locations with the same phase but in a different *type* of location might not necessarily be considered as members of the same chain. For instance, in configuration group $D$, water in the center is not considered as a member of the chain that the water corner is a member of, unless they touch each other in a corner where there is no oil layer. The water center is considered as a head of another water chain.
2. Before the displacement, the connectivity of chain heads in the target element with the chain heads in its neighbors are determined and stored using the criteria listed in Table (6.1).

3. The displacement is carried out which may omit some old phase locations while forming the new ones in the target element. Only for the newly formed phase locations must flags be assigned. The new phase locations created by piston like, snap-off, and layer formation displacement events that hold the same phase as the displacing phase location will get flags exactly the same as those of the displacing phase location. For instance, imagine an oil center in a neighbor creates an oil layer in the target element, the newly formed oil layer will get the same flags as the oil center. But if the newly born phase location contains a phase similar to that of the displaced phase location, i.e. old, then it will get the same flags as the displaced phase location. For example, consider configuration group change B to F. The oil layers will get flags the same as those of oil center before the displacement.

4. If the displacing phase location is trapped and forms new phase locations with the same flags then the new phase locations are added to the trapped cluster as new members.

5. If the displaced phase location was trapped and after the displacement it did not exist anymore, it is omitted from the list of the trapped cluster members.

6. If the target element is connected directly to the inlet or outlet and the new phase location is formed by the phase invading from the outside of the network, a continuous flag is assigned to the new phase location.

7. After the displacement, new possible chain heads are determined in the target element.

8. Connectivity of the new chain heads in the target elements with the chain heads in the neighbors are determined and stored.

9. Connectivity of every single chain head in the neighbors to the chain heads with the same phase in the target element before and after displacement are compared. If a chain head was disconnected (or connected) to the target element before the displacement and stays disconnected (or connected) after the displacement, there is no need to change the flags of the chain.
10. If a chain head in a neighbor was connected to the target element before the displacement and got disconnected after the displacement then: (I) If the chain head was continuous then its continuity is checked using the algorithm presented in Fig. (6.1) as the chain might have got trapped due to the disconnection from the target element. (II) If the chain head was trapped, disconnection from the target element might mean that a trapped cluster has broken into two or more smaller trapped clusters. This is called a local break and the next point describes how the algorithm realizes if a local break has actually broken the displaced trapped cluster to smaller ones.

11. In order to find if a local break is a break, one of the phase locations residing in a neighbor that belongs to the displaced (mother) trapped cluster is chosen. Then all the phase locations connected to it are found using the algorithm presented in Fig. (6.1). If all the other phase locations residing in the neighbor(s) that belong to the mother trapped cluster are among the found phase locations, then the disconnection has been only a local one and not a break. If not, it is a break and found phase locations form a new trapped cluster with a new identity. Now all the other phase locations in the neighbor(s) that were members of the mother trapped cluster are also picked up one by one and all the connected phase locations are found and process continues exactly the same as the first phase location until there is no any phase location left that has not been assigned to a new smaller trapped cluster.

12. If a chain head in a neighbor was disconnected from the target element before the displacement and has become connected after the displacement then: (I) If the chain in the neighbor had a trapped flag on it (as a member of trapped cluster) while the chain head in the target element is continuous then the trapped cluster has become continuous and flags of all its members are changed to continuous. The opposite case is also possible when the chain head in the target element is trapped while the one in the neighbor is continuous. (II) If the chain head in the neighbor was trapped and so was the chain head in the target element that it got connected to, then a coalescence has happened and both trapped clusters now will form a bigger trapped cluster (see section (6.3.1) for details). For all other cases there is no need to change the flags of the chains.

This clustering algorithm presents a robust and fast tool for live monitoring of the formation of new trapped clusters, and reconnection, coalescence, and breaking
of old trapped clusters which as we shall show later are vitally important.

6.2 How to Choose the Right Displacement

Based on what phase displaces what phase, there are six possible two-phase processes: oil displacing water which is controlled by an increase in $P_{c,ow}$. This could be done either by an increase in oil pressure or a decrease in water pressure. Likewise, water displacing oil (decrease in $P_{c,ow} \equiv$ increase in water pressure or decrease in oil pressure), gas displacing water (increase in $P_{c,gw} \equiv$ increase in gas pressure or decrease in water pressure), water displacing gas (decrease in $P_{c,gw} \equiv$ increase in water pressure or decrease in gas pressure), gas displacing oil (increase in $P_{c,go} \equiv$ increase in gas pressure or decrease in oil pressure), and oil displacing gas (decrease in $P_{c,go} \equiv$ increase in oil pressure or decrease in gas pressure). Every displacement belongs to one or two of these six processes. For instance, collapse of the gas layer which leads to configuration group change $G$ to $B$ could occur by either water or oil invasion which correspond to a decrease in $P_{c,ow}$ or a decrease in $P_{c,go}$, respectively. This means that this displacement belongs to both water displacing gas and oil displacing gas processes. But, for example, configuration group change $B$ to $A$ only belongs to a water displacing oil process.

A process can be carried out either by increasing the pressure of the displacing fluid or decreasing the pressure(s) of the displaced fluid(s). In two-phase processes, both methods may produce the same results but that may not necessarily be the case for three-phase systems. In this work, we shall model all the processes by increasing the pressure of the injection fluid. For example, gas injection into water and oil is carried out by increasing the gas pressure not by decreasing the pressures of oil and water.

For every single displacement, a threshold capillary pressure is calculated which might depend on the relevant contact angles, corner angles and inscribed radius of the element of interest, other capillary pressures and the configuration of nearest neighbor pores and throats. Then depending on what fluid is displacing and what is displaced, the threshold absolute pressure of the displacing fluid for a single displacement is found from:

$$P_{i}^{threshold} = P_{c,i,j}^{threshold} + P_j$$

or
where \( P_i \) and \( P_j \) are pressures of phases \( i \) and \( j \), respectively. The pressure of a fluid is referred to the pressure of a continuous cluster of that fluid and is assumed to be the same as the inlet or outlet pressure of the fluid. There might be several such clusters of one fluid but they all will have the same pressure. The foregoing procedure is used for single displacements where one continuous phase location displaces another continuous one. When one or both of them is trapped, \( P_i^{threshold} \) and \( P_j^{threshold} \) are found in a slightly different way that shall be discussed in the Multiple Displacements section (6.4). Threshold pressures of all the displacements that have the same displacing fluid are ranked into the same main sorted list. Consequently, in three-phase systems there will be three main sorted lists for gas, oil and water as displacing phases. This means that every list may include entries from two different processes with the same displacing fluid. For instance, the water list may include threshold pressures from water displacing oil and water displacing gas processes.

Initially when the network is water-filled, only oil or gas can be injected and the only processes are those that displace water by oil or gas from the elements connected to the inlet. From this stage onwards, new displacements must be added, if there were any, to the appropriate list(s) regardless of whether they could occur during the current process or not (see chapter 5 for details). The exact configuration change associated with these new displacements may not be clear at this stage; and it is not necessary, as they may occur during other processes when the conditions, i.e. pressures and target contact angles, will be different. Before a new displacement is added to an appropriate list, its threshold capillary pressure is calculated. Before a new displacement is added to a main sorted list, it must be checked to see if both displacing and displaced phase locations are continuous. If one or both of them is trapped, then, based on what fluid is displacing and what fluid is displaced, the displacement is added into an appropriate sorted sublist in one of the 18 multiple displacement search categories tabulated in Tables (6.2), (6.3) and (6.4) (see details in Multiple Displacements section (6.4)). If both phase locations are continuous then it is added to an appropriate main sorted list.

By knowing the injection fluid, the relevant main sorted list is selected, for example the water list for water injection. The list is sorted in ascending order. Imagine the invading fluid is \( i \). This means that we consider a displacement event where the volume of \( i \) in an element increases. Phase \( i \) can invade either phase \( j \) or \( k \). The threshold pressure at the top of the list belongs to the most favorable, i.e.
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easiest, displacement. This could be displacement of \( j \) or \( k \) by \( i \). If the displacement is \textit{valid} then it takes place. A displacement is valid when the displacing and displaced phase locations are \textit{present} and their continuity status flags are \textit{consistent} with the list that the threshold pressure is in. If a displacement is not valid, the event is taken off the sorted list and either discarded or moved to an appropriate list depending on the reason of invalidity. The next most favorable displacement is considered from the list. The advantage of having one list for both \( i \) to \( j \) and \( i \) to \( k \) displacements is that it assures that always the most favorable displacement is carried out \textit{first}.

Displacements in the lists might no longer be valid because of other displacements that have already taken place. For instance, consider configuration group \( G \). Collapse of the gas layer by water in the corner and oil in the center are two possible displacements that should be in the water and oil lists, respectively. If the gas layer collapsed during water invasion by increase in water pressure, the other displacement, i.e. collapsing of the gas layer by oil, is no longer valid as there is no gas layer to be collapsed.

Multiple displacement search categories listed in Tables (6.2), (6.3), and (6.4) allow us to find the most favorable multiple displacement (see later for details), which then is compared with the most favorable single displacement that is determined from the main lists. This comparison would allow us to find the \textit{globally} most favorable event.

<table>
<thead>
<tr>
<th>No.</th>
<th>Displacing</th>
<th>CS(1)</th>
<th>Displaced</th>
<th>CS</th>
<th>Name</th>
<th>CC(4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>oil</td>
<td>c(2)</td>
<td>water</td>
<td>t(3)</td>
<td>ocwt</td>
<td>wtot, wtoc, wtgt, wtgc</td>
</tr>
<tr>
<td>2</td>
<td>oil</td>
<td>c</td>
<td>gas</td>
<td>t</td>
<td>ocgt</td>
<td>gtwt, gtwc, gtot, gtoc</td>
</tr>
<tr>
<td>3</td>
<td>gas</td>
<td>c</td>
<td>water</td>
<td>t</td>
<td>gcwt</td>
<td>wtot, wtoc, wtgt, wtgc</td>
</tr>
<tr>
<td>4</td>
<td>gas</td>
<td>c</td>
<td>oil</td>
<td>t</td>
<td>gcot</td>
<td>otwt, otwc, otgt, otgc</td>
</tr>
<tr>
<td>5</td>
<td>water</td>
<td>c</td>
<td>oil</td>
<td>t</td>
<td>wcot</td>
<td>otwt, otwc, otgt, otgc</td>
</tr>
<tr>
<td>6</td>
<td>water</td>
<td>c</td>
<td>gas</td>
<td>t</td>
<td>wcgt</td>
<td>gtwt, gtwc, gtot, gtoc</td>
</tr>
</tbody>
</table>

1. Continuity Status
2. Continuous
3. Trapped
4. Chain-Categories

After a displacement, the pressure of the phase \( i \) (injection phase) is set to the \textit{maximum} of the threshold pressure and the current pressure of phase \( i \). All the
Table 6.3: Multiple displacements search categories (trapped-continuous)

<table>
<thead>
<tr>
<th>No.</th>
<th>Displacing CS(1)</th>
<th>Displaced CS</th>
<th>Name CC(4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>oil t(3)</td>
<td>water c(2)</td>
<td>otwc —</td>
</tr>
<tr>
<td>2</td>
<td>oil t</td>
<td>gas c</td>
<td>otgc —</td>
</tr>
<tr>
<td>3</td>
<td>gas t</td>
<td>water c</td>
<td>gtwc —</td>
</tr>
<tr>
<td>4</td>
<td>gas t</td>
<td>oil c</td>
<td>gtoc —</td>
</tr>
<tr>
<td>5</td>
<td>water t</td>
<td>oil c</td>
<td>wtoc —</td>
</tr>
<tr>
<td>6</td>
<td>water t</td>
<td>gas c</td>
<td>wtgc —</td>
</tr>
</tbody>
</table>

1. Continuity Status
2. Continuous
3. Trapped
4. Chain-Categories

Table 6.4: Multiple displacements search categories (trapped-trapped)

<table>
<thead>
<tr>
<th>No.</th>
<th>Displacing CS(1)</th>
<th>Displaced CS</th>
<th>Name CC(3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>oil t(2)</td>
<td>water t</td>
<td>wtot, wtoc, wtgt, wtgc</td>
</tr>
<tr>
<td>2</td>
<td>oil t</td>
<td>gas t</td>
<td>gtwt, gtwc, gtot, gtoc</td>
</tr>
<tr>
<td>3</td>
<td>gas t</td>
<td>water t</td>
<td>wtot, wtoc, wtgt, wtgc</td>
</tr>
<tr>
<td>4</td>
<td>gas t</td>
<td>oil t</td>
<td>otwt, otwc, otgt, otgc</td>
</tr>
<tr>
<td>5</td>
<td>water t</td>
<td>oil t</td>
<td>wtot, otwt, otwc, otgc</td>
</tr>
<tr>
<td>6</td>
<td>water t</td>
<td>gas t</td>
<td>gtwt, gtwc, gtot, gtoc</td>
</tr>
</tbody>
</table>

1. Continuity Status
2. Trapped
3. Chain-Categories

displacements that have threshold pressures less than the pressure of the injection phase \( i \) are carried out — *always in order of the threshold pressure* — until it is not possible to find displacement with a threshold pressure less than or equal to the current value of the phase \( i \) pressure. This is done in a way that the displacement with the *lowest* threshold pressure is *always* carried out *first*. At this time, all the configurations are stable and at *equilibrium* and the system is said to be *relaxed*.

The *maximum* of the threshold pressure and the current pressure of phase \( i \) is used because it is often the case that doing a displacement allows a subsequent displacement at a threshold pressure much lower than the current injection phase
pressure. This event is more favorable than the next displacement in the list. An example of this is oil displacement into water in a water-wet medium. $P_{oil}$ may be high to allow oil to fill a throat, but oil can then fill an adjoining pore at a lower oil pressure. If we used this new lower value of $P_{oil}$ to compute radii of curvature, then we would find that in some elements the radius is inconsistent with the fluid configuration - for instance, water AM in a corner would have a radius of curvature too large to fit in an element. In strict capillary equilibrium, the fluid would rearrange throughout the network to give configurations consistent with the prevailing capillary pressure. This is, however, a very difficult task for a general three-phase model. Instead, phase pressures are defined as the maximum value ever reached during the whole simulation. In other words, the pressure of the invading phase never acquires a lower value than its current one. Whenever a phase pressure reaches a new maximum, the fluid configurations are truly in a position of capillary equilibrium. In a simulation involving a complex displacement path, the phase pressures will continue to increase. However, since it is only pressure differences that control the displacement sequence, this is not a problem.

As it is mentioned earlier, threshold capillary pressures of the displacements may be affected by the change in capillary pressure. In such circumstances, threshold capillary pressures of those displacements are recomputed taking into account the new arrangements of fluid and capillary pressures and re-ordered in the sorted lists. The new phase saturations and relative permeabilities are computed (see sections (6.5) and (6.6)) when the system is relaxed. If a new phase is injected then the sorted lists for displacements are re-ordered to account for latest changes in capillary pressures.

### 6.3 How to Treat the Trapped Clusters, Associated Radii of Curvatures and Displacements

Injection of different phases, wettability, capillary pressures, geometry of elements and different displacement mechanisms are amongst the main reasons that cause trapping of different phases in porous media. The trapped phases will be in the form of clusters of phase locations. When a cluster of phase locations becomes trapped, (1): A number is assigned to it. (2): The phase of the cluster is stored. (3): Addresses of all the phase locations belonging to it are stored. (4): Two flags are assigned to every single phase location indicating that they are trapped and the cluster number that they belong to. (5): All the current capillary pressures,
i.e. phase pressures, are stored. (6): The volume of the trapped cluster, which is
the summation of volume of its phase locations, when it is trapped is stored as the
original volume of the cluster. The original volume is used in saturation calculations
to account for volume errors caused by multiple displacements (see section (6.5)).
(7): If any of the phase locations of the cluster is involved in a displacement then
it is moved to an appropriate sublist in one of the multiple displacement search
categories. This could be a move from the main sorted lists to the categories listed
in Tables (6.2) and (6.3). If any of the phase locations is involved in displacements
that are already in the search categories listed in Tables (6.2) and (6.3), then they
need to be moved into corresponding categories in Table (6.4).

Every multiple displacement search category may contain several sorted sub-
lists. Every sorted sublist within the categories named in Tables (6.2) and (6.3)
has a cluster number associated with it and contains threshold pressure of the valid
displacements at the nudging points of a trapped cluster with a continuous fluid.
Categories listed in Table (6.2) contain displacements that the displaced phase loca-
tion is trapped while the categories named in Table (6.3) have an opposite situation.
All the sublists are always sorted in ascending order. One should note that the sub-
lists within each category are completely independent from each other.

During different three-phase processes, there may be cases where a trapped clus-
ter touches one, two or several other trapped clusters with different phases. WAG
flooding with several injection cycles is an example of such a case. The touching
points represent displacements whose threshold pressures are stored in sublists
within categories tabulated in Table (6.4). For every displacement both displacing
and displaced phase locations are trapped. One trapped cluster might be involved
in several sublists as every sublist represents the touching points between only two
trapped clusters with different fluids. For every sublist displacing and displaced
cluster, numbers are also stored.

When a trapped cluster forms, the curvature of all interfaces associated with
it need to be kept fixed as long as the cluster is trapped and it has not become
involved in multiple displacements. The conventional method in previously devel-
oped network models was that the interfaces were considered frozen. This was done
regardless of the pressure of the phase inside the trapped cluster and pressures of
the surrounding fluids. In this work, the pressure of the fluid inside the cluster is
not a dummy value. It has a physical meaning during the modeling of different
processes. The initial pressure of the cluster is the pressure of the phase when it
was first trapped. However, the pressure of the cluster changes according to the
change in the pressure of the surrounding phases in order to maintain the curvature of the interfaces at the same value as when the trapped cluster first formed. As an example, imagine water flooding into a two-phase water-wet system with connate water saturation. Trapped clusters of oil form at different stages of water injection, i.e. at different oil/water capillary pressures. Once each trapped cluster forms, it gets the current pressure of oil, i.e. $P_{oil}$. But since $P_{oil}$ is fixed during water flooding, all the trapped clusters will have the same oil pressure regardless of when they have trapped while water pressure is increasing. To deal with this problem, we update the pressure of the trapped oil clusters according to the increase in pressure of water using:

$$
P_{cluster k, new}^{i} = P_{cluster k, old}^{c,ij} + P_{j, new}
$$

or

$$
P_{cluster k, new}^{j} = P_{i, new} - P_{cluster k, old}^{c,ij}
$$

where $P_{cluster k, old}^{c,ij} = (P_{cluster k, old}^{i, old} - P_{j, old})$ or $P_{cluster k, old}^{c,ij} = (P_{i, old} - P_{cluster k, old}^{j, old})$ is the capillary pressure exactly at the moment that the trapped cluster $k$ formed. For the above water flooding example, it becomes:

$$
P_{oil, new}^{cluster k} = (P_{oil, old}^{cluster k} - P_{water, old}) + P_{water, new}
$$

The change in pressure of the trapped clusters has very important effect on the selection of the most favorable multiple displacement as we shall describe later.

### 6.3.1 Coalescence

During different three-phase processes, trapped clusters may have to move under multiple displacement mechanisms in order to predict a physically correct occupancy. It is quite often the case that the moving trapped clusters meet other trapped clusters of the same phase. This will lead to a coalescence event. A coalescence event might also happen when a trapped cluster starts forming layers, if it is possible, between phase locations of the two other phases in the neighboring pores and throats. Layer reformation allows the trapped clusters to extend their margins and meet other trapped clusters. This phenomenon is very well known when gas injection is carried out into water flood residual oil in a water-wet system [59, 61, 63, 64, 287]. But there are some subtleties associated with coalescence. It may well be the case
that the merging trapped clusters have different pressures and sizes, i.e. volumes, as they might have trapped at different times during different processes. In such circumstances, it is sensible to think that after coalescence the resultant trapped cluster would have a \textit{volume weighted} average pressure of the the merging trapped clusters. The \textit{original} volume of the merging trapped clusters may be used in an average pressure calculation as follows:

\[
P_{\text{cluster}} = \frac{\sum_{k=1}^{n} V_{\text{cluster } k}^{\text{original}} \times P_{\text{cluster } k}}{\sum_{k=1}^{n} V_{\text{cluster } k}^{\text{original}}} \tag{6.6}
\]

where \(n\) is the number of merging trapped clusters.

The calculated average pressure of the newly formed trapped cluster is used in saturation calculations and also multiple displacements. The volume of the trapped cluster formed by coalescence is given by:

\[
V_{\text{cluster}} = \sum_{k=1}^{n} V_{\text{cluster } k}^{\text{original}} \tag{6.7}
\]

When a coalescence happens, all the phase locations of the merging trapped clusters are stored together and are assigned the same cluster number. If there are groups of displacements in categories listed in Tables (6.2) and (6.4) that any of the merging clusters were involved in, their threshold pressures are changed according to new average pressure of the resultant trapped cluster. This is done by:

\[
P_{\text{threshold } i, \text{ new}} = P_{\text{cluster } j, \text{ new}} + P_{\text{threshold } i, \text{ old}} - P_{\text{cluster } k, \text{ old}} \tag{6.8}
\]

or

\[
P_{\text{threshold } j, \text{ new}} = P_{\text{cluster } i, \text{ new}} - P_{\text{cluster } k, \text{ old}} - P_{\text{threshold } j, \text{ old}} \tag{6.9}
\]

For the displacements in the categories listed in Table (6.3), threshold pressures are updated if the pressure of the displaced phase which is continuous changes.

In every multiple displacement search category listed in Tables (6.2), (6.3), and (6.4) all sublists associated with the merging clusters are re-ordered to represent one bigger cluster.

It is often the case that a trapped cluster meets a continuous cluster of the same phase. In such circumstances, the pressure of the continuous fluid is changed to an average pressure given by:
\[ P_{new} = \left( \frac{V_{\text{cluster}}}{V_{\text{cluster}}} \times P_{\text{cluster}} \right) + \left[ V_{\text{continuous}} \times P_{\text{old}} \right] \]

where \( V_{\text{continuous}} \) is the volume of continuous phase \( i \). All the volume error associated with that trapped cluster is ignored as the system is in contact with the inlet or outlet and the volume error would be compensated automatically. Note that this allows the phase pressures to change due to contact with previously trapped clusters. This method to update pressure is similar to the work of Van Dijke et al. [151, 152] but different from Fenwick & Blunt [141, 142] who kept the continuous cluster pressure constant. All the displacements associated with the trapped cluster are now transferred to the other lists, i.e. main sorted lists or sublists within search categories, as appropriate.

### 6.3.2 When a Trapped Cluster Breaks into Smaller Ones

In three-phase systems when multiple displacements take place, a trapped cluster might break into two or more smaller ones. For instance, consider an angular element with trapped oil in the center that is invaded by gas. It is possible that the displaced trapped cluster can not leave oil layers in the corners of the element and this might disconnect the other phase locations of the displaced trapped cluster that are residing in the neighboring elements. This might also happen, for instance, when an existing layer phase location which is a member of a trapped cluster collapses.

After every multiple displacement, it must be checked if it has caused any local disconnection among the phase locations of the displaced trapped cluster(s) residing in neighboring elements. If this has happened, it does not necessarily mean that the displaced clusters have broken into smaller ones as the phase locations might be connected to each other through other routes in the network, or the displaced phase location that has caused the local disconnection might be simply the dead end of a branch of the trapped cluster. If a break has happened then the number of the resultant smaller clusters and their members are determined and stored using the clustering algorithm described in section (6.1.2).

When a trapped cluster breaks into two or more smaller trapped clusters, the pressure of the smaller clusters are assumed to be exactly the same as that of the mother cluster at the time when the break took place. Now since the smaller trapped clusters have their own new independent identity, all the displacements associated with the mother trapped cluster in the different multiple displacement search categories must be distributed among the smaller clusters based on which cluster the
trapped phase location involved in every displacement is associated with. The original volume of the mother cluster is assigned to the largest of the smaller clusters. The volume of the other clusters is set to zero. This does not create any problem as we shall show in section (6.5).

### 6.4 Multiple Displacements

One unique feature of three-phase flow at the pore level is multiple displacement. This displacement mechanism is involved in rearrangement of different trapped clusters to produce a physically correct occupancy. An invasion of phase \( j \) by phase \( i \) may be composed of a series of displacements starting with a displacement where \( i \) is the displacing fluid and ending with a displacement where \( j \) is the displaced fluid. If all the phases are continuous, this is simply equivalent to separate single displacements. However, the intermediate phases in the chain may be trapped. This means that a cascade of trapped clusters nudge each other before a final displacement of a continuous phase. Trapped clusters of the intermediate phases can rearrange themselves in the pore space and/or reform layers, and may coalesce with other trapped clusters of the same phase to make bigger trapped clusters or become continuous by meeting continuous clusters. This happens simply due to capillary forces. Multiple displacements that involve more than one intermediate stage are only possible if two phases are trapped [151]. If only one phase is trapped, a simpler version of multiple displacement, *double displacement*, may take place and this has been observed in micromodel experiments [63, 68, 71, 262] and coded into network models [137, 141, 142, 151], where one phase invades part of a trapped cluster that in turn displaces the third, continuous phase.

Six possible double displacements are possible [141]. Table (6.5) lists all the possible cases for strongly water-wet system and Figs. (6.2)-(6.4) schematically illustrate three of them. Likewise, six double displacements can be considered in weakly and strongly oil-wet systems. They are tabulated in Tables (6.7) and (6.6), respectively.

Here we present a search algorithm that is capable of finding the most favorable multiple displacement. In this work, we use it to find the most favorable double displacement. During each process, the most favorable double displacement is compared with the most favorable single displacement. The one that requires the lower pressure of the injection phase is the one that takes place. In order to find the most favorable double displacement, all the possible double events for all the trapped
Table 6.5: Possible double displacements in strongly water-wet systems.

<table>
<thead>
<tr>
<th>No.</th>
<th>Mechanism</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Gas Displaces Oil Displaces Water</td>
<td>Double Drainage</td>
</tr>
<tr>
<td>2</td>
<td>Gas Displaces Water Displaces Oil</td>
<td>Drainage-Imbibition</td>
</tr>
<tr>
<td>3</td>
<td>Oil Displaces Gas Displaces Water</td>
<td>Imbibition-Drainage</td>
</tr>
<tr>
<td>4</td>
<td>Water Displaces Oil Displaces Gas</td>
<td>Double Imbibition</td>
</tr>
<tr>
<td>5</td>
<td>Water Displaces Gas Displaces Oil</td>
<td>Imbibition-Drainage</td>
</tr>
<tr>
<td>6</td>
<td>Oil Displaces Water Displaces Gas</td>
<td>Drainage-Imbibition</td>
</tr>
</tbody>
</table>

Figure 6.2: Double drainage in water-wet systems, (a) Trapped oil is in contact with water and gas in neighboring elements, (b) Gas displaces oil which in turn displaces water [141].

Table 6.6: Possible double displacements in strongly oil-wet systems

<table>
<thead>
<tr>
<th>No.</th>
<th>Mechanism</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Water Displaces Gas Displaces Oil</td>
<td>Double Drainage</td>
</tr>
<tr>
<td>2</td>
<td>Water Displaces Oil Displaces Gas</td>
<td>Drainage-Imbibition</td>
</tr>
<tr>
<td>3</td>
<td>Gas Displaces Water Displaces Oil</td>
<td>Imbibition-Drainage</td>
</tr>
<tr>
<td>4</td>
<td>Oil Displaces Gas Displaces Water</td>
<td>Double Imbibition</td>
</tr>
<tr>
<td>5</td>
<td>Oil Displaces Water Displaces Gas</td>
<td>Imbibition-Drainage</td>
</tr>
<tr>
<td>6</td>
<td>Gas Displaces Oil Displaces Water</td>
<td>Drainage-Imbibition</td>
</tr>
</tbody>
</table>
Table 6.7: Possible double displacements in weakly oil-wet systems

<table>
<thead>
<tr>
<th>No.</th>
<th>Mechanism</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Gas Displaces Water Displaces Oil</td>
<td>Double Drainage</td>
</tr>
<tr>
<td>2</td>
<td>Gas Displaces Oil Displaces Water</td>
<td>Drainage-Imbibition</td>
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<tr>
<td>3</td>
<td>Oil Displaces Gas Displaces Water</td>
<td>Imbibition-Drainage</td>
</tr>
<tr>
<td>4</td>
<td>Oil Displaces Water Displaces Gas</td>
<td>Double Imbibition</td>
</tr>
<tr>
<td>5</td>
<td>Water Displaces Gas Displaces Oil</td>
<td>Imbibition-Drainage</td>
</tr>
<tr>
<td>6</td>
<td>Water Displaces Oil Displaces Gas</td>
<td>Drainage-Imbibition</td>
</tr>
</tbody>
</table>

Figure 6.3: Double imbibition in water-wet systems, (a) Water imbibes into trapped oil which contacts gas, (b) Oil in turn displaces gas [141].

clusters in the system need to be considered.

The algorithm for considering such events is somewhat involved, since multiple events for all clusters need to be considered [151]. Here we present how the most favorable multiple displacement is found every time:

First, based on what fluid is being injected into the system, the two categories from Table (6.2) that have the same displacing fluid as the injection fluid are considered and called starting categories. For instance, categories gcwt and gcot are considered (c indicates continuous and t trapped) when gas is being injected. Now all the categories that could chain up with the starting categories are determined from Tables (6.2), and (6.4) and are called chain-categories. Chain-categories for gcwt and gcot would be wtot, wtoc, wtgc, otwt, otwc, otgt, and otgc. As men-
tioned earlier, every category might include several sublists with one or two trapped cluster numbers associated with each one. The displacements at the top of each sublist within the starting categories can now chain up with the displacements at the top of the sublists within the chain-categories, if there are any, provided that the displacing trapped cluster number of the sublist within the chain-category is the same as the displaced trapped cluster number of the sublist within the starting category. This means that every trapped cluster involved in a multiple displacement contributes to two displacements. One should note that the displaced phase of a category must be always the same as the displacing phase of the category that it is going to chain up with. The displacement at the top of each sublist is the easiest, i.e. lowest invasion pressure, displacement of the sublist. So every multiple displacement is a chain of easiest displacements from sublists within categories that are allowed to chain up with each other. Chaining up with categories continues until the next category is one of those tabulated in Table (6.3). For example, the chain of gcot, otwt, wtgt and gtwc could give multiple displacements provided that sublists satisfying the foregoing conditions exist within above categories. This in turn means that oil, water, and gas trapped clusters existed in the system. Continuous gas is touching trapped oil clusters which in turn touch trapped water clusters which in turn touch trapped gas clusters which in turn touch continuous water. For a multiple displacement with \( n \) trapped clusters involved, a series of \( n + 1 \) chainlike displacements are
carried out. Using the foregoing algorithm, all the possible multiple displacements are determined and their threshold absolute pressure are calculated using:

\[ P_{\text{threshold}}^{i, \text{MD}} = P_{\text{threshold}}^i + \sum_{k=1}^{n} \left[ (P_{\text{threshold}}^j)_{\text{cluster } k} - P_{\text{cluster } k}^j, \text{old} \right] \] (6.11)

where \( n \) is the number of trapped clusters involved, \( \text{MD} \) stands for multiple displacement, \( P_{\text{threshold}}^i \) is the threshold pressure of the first displacement of the multiple displacement where the injection fluid is the displacing fluid, \( j \) is the fluid that cluster \( k \) accommodates, \( (P_{\text{threshold}}^j)_{\text{cluster } k} \) is the threshold absolute pressure of the displacement for which trapped cluster \( k \) is the displacing fluid, and \( P_{\text{cluster } k}^j, \text{old} \) is the old pressure of the trapped cluster \( k \), i.e. before the multiple displacement.

Eq. (6.11) has been derived by summing up the threshold capillary pressures of all the displacements. One should note that the threshold capillary pressure of each displacement in a multiple displacement is calculated using a contact angle that is defined according to what fluid is displacing what, regardless of what fluid is being injected into the system. When a multiple displacement is carried out pressures of the involved trapped clusters are increased to the value given by:

\[ P_{\text{cluster } k}^j, \text{new} = (P_{\text{threshold}}^j)_{\text{cluster } k} \] (6.12)

We give an example of applying this algorithm by considering a double displacement which is used in this work. Imagine gas is being injected into oil and water where some of the oil is in trapped clusters. Since there are only trapped oil clusters the only possible multiple displacement is double displacement where continuous gas displaces trapped oil which in turn displaces continuous water. The double displacements could be determined by chaining up categories \( \text{gcot} \) and \( \text{otwc} \) provided that the required sublists are present within each category. The threshold capillary pressure of the double displacement is:

\[ P_{\text{threshold}}^{\text{gas, DD}} = P_{\text{threshold}}^{\text{gas}} + \left[ (P_{\text{threshold}}^\text{oil})_{\text{cluster } k} - P_{\text{cluster } k}^\text{oil, old} \right] \] (6.13)

where DD stands for double displacement. The new pressure of the trapped oil cluster is:

\[ P_{\text{cluster } k}^\text{oil, new} = (P_{\text{threshold}}^\text{oil})_{\text{cluster } k} \] (6.14)

Once a multiple displacement is recognized as a \textit{global} most favorable event, it is carried out. But there is one subtlety involved. It is quite often the case that
$P^{\text{threshold}}_{i, MD}$ is smaller than $P^{\text{global}}_{i}$. In other words, the multiple displacement could be carried out without any increase in pressure of phase $i$. The difference between these two pressures needs to be accounted for in the pressures of trapped clusters involved in multiple displacement by increasing them by $(P_{i} - P^{\text{threshold}}_{i, MD})$.

When it comes to calculate the threshold pressure of a multiple displacement, one may use threshold pressures of the displacements involved regardless of their type. This means that displacements may well be layer formation or collapse events. Theoretically this is fine but not technically. (I) This approach might increase the volume error associated with multiple displacement as piston-like, pore-body filling and snap-off events might chain up with the layer formation or collapse events which would obviously be detrimental for volume-mass conservation. (II) The simulator might be trapped in an infinite loop of forming and collapsing layers. To prevent these problems, we shall use a slightly different approach where only threshold pressures of piston-like, pore-body filling and snap-off events are used in calculating the threshold pressure of a multiple displacement. In this approach, when a multiple displacement is to be carried out, all the layer formation or collapse events in the involved sublists that are more favorable to the displacements used in $P^{\text{threshold}}_{i, MD}$ calculations, are carried out first.

As we mentioned earlier, when a multiple displacement is taking place, pressures of the involved trapped clusters increase. Once this happens, we then update all the AM’s associated with the trapped clusters according to their new pressures. This means that the volumes of the trapped clusters are always kept updated. Also the new AM’s formed during the multiple displacements will have radii of curvatures according to the new pressures of the trapped clusters that they belong to.

After every multiple displacement event, new displacements that are now available have to be added to the sublists within the correct categories. This means that we might have new chains of displacements, i.e. multiple displacements, for the next round. Also there might be phase locations that must be added to or omitted from the involved trapped cluster(s). For example, imagine a trapped gas cluster is to displace trapped oil in the center of a triangular throat. Before the displacement, configurations in all the corners are from group $B$ and the center phase location is a member of a trapped oil cluster. Also imagine corner half angles, contact angles and capillary pressures allow oil to reside as a layer at least in one corner after the oil in the center is displaced by gas. After the displacement, the configuration in two corners are changed to $C$ and in one corner to $F$. Once the configurations are changed, the center phase location must be omitted from the trapped oil cluster and
added to the trapped gas cluster as it now accommodates gas. Also one oil layer phase location residing in one of the corners must be added to the displaced trapped oil cluster. The new displacements that must be added to the appropriate lists are:

- oil layer collapse by water in the corner to be added into the right sublist, i.e. the sublist with the same cluster number, within the wcot category provided that water in the corner is continuous,
- oil layer collapse by gas in the center to be added into the right sublist within the gtot category,
- snap-off of the gas in the center by oil layer to be added into the right sublist within the otgt category,
- snap-off of gas in the center by water in the corners to be added into the right sublist within the wcgt category and other displacements in connection with continuous and trapped fluids residing in the neighboring elements.

### 6.5 Saturation Computation

Saturation is computed when the phase pressure reaches a new maximum - this means that the system is at equilibrium and it is not possible to carry out any displacements with the current phase pressures. If $V^i_p$ is the volume of phase $p$ in element $i$ (including the water volume in clay) then the saturation of phase $p$ is given by:

$$S_p = \frac{\sum_{i=1}^{n_e} V^i_p + V^{error}_p}{\sum_{p=1}^{n_p} \sum_{i=1}^{n_e} V^i_p + \sum_{j=1}^{n_e} V^j_p}$$  \hspace{1cm} (6.15)$$

where $n_p$ is the number of phases, $n_e$ is the total number of pores and throats, and $V^{error}_p$ is the volume error of phase $p$ caused by multiple displacements and is given by:

$$V^{error}_p = \sum_{i=1}^{n_p^c} (V_{\text{original}}^p - V_{\text{present}}^p)$$ \hspace{1cm} (6.16)$$

where $n_p^c$ is the number of trapped clusters of phase $p$. The total volume, inscribed radius, and shape of each element are read in as input data. The volume of a phase in an element is the total volume multiplied by the fraction of the cross-sectional area occupied by that phase. One should note that saturation is computed within the selected region, i.e. between inlet and outlet surfaces of the network rather than over the whole network (see section (6.6) for details). Expressions used to compute areas are given next.
6.5.1 Area Open to Flow

The equations used to compute the total area of a pore or throat with different cross-sections are:

\[ A_t = \pi R^2 \quad \text{Circular cross-section} \quad (6.17) \]

\[ A_t = 4R^2 \quad \text{Square cross-section} \quad (6.18) \]

\[ A_t = \frac{R^2}{4G} \quad \text{Triangular cross-section} \quad (6.19) \]

where \( R \) and \( G \) are the inscribed radius and shape factor of the pore or throat, respectively.

The corner area open to flow is calculated using:

\[ A_c = r^2 \left[ \cos \theta (\cot \alpha \cos \theta - \sin \theta) + \theta + \alpha - \frac{\pi}{2} \right] \quad (6.20) \]

\[ A_c = \left[ r \frac{\cos(\theta + \alpha)}{\sin \alpha} \right]^2 \sin \alpha \cos \alpha \quad if \quad \alpha + \theta = \frac{\pi}{2} \quad (6.21) \]

where \( r \) is the radius of curvature which corresponds to the ratio of interfacial tension to the capillary pressure of the interface, \( \alpha \) is the corner half angle and \( \theta \) is the angle that the interface makes with the solid surface towards the corner not necessarily the contact angle of the interface, e.g. \( \theta_I \) and \( \theta_{II} \) in Fig. (6.5).

If a layer is present in the corner, the layer area is the total area of the corner including the layer minus the corner area excluding the layer and both are calculated using Eqs. (6.20) and (6.21) but with pertinent \( r \) and \( \theta \). For instance, in configuration group F, first the total corner area, \( A_c = A_{w\,\text{corner}} + A_{o\,\text{layer}} \), is calculated with \( r \) and \( \theta \) of the gas/oil interface and then \( A_{w\,\text{corner}} \) is found using \( r \) and \( \theta \) of the oil/water interface. Then \( A_{o\,\text{layer}} = A_c - A_{w\,\text{corner}} \). The same procedure is used to calculate the area of the the second layer, if present.

The area open to flow to a phase in the center of an angular element is the total area of the element minus the summation of the corner areas, including the layers (if present).
6.6 Conductances - Absolute and Relative Permeabilities

When saturation is computed, relative permeability and capillary pressure can also be found. This is not done after every saturation computation to save computer time. Typically, relative permeability is calculated around 20 - 40 times during a simulation. To compute absolute and relative permeability, conductances of each continuous phase location in each element are first computed. Normally exact analytic results are not possible, and empirical expressions derived from solutions of the Stoke’s equation for flow in pores of different geometries and for different fluid configurations are used [75–77, 125, 260, 288, 289]. See later for expressions for the conductances of each phase for the configurations shown in Figs. (5.1) and (5.2). Then the average conductance for each phase in the whole network is computed by explicitly calculating the flow through the network assuming conservation of volume. From this absolute and relative permeability can be found [76, 125, 141, 285].

Solving the system of linear equations for each phase gives the pressure of that phase in all the pores that contain that continuous phase. If there is an interface between any of the phases in a pore or between the pore and connected throats then the difference between the pressures of those two phases in that pore corresponds to capillary pressure between those two phases [143].

In order to minimize end effects on calculated macroscopic properties, we calculate the properties within two surfaces perpendicular to the main flow direction.
bounding the central 90% of the network. However, the pressure is solved over whole network to find the pressure in each pore. The pressure of the fluid whose permeability is being calculated is found at the two surfaces by:

\[ P_a = \frac{\sum_{i=1}^{n} P_a^i A_a^i}{\sum_{i=1}^{n} A_a^i} \]  

(6.22)

where \( P_a \) is the pressure of phase \( a \) at the surface, \( P_a^i \) is the pressure of phase \( a \) in a pore or throat at the point that touches the surface, \( A_a^i \) is the area open to flow for phase \( a \) through that pore or throat, and \( n \) is the number of pores and throats touching the surface. When the element that touches the surface is a pore then the pressure of the phase \( a \) at the touching point will be the pore pressure of fluid \( a \) and is known after the pressure is solved over the whole network. But if it is a throat, then the pressure at the touching point is found by a linear interpolation between the pressures of phase \( a \) in two connecting pores located in two sides of the surface. This is similar to the procedure used by Øren et al. [76].

The absolute permeability of the network is calculated using Darcy’s law:

\[ K = \frac{\mu_a Q_{a\text{total}} L}{A \Delta P} \]  

(6.23)

where \( K \) is the absolute permeability, \( \mu_a \) the viscosity of fluid \( a \), \( L \) is the distance and \( \Delta P \) is the corresponding pressure drop between the vertical surfaces. \( A \) is the cross-sectional area perpendicular to the main direction of flow, \( Q_{a\text{total}} \) is the total flow rate of fluid \( a \).

First it is assumed that the network is completely filled with only one phase, e.g. \( a \). Conductance is calculated using the following equations [76, 290]:

\[ g = \frac{0.5GA^2}{\mu} \] \hspace{1cm} Circular cross-section \hspace{1cm} (6.24)

\[ g = \frac{0.5623GA^2}{\mu} \] \hspace{1cm} Square cross-section \hspace{1cm} (6.25)

And for triangular cross-sections:

\[ g = \frac{3R^2A}{20\mu} \]  

(6.26)

A pore might be connected to several other pores by throats (see Fig. (6.6)). The conductance of a phase \( a \), through an assembly of two pores connected to each other by a throat, is considered to be the harmonic mean of the conductance to the
phase through the pores and the connecting throat [141]:

\[
\frac{L_{ij}}{g_{ij}^a} = \frac{L_{tij}}{g_{ij}^a} + \frac{L_{pij}}{g_{ij}^a} + \frac{L_{pji}}{g_{ij}^a} \tag{6.27}
\]

where \( L_{ij} \) is the distance between the centers of two connected pores, \( g_{ij}^a \) is the conductance of the assembly to phase \( a \), \( L_{tij} \) is the throat length, \( g_{ij}^a \) the throat conductance to phase \( a \), \( L_{pij} \) and \( L_{pji} \) are the half length of the pores, and \( g_{ij}^a \) and \( g_{ij}^a \) are conductance of the pores \( i \) and \( j \) to phase \( a \), respectively, see Fig. (6.6).

The flow rate of the phase between two connected pores, i.e. \( q_{ij}^a \) is then given by [141]:

\[
q_{ij}^a = \frac{g_{ij}^a}{L_{ij}} (P_{ap_i} - P_{ap_j}) \tag{6.28}
\]

where \( P_{ap_i} \) and \( P_{ap_j} \) are the pressures of fluid \( a \) in pores \( i \) and \( j \) respectively.

Conserving volume for fluid \( a \) in each pore gives:

\[
\sum_{i=1}^{m_i} q_{ij}^a = 0 \tag{6.29}
\]

where \( m_i \) is the number of connected throat-pores containing continuous phase \( a \). If Eq. (6.27) is written for all such throat-pores and then inserted into Eq. (6.29), a system of linear equations is formed:

\[
P_{p1}^a \sum_{j=1}^{m_1} \frac{g_{1j}^a}{L_{1j}} - \sum_{j=1}^{m_1} \frac{g_{1j}^a}{L_{1j}} P_{p_j}^a = 0
\]

\[
P_{p2}^a \sum_{j=1}^{m_2} \frac{g_{2j}^a}{L_{2j}} - \sum_{j=1}^{m_2} \frac{g_{2j}^a}{L_{2j}} P_{p_j}^a = 0
\]

\[
\ldots
\]

\[
P_{pn}^a \sum_{j=1}^{m_n} \frac{g_{nj}^a}{L_{nj}} - \sum_{j=1}^{m_n} \frac{g_{nj}^a}{L_{nj}} P_{p_j}^a = 0 \tag{6.30}
\]

The resultant system of linear equations for the pore pressures is solved using the Conjugate Gradient method [76, 125]. Having the pore pressures allows us to calculate the total flow rate of the phase, i.e. \( Q_{\text{total}}^a \), which in turn is used in Eq. (6.23) to calculate the absolute permeability of the network, \( K \).

Relative permeabilities are computed only when the network contains more than one phase. They are calculated only for phases that have at least one network-
spanning cluster (a cluster that is continuous from inlet to outlet).

First the conductance in all the pore and throats containing continuous phase \(a\) is computed. Then using the same procedure used for the calculation of absolute permeability, the pressures of the phase in the pores that are a member of spanning cluster(s) are found which in turn allows us to calculate relative permeability of the phase by:

\[
k^a_r = \frac{Q^a_{total}}{Q_{single\ phase}^{single\ phase}} \tag{6.31}
\]

Relative permeabilities are calculated only when the system is relaxed otherwise...
there will be configurations that are not stable at the pressure at which the relative permeabilities are calculated. The number of linear equations to be solved will be lower than that for single-phase flow simply because the network is filled by multiple phases meaning that not all the elements might contain continuous phase $a$.

When a network has elements with non-circular cross-section, a single element might accommodate up to three fluids in it. A fluid, as it was shown in Figs. (5.1) and (5.2), might be residing in corners, layers or the center of a non-circular element. For the fluid flowing through the center of an element, Eqs. (6.24), (6.25), and (6.26) are still used with $A$ being only the area open to flow to the fluid at the center.

Fluid flow through the corners and layers is yet more complex considering the involved physics. Parameters such as wettability, fluid-fluid and fluid-solid boundary conditions, corner half angle, surface shear viscosity and physical properties of fluids affect the conductances. This have been investigated by several authors. One group has tried to solve the fluid flow numerically using Navier-Stokes equations and then empirically correlate the numerical results and propose expressions for laminar corner flow [76, 110, 288, 291–293]. Another approach is to apply the hydraulic diameter approximation which was used by Lenormand and Zarcone [294] for flow in square cross-section tubes. Blunt et al. [67] used a thin film flow approximation to study the oil layer flow regime in a gravity drainage process. Later, Zhou et al. [289] combined the hydraulic diameter and the thin film flow approximations to derive expressions for corner and layer flow which were later modified by Hui & Blunt [260, 261]. The proposed expressions were successful in predicting experimental measurements [289, 295]. The authors found free and no-flow boundary conditions suitable for gas/oil and oil/water interfaces, respectively.

In this work, we use the expressions proposed by Hui & Blunt [260, 261] to compute the conductance of wetting and spreading layers.

When $\theta_l \leq \frac{\pi}{2} - \alpha$, see Fig. (6.5)-(a), the conductance of the element to the phase flowing at the corner can be estimated by:

\[
g = \frac{A^2 (1 - \sin \alpha)^2 (\varphi_2 \cos \theta - \varphi_1) \varphi_3^2}{12 \mu \sin^2 \alpha (1 - \varphi_3)^2 (\varphi_2 + f \varphi_1)^2} \tag{6.32}
\]

\[
\varphi_1 = \left( \frac{\pi}{2} - \alpha - \theta \right) \tag{6.33}
\]

\[
\varphi_2 = \cot \alpha \cos \theta - \sin \theta \tag{6.34}
\]
\[ \varphi_3 = \left( \frac{\pi}{2} - \alpha \right) \tan \alpha \]  

(6.35)

where \( \theta = \theta_I \), \( A_c = A_I \), \( f = 1 \) for a no-flow boundary condition suitable for oil/water interfaces, and \( f = 0 \) when a free boundary condition is applied for gas/oil or gas/water interfaces.

If \( \theta_I > \frac{\pi}{2} - \alpha \), see Fig. (6.5)-(b), the corner conductance is calculated using:

\[ g = \frac{A_c^2 \tan \alpha (1 - \sin \alpha)^2 \varphi_3^2}{12 \mu \sin^2 \alpha (1 - \varphi_3)(1 + f \varphi_3)^2} \]  

(6.36)

When there is a fluid layer sandwiched between the phases residing in the corner and center, corner and layer or layer and center (see Figs. (5.1) and (5.2)), the conductance of the element to the sandwiched phase can be estimated by:

\[ g = \frac{A_1^3 (1 - \sin \alpha)^2 \tan \alpha \varphi_3^2}{12 \mu A_c \sin^2 \alpha (1 - \varphi_3) \left[ 1 + f_1 \varphi_3 - (1 - f_2 A_2) \sqrt{\frac{A_2}{A_c}} \right]^2} \]  

(6.37)

where \( A_1 \) is the area of the layer that the conductance is being calculated for, \( A_c \) is a summation of areas of corner and layer (if present) above the layer of interest, and \( A_2 = A_c - A_1 \). For instance, to calculate the conductance of the gas layer in configuration group J, see Fig. (5.2), \( A_1 = A_{g\text{layer}} \), \( A_c = A_{w\text{corner}} + A_{o\text{layer}} + A_{g\text{layer}} \), and \( A_2 = A_{w\text{corner}} + A_{o\text{layer}} \). The corner and layer areas are calculated using Eqs. (6.20) and (6.21).

### 6.7 Saturation Path Tracking

As several authors have shown (see section (3.1)), macroscopic properties in three-phase systems are strongly dependent on the saturation history of the system. This means that prediction of experimental measurements is possible only if the experimental saturation history is reproduced by the model. It is only then that the computed properties are comparable with their experimental counterparts. In this work, we present an algorithm to track the experimental saturation paths on a point by point basis.

The network model is designed to compute capillary pressure and relative permeability for a given input saturation path. Every given saturation path is composed of a series of points in the saturation space. The first saturation target (of oil, water, and gas) is specified. The difference between the present saturations and the target saturations are found. The phase with the most negative difference is the next to
be injected. Imagine this is phase $i$. This means that we consider a displacement
where the volume of $i$ in an element increases. Injection of phase $i$ continues until
the difference between the present and the target saturation of phase $i$ is not the
most negative difference. Another phase with the most negative difference is then
injected. This continues until the saturation differences fall within a predefined tol-
erance. Then a new saturation target is considered. This process continues until
the desired saturation path is produced, see Fig. (6.7).

\[ S_o, S_w, S_g \]

\[ S_{o}^{n+1}, S_{w}^{n+1}, S_{g}^{n+1} \]

\[ S_{o}^{n}, S_{w}^{n}, S_{g}^{n} \]

Figure 6.7: Schematic presentation of saturation tracking method

Tracking an experimental path using a network model is practically very complex
and difficult. This is because of finite size effects, the percolation nature of the
processes and hysteresis. For instance, in some cases during a saturation tracking
procedure, the system does not relax before several thousand displacements have
been performed which will take the saturations far away from the desired path.
However, in the cases we present in this work, this does not significantly affect the
results.
Chapter 7

Two- and Three-Phase Relative Permeabilities

In this chapter, we use our model to simulate different two- and three-phase processes at the pore-level and compare the results with their experimental counterparts. Tables (7.1) and (7.2) present the interfacial tensions and contact angles that have been used throughout this chapter.

Table 7.1: Interfacial tensions and spreading coefficients (mN/m) used in this work.

<table>
<thead>
<tr>
<th>Fluids</th>
<th>$\sigma_{ow}$</th>
<th>$\sigma_{go}$</th>
<th>$\sigma_{gw}$</th>
<th>$C_s$</th>
<th>Reference(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hexane-water-air</td>
<td>48</td>
<td>19</td>
<td>67</td>
<td>0</td>
<td>[260, 295]</td>
</tr>
</tbody>
</table>

Table 7.2: Contact angles (degrees) used in this work.

<table>
<thead>
<tr>
<th>$\theta_{PD}$</th>
<th>$\theta_{gw}$</th>
<th>$\theta_{ow}$</th>
<th>$\theta_{go}$</th>
<th>$\theta_{ao}$</th>
<th>$\theta_{rgw}$</th>
<th>$\theta_{rgw}$</th>
<th>$\theta_{rgo}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>10-60</td>
<td>30-80</td>
<td>0</td>
<td>0</td>
<td>8.5-50.1</td>
<td>25.3-65.9</td>
</tr>
</tbody>
</table>

7.1 Two-Phase Simulations

7.1.1 Primary Drainage and Comparison with Experiment

We compare the network model predictions with experimental two-phase data from water-wet Berea cores [1]. During drainage, the receding contact angle is assumed to be $0^\circ$; there are no other parameters to adjust. Fig. 7.1 shows the prediction. We
are able to predict the relative permeabilities accurately. These results are similar to those obtained using a two-phase code by Valvatne & Blunt [133].

![Comparison of experimental and predicted relative permeabilities during primary drainage](image)

**Figure 7.1:** Comparison of experimental [1] and predicted relative permeabilities during primary drainage in Berea sandstone.

### 7.1.2 Water Flooding and Comparison with Experiment

To predict the imbibition data, we assumed a uniform distribution of advancing contact angles with a minimum of $30^\circ$ and adjusted the maximum value of contact angle to fit the data. The best match, shown in Fig. (7.2), was obtained using a maximum advancing contact angle of $80^\circ$. Small changes in the contact angle distribution did not adversely affect the match.

### 7.1.3 Effects of Wettability

In order to investigate the effects of wettability on water flooding results, two different uniformly distributed advancing oil/water contact angles, i.e. (I) strongly water-wet, $\theta_{ow}^a = 30^\circ - 80^\circ$, and (II) strongly oil-wet, $\theta_{ow}^o = 110^\circ - 180^\circ$, were used to run the model.

Fig. (7.3) shows oil and water relative permeabilities for these two cases. The water relative permeability for the strongly oil-wet system at low water saturation is
lower than that of the water-wet case because at low water saturation there are not many network-spanning water-filled oil-wet elements since it is a drainage process and the biggest pores and throats are filled first. At higher water saturation the water relative permeability in the oil-wet system is larger since water occupies the larger pore spaces. When the wettability changes from water-wet to oil-wet, the oil relative permeability decreases since oil becomes the wetting phase and occupies the smaller pores and throats.

Table (7.3) indicates the residual oil saturation for systems with different wettability. The water-wet system has the highest residual oil saturation because snap-off traps oil. The lowest residual oil saturation is found in the oil-wet system since oil layers prevent trapping. Oil and water occupancy in systems with different wettability are also illustrated in Figs. (7.4) and (7.5). This behavior is consistent with that found by other authors such as McDougall & Sorbie [111] and Dixit et al. [118, 120, 296, 297].
Figure 7.3: Oil and water relative permeability of water flooding in: (I) strongly water-wet, $\theta_{ow} = 30^\circ - 80^\circ$, and (II) strongly oil-wet, $\theta_{ow} = 110^\circ - 180^\circ$ Berea sandstone.

Table 7.3: Residual oil saturation at the end of water flooding in Berea sandstone with different wettabilities.

<table>
<thead>
<tr>
<th>$\theta_{ow}$</th>
<th>Residual Oil Saturation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$30^\circ - 80^\circ$</td>
<td>0.374</td>
</tr>
<tr>
<td>$110^\circ - 180^\circ$</td>
<td>0.0055</td>
</tr>
</tbody>
</table>

7.2 Three-Phase Simulations

7.2.1 Comparison with Experiment

Fig. (7.6) shows a comparison of predicted three-phase oil relative permeability with the measured steady-state values published by Oak [1]. The predicted results are produced by tertiary gas injection into different initial oil saturations maintaining a constant oil/water capillary pressure. As it is seen, an excellent agreement has been obtained. The experimental data and predictions are scattered in a quite similar manner. The scatter arises because in a water-wet system oil is the intermediate-wet phase and its relative permeability is a strong function of saturation history and initial oil saturation [148–150, 260, 261]. These predictions are similar to those
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Figure 7.4: Oil and water occupancy at the end of water flooding in a strongly water-wet Berea sandstone, $\theta_{ow} = 30^\circ - 80^\circ$.

Figure 7.5: Oil and water occupancy at the end of water flooding in a strongly oil-wet Berea sandstone, $\theta_{ow} = 110^\circ - 180^\circ$.

obtained using a water-wet three-phase network model by Lerdahl et al. [146].

Fig. (7.7) illustrates the comparison between predicted and measured three-
phase gas relative permeability. Again the predictions are in a very good agreement with the measured values. At high gas saturation, predictions and experimental data are not very scattered because gas is the most non-wetting phase in a water-wet system, and its relative permeability is a function of only its own saturation. However, the measured values at low gas saturations are quite scattered and this is because of difficulties in the experiments [1, 146]. Predicted values at low gas saturation are zero due to finite size effects. This is again in agreement with the work by Lerdahl et al. [146].

Fig. (7.8) presents the comparison between predicted three-phase water relative permeability and measured values. As it is seen, the water relative permeability is slightly over estimated. The reason is not known but it may be due to measurement difficulties because in water-wet systems it is expected that the water relative permeability to be a function of only its own saturation but this is not quite the case in the reported experiments.

While these results are very encouraging, we are comparing two clouds of points with considerable scatter. In the next section we go one step further and attempt a more rigorous analysis by comparing experiments on a point-by-point basis.
Figure 7.7: Comparison of measured and predicted three-phase gas relative permeability. Points represent the measured values and the curves are the predicted ones.

Figure 7.8: Comparison of measured and predicted three-phase water relative permeability. Points represent the measured values and the curves are the predicted ones.
7.2.2 Comparison with Experiment Using Saturation Tracking

We apply our saturation tracking algorithm presented in section (6.7) to produce identical saturation paths as the measured ones and then compare the predicted and measured relative permeabilities. This is of interest in three-phase flow due to the fact that three-phase macroscopic properties are a strong function of saturation history (path).

We analyze two experiments with high and low initial oil saturations, Experiment 9 - Sample 13 and Experiment 5 - Sample 14 by Oak [1].

- **High Initial Oil Saturation**

Fig. (7.9) indicates the predicted and measured saturation path for a high initial oil saturation experiment, Experiment 9 - Sample 13. The initial point was produced by primary drainage and the saturation tracking algorithm was used to reproduce the experimental path. We were able to reproduce the same path as the experiment.

![Figure 7.9: Comparison of measured and predicted saturation paths for Experiment 9 of Sample 13 of Oak experiments [1].](image)

Fig. (7.10) compares the predicted and measured three-phase oil relative permeability for Experiment 9 - Sample 14. The prediction compares well with
the measured values at high oil saturations but tends to over-predict at low oil saturations. The reason for this is not very clear at this stage but it may be due to scatter in the data, the uncertainty associated with the layer conductance estimations and also the representation of the void space of the rock by different idealized angular geometries.

Fig. (7.11) illustrates the comparison between the predicted and measured three-phase gas relative permeability. The agreement is excellent. Due to finite size effects the predicted values at low gas saturations were zero.

Fig. (7.12) compares the predicted three-phase water relative permeability with the measured values. The agreement is fairly good. We slightly overestimate the relative permeability, as discussed in the previous section.

- **Low Initial Oil Saturation**

  The physics involved with gas injection into very low water flood residual oil is very complex. This is because all the residual oil is trapped and several micromodel experiments [59–68, 70, 71] have shown that when gas is injected into such a spreading system the two phenomena of double displacement and oil layer formation make the oil continuous which allows it to drain to very low saturation. This in turn involves coalescence, formation and break-up of
trapped clusters of oil. Reproduction of this behavior is very difficult as it is very complex. We have implemented these processes in our model and here we compare the results with the measured values of relative permeabilities.
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Figure 7.13: Comparison of measured and predicted saturation paths for Experiment 5 of Sample 14 of Oak experiments [1].

Fig (7.13) compares the predicted and measured saturation path for a low initial oil saturation experiment, Experiment 5 - Sample 14 by Oak [1].

Figure 7.14: Comparison of measured and predicted three-phase oil relative permeabilities for Experiment 5 of Sample 14 of Oak experiments [1].
Fig. (7.14) shows the comparison between predicted and measured three-phase oil relative permeability for this experiment. Since it is not clear if the initial point of the experiment was actually produced by primary drainage or water flooding, we present results for both scenarios. The very low values of three-phase oil relative permeability and the oil saturation range of the experiment suggests that the initial point was produced by water flooding and the process was tertiary gas injection. The agreement between the measured and predicted values is very good. However, if it is assumed that the initial point was reached by primary drainage, the predicted oil relative permeability would be higher, as indicated in Fig. (7.14). This is because the oil/water capillary pressure is higher and consequently the oil layers are more stable.

![Graph showing comparison between measured and predicted three-phase gas relative permeabilities](image)

Figure 7.15: Comparison of measured and predicted three-phase gas relative permeabilities for Experiment 5 of Sample 14 of Oak experiments. [1]

Fig. (7.15) compares the predicted and measured three-phase gas relative permeability. The agreement is excellent. The gas relative permeability if the initial point was reached by primary drainage is higher than that of the water flooding case. This is due to blocking by trapped blobs of oil in the latter case which prevents gas entering larger elements. However, later in the displacement gas pushes the trapped clusters of oil into the intermediate size elements by double displacement.

Fig (7.16) shows the comparison between the measured and predicted three-
Figure 7.16: Comparison of measured and predicted three-phase water relative permeabilities for Experiment 5 of Sample 14 of Oak experiments [1].

Three-phase water relative permeability for Experiment 5 - Sample 14. The agreement is very good. The predictions when the initial point is produced by primary drainage are slightly higher than that for water flooding. This is because water is pushed into smaller pores and throats by the double displacement mechanism in the latter case which in turn means lower water relative permeability.

Figs. (7.17), (7.18), (7.19), and (7.20) show predicted oil, water and gas occupancy for Experiment 5 of Sample 14 at different oil saturations. As it is seen, gas tends to push oil to smaller elements while it is recovered.
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Figure 7.17: Predicted oil, water, and gas occupancy for Experiment 5 of Sample 14 at oil saturation about 27%.

Figure 7.18: Predicted oil, water, and gas occupancy for Experiment 5 of Sample 14 at oil saturation about 15%.
Figure 7.19: Predicted oil, water, and gas occupancy for Experiment 5 of Sample 14 at oil saturation about 8%.

Figure 7.20: Predicted oil, water, and gas occupancy for Experiment 5 of Sample 14 at oil saturation less than 1%.
7.2.3 Secondary Gas Injection and the Effects of Initial Oil Saturation

We now use our model to study different cases that have not necessarily been studied experimentally. Here we simulate gas injection into different initial oil saturations after primary drainage, i.e. secondary gas injection assuming a fixed oil/water capillary pressure. Fig. (7.21) presents the saturation paths taken by each simulation. Since the gas/oil interfacial tension is lower than that of the gas/water, gas displaces oil first and then at residual oil saturation (close to zero) starts displacing water.

\[ \text{Soi} = 0.05 \]
\[ \text{Soi} = 0.15 \]
\[ \text{Soi} = 0.25 \]
\[ \text{Soi} = 0.35 \]
\[ \text{Soi} = 0.45 \]
\[ \text{Soi} = 0.55 \]
\[ \text{Soi} = 0.65 \]
\[ \text{Soi} = 0.76 \]

Figure 7.21: Saturation paths for secondary gas injection with different initial oil saturations in a spreading system.

Fig. (7.22) compares the three-phase oil relative permeability for secondary gas injection with different initial oil saturations. At high oil saturation, the higher the oil saturation, the lower the oil relative permeability and this a consequence of the fact that at the same oil saturation, oil stays in larger elements for low initial oil saturation while it will reside in the smaller ones when the initial oil saturation is high, Van Dijke et al. [148–150] and Hui & Blunt [260, 261]. But at low oil saturations, the higher the initial oil saturation the higher the oil relative permeability. This is due to direct effect of initial oil saturation on oil layer stability. At higher initial oil saturations the oil/water capillary pressure, or oil pressure, is higher which in turn means the oil layers are thicker compared to the lower initial oil saturation.
saturations where oil/water capillary pressure is lower (see section (4.5.2) for layer stability analysis). Thicker layers have a larger conductance and will collapse later in the displacement.

Figure 7.22: Three-phase oil relative permeabilities for secondary gas injection with different initial oil saturations.

Figs. (7.23) and (7.24) illustrate three-phase gas and water relative permeabilities for secondary gas injection with different initial oil saturations respectively. Since the system is water-wet, gas and water relative permeabilities are a function of only their own saturations and this is why initial oil saturation does not show any effect on their behavior.

Figs. (7.25) and (7.26) indicate gas/oil and gas/water capillary pressures for the secondary gas injections. The gas/water capillary pressure for secondary gas injection into an initial oil saturation of 0.76 exhibits much higher values than the others in Fig. (7.26). This is because gas injection has been done into very high initial oil saturation (connate water saturation) corresponding to a very high oil/water capillary or oil pressure.
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Figure 7.23: Three-phase gas relative permeabilities for secondary gas injection with different initial oil saturations.

Figure 7.24: Three-phase water relative permeabilities for secondary gas injection with different initial oil saturations.
Figure 7.25: Gas/oil capillary pressure for secondary gas injection with different initial oil saturations.

Figure 7.26: Gas/water capillary pressure for secondary gas injection with different initial oil saturations.
7.2.4 Tertiary Gas Injection and the Effects of Initial Oil Saturation

In this section, we present results for gas injection into different oil saturations after water flooding, tertiary gas injection assuming a fixed oil/water capillary pressure. The effects of initial oil saturation on the predicted relative permeabilities are discussed. Fig. (7.27) indicates the saturation paths for tertiary gas injection with different initial oil saturations. The higher the initial oil saturation the lower the tertiary gas injection residual oil saturation (the reason for this behavior is discussed shortly).

![Saturation paths for tertiary gas injection with different initial oil saturations](image)

Figure 7.27: Saturation paths for tertiary gas injection with different initial oil saturations in a spreading system.

Fig. (7.28) shows the three-phase oil relative permeability for tertiary gas injection into different initial oil saturation. Similar to those of secondary gas injection, at high oil saturations, the oil relative permeability is higher for lower initial oil saturation which is not the case at low oil saturations. The reason for this kind of behavior is similar to that of the secondary gas injection as discussed above. As mentioned before, when the initial oil saturation is higher, oil layers stay stable until a higher gas pressure. This will maintain the connectivity of oil that results in lower residual oil saturation for gas injection into higher initial oil saturation.

Figs. (7.29) and (7.30) indicate the three-phase gas and water relative perme-
Figure 7.28: Three-phase oil relative permeabilities for tertiary gas injection with different initial oil saturations.

abilities for tertiary gas injection. They all behave similarly as gas and water relative permeabilities depend only on their own saturation although there are some subtle differences, as discussed when analyzing the experimental data. Figs. (7.32) and (7.31) show gas/water and gas/oil capillary pressures for the different tertiary gas injections. Gas/oil and gas/water capillary pressures are quite similar to each other since the oil/water capillary pressure is low due to water flooding before gas injection.
Figure 7.29: Three-phase gas relative permeabilities for tertiary gas injection with different initial oil saturations.

Figure 7.30: Three-phase water relative permeabilities for tertiary gas injection with different initial oil saturations.
Figure 7.31: Gas/oil capillary pressure for tertiary gas injection with different initial oil saturations.

Figure 7.32: Gas/water capillary pressure for tertiary gas injection with different initial oil saturations.
7.2.5 Comparison of Secondary and Tertiary Gas Injection

Here we compare secondary with tertiary gas injection. Figs. (7.33), (7.34), and (7.35) illustrate three-phase oil, gas, and water relative permeabilities for secondary and tertiary gas injections into an initial oil saturation of 0.55. Fig. (7.33) shows that the three-phase oil relative permeability for secondary gas injection is not very different from tertiary gas injection at high oil saturations where layer flow is not dominant, but that is not the case at low oil saturation. At low oil saturations, oil flows mainly through the spreading layers that are more stable during secondary gas injection due to the higher oil/water capillary pressure in compare with tertiary gas injection, where the oil layers are less stable due to the low oil/water capillary pressure caused by water flooding. This means higher oil relative permeability for secondary gas injection than for tertiary gas injection with the same initial oil saturation.

Figure 7.33: Comparison of three-phase oil relative permeability for secondary and tertiary gas injection with an initial oil saturation of 0.55.

In Fig. (7.33) at high oil saturation we see, approximately, \( k_{ro} \propto S_o^4 \). The oil relative permeability is controlled by the network of pores and throats filled with oil in the centers and it drops rapidly with oil saturation as this network becomes less well connected. For secondary gas injection, at an oil saturation approximately
equal to the water flood residual, we see a cross-over to a layer drainage regime where approximately $k_{ro} \propto S_o^2$. This is easily explained theoretically [53, 142, 298–300]. The hydraulic conductance of the layers is proportional to the square of the cross-sectional area of oil. When most oil is flowing in layers, the oil saturation is proportional to the oil area, leading to the quadratic relative permeability. This behavior has been observed in other gas injection and gravity drainage experiments [142, 259, 298–300]. Notice that the apparent log-log slope at low saturation is slightly larger than 2. This is because some small throats are still oil-filled in the layer drainage regime and when they are occupied by gas, their contribution to the oil relative permeability drops significantly. For tertiary gas injection, this oil layer drainage regime is not observed - this is because oil layers collapse during the displacement leading to very low oil relative permeabilities.

Figs. (7.34) and (7.35) do not show a significant difference in three-phase gas and water relative permeabilities of secondary and tertiary gas injections, respectively. Again this is because they depend on only their own saturations.

Figure 7.34: Comparison of three-phase gas relative permeability for secondary and tertiary gas injection with an initial oil saturation of 0.55.
Figure 7.35: Comparison of three-phase water relative permeability for secondary and tertiary gas injection with an initial oil saturation of 0.55.

7.2.6 Effects of Wettability

We will now use our model to predict relative permeability for three-phase mixed-wet systems. In this case, we do not have experimental data to compare against, but the success of network modeling predictions for mixed-wet two-phase systems [133, 301] and water-wet two- and three-phase systems gives us some confidence that our results are valid. We consider primary drainage to connate water saturation followed by water flooding to $S_w = 0.4$ ($S_{oi} = 0.6$). Then gas is injected at a constant oil/water capillary pressure. We study two cases: water-wet, where the distribution of advancing oil/water contact angles is the same as used to predict the two-and three-phase data (uniform from $30^\circ - 80^\circ$); and oil-wet where the distribution of advancing contact angles ($110^\circ - 180^\circ$) is the same as used to predict mixed-wet water flood data [301].

Fig. (7.36) shows the oil relative permeability. In the oil-wet case, oil remains in smaller pores and throats after water flooding than for a water-wet medium, giving a lower relative permeability. This is seen in Fig. (7.36) for oil saturations larger than approximately 0.4. At lower oil saturations, gas has invaded most of the oil-filled elements. The relative permeability is limited by the connectivity of the oil phase. In the water-wet medium, oil layers collapse during gas injection, whereas oil layers
remain stable throughout the displacement for the oil-wet case (see layer stability analysis in section (4.5.2)). Thus, the oil-wet relative permeability is larger at low oil saturation.

![Figure 7.36: Effects of wettability on three-phase oil relative permeability. Curves for tertiary gas injection into a water-wet and oil-wet system with initial oil saturation of 0.6 are shown.](image)

The water-wet gas relative permeability in Fig. (7.37) is larger than the oil-wet case at high gas saturation. In a water-wet medium, the gas always occupies the largest pores and throats. For an oil-wet system, gas is not the most non-wetting phase in the presence of water and will displace water from some of the smaller pores, resulting in poorer connectivity and conductance. This effect of wettability has been discussed previously [260] and is well established experimentally [145, 299, 300]. This result is a direct consequence on the constraint on contact angles, Eq. (2.6) [244]. At low gas saturation, the gas relative permeability in the water-wet system is lower than for oil-wet case since in the water-wet system gas is the most non-wetting phase and fills the biggest pores and throats leading to lower number of network-spanning gas clusters.

The water relative permeability in Fig. (7.38) is at first sight surprising. One might expect that the water relative permeability for the oil-wet case to be higher than for the water-wet medium, since water can be non-wetting to both oil and gas in oil-wet systems, occupying the larger pore spaces. The explanation is that during
Figure 7.37: Effects of wettability on three-phase gas relative permeability. Curves for tertiary gas injection into a water-wet and oil-wet system with initial oil saturation of 0.6 are shown.

Water flooding water invades the larger pores and throats in the oil-wet medium. This results in an increase in water saturation, but the oil-wet water-filled elements fail to span the network, meaning that the water relative permeability remains very low. During gas injection, since gas displaces water, the water relative permeability can only decrease from its already negligible value. Figs. (7.39) and (7.40) show the effects of wettability on gas/oil and gas/water capillary pressures. The gas/water capillary pressure in the oil-wet system is lower than that of the water-wet case because the oil/water capillary pressure of the oil-wet case is lower than for the water-wet system.

We shall not discuss the effects of spreading coefficient on fluid flow behavior as they have been investigated extensively by several authors [24, 59, 61, 63, 64, 66, 67, 70, 139, 242, 287, 302, 303].
Figure 7.38: Effects of wettability on three-phase water relative permeability. Curves for tertiary gas injection into a water-wet and oil-wet system with initial oil saturation of 0.6 are shown.

Figure 7.39: Effects of wettability on gas/oil capillary pressure. Curves for tertiary gas injection into a water-wet and oil-wet system with initial oil saturation of 0.6 are shown.
Figure 7.40: Effects of wettability on gas/water capillary pressure. Curves for tertiary gas injection into a water-wet and oil-wet system with initial oil saturation of 0.6 are shown.
Chapter 8

Summary and Conclusions

8.1 Model Development

Based on today’s knowledge on physics of two- and three-phase flow in porous media at the pore-level, a definitive capillary dominated three-phase network model was developed that combines three essential components:

1. A description of the pore space and its connectivity that mimics real systems
2. A physically-based model of wettability alteration
3. A full description of fluid configurations for two- and three-phase flow

We described in detail how the model was developed and works. We also presented a new and robust clustering algorithm that is critically important to capture different displacement mechanisms. The model includes the following features:

- Mixed wettability
- Wetting layers
- Spreading layers
- Hysteresis and wettability alteration are fully accounted for. Any values of receding and advancing oil/water, gas/water, and gas/oil contact angles can be considered.
- Any random/regular two- and three-dimensional networks can be used.
- Direct two-phase displacements
Section 8.2 Validation

Different abilities of the model enabled us to successfully predict measured values of water-wet two- and three-phase relative permeabilities using a geologically realistic network based on Berea sandstone. We were able to predict the three-phase relative permeabilities on a point-by-point basis. Then we simulated secondary and tertiary gas injection into different initial oil saturations in a strongly water-wet system to see the effects of initial oil saturation. We also compared secondary and tertiary gas injection results for the same initial oil saturation. The behavior of the two- and three-phase relative permeabilities were in agreement with those published by other authors. Then we predicted three-phase relative permeabilities for systems with different wettabilities and found some surprising results. We interpreted the results using the physics of three-phase flow at the pore-level.

Section 8.3 Recommendations for Future Work

Still there is a great amount of work that can be done to improve, even further, the abilities of the two- and three-phase pore-scale network models:

- More accurate layer conductance models for different boundary conditions which are critically important for prediction of relative permeabilities at low saturation
- Improved pore-body filling models
- Better estimations of three-phase equilibrium interfacial tensions
- More representative networks for different types of rocks, in particular carbonates

Also there are many interesting subjects to be studied using three-phase network modeling:
• Solution gas drive

• Effects of asphalt precipitation on three-phase relative permeabilities due to composition variation, e.g. $CO_2$ sequestration, or pressure drop below the bubble point

• Gas condensates

• Coupling pore-scale network model to a 3D simulator to capture displacement paths

• Dispersion in three-phase systems

• Water alternative gas (WAG) injection
Bibliography


Appendix A

Threshold Layer Collapse
Capillary Pressure

Figure A.1: A layer sandwiched between identical fluids residing in the corner and the center

Consider the triangle OEB:

\[
\frac{r}{\sin \alpha} = \frac{OB}{\sin(\pi - \psi)} \quad (A.1)
\]
\[ \psi = \theta_{12}^{b_2} - \frac{\pi}{2} \]

\[ \therefore \quad \frac{r}{\sin \alpha} = \frac{OB}{\sin \left( \frac{3\pi}{2} - \theta_{12}^{b_2} \right)} \quad (A.2) \]

\[ OB = \frac{r}{\sin \alpha} \sin \left( \frac{3\pi}{2} - \theta_{12}^{b_2} \right) \]

\[ \sin \left( \frac{3\pi}{2} - \theta_{12}^{b_2} \right) = -\cos \theta_{12}^{b_2} \]

\[ \therefore \quad OB = -r \frac{\cos \theta_{12}^{b_2}}{\sin \alpha} \quad (A.3) \]

\[ OC = OB - r = -r \left[ 1 + \frac{\cos \theta_{12}^{b_2}}{\sin \alpha} \right] \quad (A.4) \]

Consider triangle AOF:

\[ \frac{r}{\sin(\pi - \alpha)} = \frac{b_1}{\sin \beta} \quad (A.5) \]

\[ \sin(\pi - \alpha) = \sin \alpha \]

\[ \therefore \quad \sin \beta = \frac{b_1}{r} \sin \alpha \quad (A.6) \]

\[ \gamma = \pi - (\pi - \alpha) - \beta = \alpha - \beta \quad (A.7) \]

In triangle AOF:

\[ \frac{AO}{\sin \gamma} = \frac{b_1}{\sin \beta} \quad (A.8) \]

From Eqs. (A.6), (A.7), and (A.8):

\[ \frac{AO}{\sin(\alpha - \beta)} = \frac{r}{\sin \alpha} \quad (A.9) \]

\[ AO = \frac{r}{\sin \alpha} \sin(\alpha - \beta) = \frac{r}{\sin \alpha} (\sin \alpha \cos \beta - \cos \alpha \sin \beta) \quad (A.10) \]
From Eqs. (A.6) and (A.10):

\[ AO = r \cos \beta - b_1 \cos \alpha \quad (A.11) \]

\[ OC = r - AO \quad (A.12) \]

\[ OC = r - r \cos \beta + b_1 \cos \alpha \quad (A.13) \]

From equating Eqs. (A.4) and (A.13):

\[ r(2 + \cos \theta h_2 h_2 \sin \alpha) + b_1 \cos \alpha = r \cos \beta \quad (A.14) \]

\[ r^2 (4 + 4 \frac{\cos \theta h_2}{\sin \alpha} + \cos^2 \theta h_2 \sin^2 \alpha) + b_1^2 \cos^2 \alpha + 2b_1 r \cos \alpha (2 + \frac{\cos \theta h_2}{\sin \alpha}) = r^2 \cos^2 \beta \quad (A.15) \]

\[ r^2 \cos^2 \beta = r^2 (1 - \sin^2 \beta) = r^2 (1 - \frac{b_1^2}{r^2} \sin^2 \alpha) = r^2 - b_1^2 \sin^2 \alpha \quad (A.16) \]

\[ r^2 (3 + 4 \frac{\cos \theta h_2}{\sin \alpha} + \cos^2 \theta h_2 \sin^2 \alpha) + b_1^2 + 2b_1 r \cos \alpha (2 + \frac{\cos \theta h_2}{\sin \alpha}) = 0 \quad (A.17) \]

\[ r = -\frac{2b_1 \cos \alpha [2 + (\cos \theta h_2 / \sin \alpha)] \pm [A]}{[6 + 8(\cos \theta h_2 / \sin \alpha) + 2(\cos^2 \theta h_2 / \sin^2 \alpha)]} \quad (A.18) \]

\[ A = \left[ 4b_1^2 \cos^2 \alpha (4 + 4 \frac{\cos \theta h_2}{\sin \alpha} + \frac{\cos^2 \theta h_2}{\sin^2 \alpha}) - 12b_1^2 - 16b_1 \frac{\cos \theta h_2}{\sin \alpha} - 4b_1^2 \frac{\cos^2 \theta h_2}{\sin^2 \alpha} \right]^{\frac{1}{2}} \quad (A.19) \]

\[ \frac{r}{b_1} = -\frac{2 \sin^2 \alpha \cos \alpha - \cos \alpha \sin \alpha \cos \theta h_2 \pm [A]}{3 \sin^2 \alpha + 4 \sin \alpha \cos \theta h_2 + \cos^2 \theta h_2} \quad (A.20) \]

\[ A = [4 \cos^2 \alpha \sin^4 \alpha + 4 \sin^3 \alpha \cos \theta h_2 \cos^2 \alpha + \cos^2 \alpha \sin^2 \alpha \cos^2 \theta h_2 - 3 \sin^4 \alpha - 4 \cos \theta \sin^3 \alpha - \cos^2 \theta h_2 \sin^2 \alpha]^{\frac{1}{2}} \quad (A.21) \]
\[ \frac{r}{b_1} = -\cos \alpha \sin \alpha (2 \sin \alpha + \cos \theta_{12}^h) \pm \sin^2 \alpha \left[-4 \sin \alpha \cos \theta_{12}^h - 3 + 4 \cos^2 \alpha - \cos^2 \theta_{12}^h\right]^{\frac{1}{2}} \]
\[ 3 \sin^2 \alpha + 4 \sin \alpha \cos \theta_{12}^h + \cos^2 \theta_{12}^h \] (A.22)

\[ P_{c12} = -\frac{\sigma_{12}}{r} \] (A.23)

\[ P_{c12} = \frac{\sigma_{12} (3 \sin^2 \alpha + 4 \sin \alpha \cos \theta_{12}^h + \cos^2 \theta_{12}^h)}{b_1 [\cos \alpha \sin (2 \sin \alpha + \cos \theta_{12}^h) + \sin^2 \alpha \sqrt{4 \cos^2 \alpha - 3 - \cos^2 \theta_{12}^h - 4 \sin \alpha \cos \theta_{12}^h]} \] (A.24)

For \( b_1 \):

\[ \gamma + \theta_{12}^h = \frac{\pi}{2} \] (A.25)

From Eqs. (A.6), (A.7), and (A.25):

\[ \beta = (\alpha + \theta_{12}^h) - \frac{\pi}{2} \] (A.26)

\[ b_1 = \frac{r}{\sin \alpha} \sin[(\alpha + \theta_{12}^h) - \frac{\pi}{2}] \]

\[ \sin[(\alpha + \theta_{12}^h) - \frac{\pi}{2}] = -\cos(\alpha + \theta_{12}^h) \]

\[ \therefore b_1 = \frac{r}{\sin \alpha} [-\cos(\alpha + \theta_{12}^h)] \] (A.27)

Since the curvature is negative then:

\[ b_1 = r \frac{\cos(\alpha + \theta_{12}^h)}{\sin \alpha} \] (A.28)

For \( b_2 \), consider triangle OEB:

\[ \frac{r}{\sin \alpha} = \frac{b_2}{\sin(\varphi)} \] (A.29)
\[
\varphi = \pi - \left(\frac{3\pi}{2} - \theta_{12}^b\right) - \alpha \\
\varphi = -\frac{\pi}{2} + \theta_{12}^h - \alpha \\
\theta_{12}^h = \pi - \phi \\
\therefore \varphi = \frac{\pi}{2} - (\alpha + \phi) \tag{A.30}
\]

From Eqs. (A.29) and (A.30):

\[
\sin \varphi = \sin \left[\frac{\pi}{2} - (\alpha + \phi)\right] = \cos (\alpha + \phi) \\
\therefore b_2 = r \frac{\cos (\alpha + \phi)}{\sin \alpha} \tag{A.31}
\]