Imperial College Consortium on Pore-Scale Modelling

Yearly progress report

December 30, 2006

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Matthew Rhodes and Hu Dong
Executive Summary

This is the third and final report of Phase 2 of the Imperial College Consortium on Pore-Scale Modelling. In our project meeting we will highlight the major progress made in Phase 2 – on network extraction, three-phase flow, dispersion and upscaling – and discuss our plans for Phase 3.

The main highlight of the year was Sander completing his PhD on three-phase pore-scale modelling; he is now working for Saudi Aramco. We welcomed two new PhD students from Abu Dhabi, Saleh Al-Mansoori and Saif Al-Sayari. While they are not working directly on pore-scale modelling, their laboratory studies will provide benchmarks for the testing and validation of our numerical predictions. We are also hosting a visitor from China – Congjiao Xie – who is working on pore-scale imaging of fluid distributions; she will present her work at the project meeting.

This report contains five parts comprising a PhD thesis and papers that have recently been submitted for publication. Part 1 is Sander Suijmez’s PhD thesis, “Pore-scale simulation of three-phase flow.” Part 2 is a paper written by Matthew Rhodes for the Reservoir Simulation Symposium in February on pore-to-field upscaling in single-phase flow using continuous time random walks – it is an extension of the dispersion studies started by Branko Bijeljic. Part 3 presents some of our work on imaging and network extraction performed by Hu Dong in collaboration with Saudi Aramco – details of how the networks are extracted are being written up and will be presented at the project meeting.

The current researchers in the group are:

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

Branko Bijeljic, Research Fellow – dispersion and reaction in porous media.

Gady Frenkel, post-doctoral research associate – statistical mechanics of grain packings.

Congjiao Xie, visiting scholar – imaging fluid distribution at the pore scale.

Anwar Al-Kharusi, 3rd year PhD student – analysis of carbonates.

Hu Dong – 3rd year PhD student – imaging and analysis of the pore space of sandstones and carbonates.

Taha Sochi – 3rd year PhD student – non-Newtonian flow in porous media.

Matthew Rhodes – 3rd year PhD student – general transport models.

Olu Talabi – 2nd year PhD student – prediction of electrical and NMR responses as a function of wettability.

Nasiru Idowu – 2nd year PhD student – pore-to-reservoir upscaling.

Saleh Al-Mansoori – 1st year PhD student – experimental studies of trapping in three-phase flow.

Saif Al-Sayari – 1st year PhD student – experimental studies of the effects of wettability on relative permeability, resistivity index and NMR response.
All our publications, theses, reports and presentations are available on our Website: http://www3.imperial.ac.uk/earthscienceandengineering/research/perm/porescalemodelling

**Project publications in 2006**

**Journal publications**


**Conference Proceedings**


Our current sponsors are: BHP, ENI, JOGMEC, Saudi Aramco, Schlumberger, Shell, Statoil and Total as well as the DTI. 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 2006
Part 1

PORE SCALE SIMULATION OF THREE-PHASE FLOW

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

Vural Sander Suicmez

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Abstract

We use a three-dimensional mixed-wet random network model representing Berea sandstone to compute displacement paths and relative permeabilities for water alternating gas (WAG) flooding. First we reproduce cycles of water and gas injection observed in previously published experimental studies. We predict the measured oil, water and gas relative permeabilities accurately. We discuss the hysteresis trends in the water and gas relative permeabilities and interpret the results in terms of pore-scale displacements. In water-wet media the water relative permeability is lower in the presence of gas during waterflooding due to an increase in oil/water capillary pressure that causes a decrease in wetting layer conductance. The gas relative permeability is higher for displacement cycles after first gas injection at high gas saturation due to cooperative pore filling, but lower at low saturation due to trapping.

We then perform a study of the effect of wettability and spreading coefficient on relative permeability for WAG flooding. In oil-wet media, the water relative permeability remains low until water-filled elements span the system at which point the relative permeability increases rapidly. The gas relative permeability is lower in the presence of water than oil because it is no longer the most non-wetting phase. The amount of trapping during gas injection is controlled by the stability of oil layers that is in turn determined by the gas/oil contact angle.

We also show how to use network modelling to develop a physically-based empirical model for three-phase relative permeability. We demonstrate that the relative permeabilities are approximately independent of saturation path when plotted as a function of flowing saturation. The flowing saturation is the saturation minus the amount that is trapped. The amount of oil and gas that is trapped shows a surprising trend with wettability – weakly water-wet media show more trapping of oil and gas than a water-wet system due to the complex competition of different three-phase displacement processes. Further work is needed to explore the full range of behaviour as a function of wettability and displacement path.

The following articles have been based on the material presented in this thesis:


Acknowledgements

Looking back to three years ago, I now strongly believe that the best decision of my life was coming to Imperial College London for my PhD studies. I feel extremely lucky that I had a chance to work with some of the greatest people in the specific area of “Fluid Flow in Porous Media”.

Financial support for this study was provided by Imperial College Consortium on Pore-scale Network Modelling (BHP, DTI, ENI, JOGMEC, Saudi Aramco, Schlumberger, Shell, Statoil and Total). These contributions are gratefully acknowledged. I would also like to thank Dr. Pål-Eric Øren of Numerical Rocks for providing us with the Berea network data used in this work.

I would like to sincerely express the gratitude to Prof. Martin J. Blunt of Imperial College London and Prof. Mohammad Piri of University of Wyoming for their constant support, guidance, trust and encouragement during this study. None of this work would have been done without their assistance. I have enormously benefited from them that I am sure will be helpful during both my further studies at Saudi Aramco, Reservoir Engineering Technology Division, Dhahran, Saudi Arabia and in my future life. They both mean much more than a supervisor to me.

Living three years in London, I enjoyed every minute of it. This is a town that can offer anything you want. I feel very fortunate that I had the opportunity of meeting many nice people in these years which made this stay memorable for me. I am very much grateful to the faculty members, administrative and technical staff of the Department of Earth Science & Engineering. They are always there and ready to help.

I also would like to thank all my colleagues from Petroleum Engineering and Rock Mechanics (PERM) research group. I very much enjoyed the weekly seminars and learnt a lot from the presentations, comments and stimulating discussions. Among many friends in London, special thanks should go to Dr. Ehat Omer, Anwar Al-Kharusi, Hu Dong, Nabil Al-Bulushi, Dr. Per Valvatne, Dr. Hiroshi Okabe, Dr. Xavier Lopez, Dr. Mohammed Al-Gharbi, Dr. Branko Bijeljic, Dr. Zohreh Tavassoli and Dr. Ginevra Di Donato.

My gratitude extends to Prof. Peter King of Imperial College London and Dr. Rink van Dijke of Heriot-Watt University for serving on my PhD defence exam
committee and Dr. Matthew Jackson and Dr. Mariela Araujo-Fresky on my MPhil/PhD transfer exam committee.

Last, but by no means the least, my family. Being far away from home, I once again realised how valuable they are. I would like to take this opportunity to thank them for their understanding, care, love and endless support. At this point, I would like to dedicate this work to them, my grandmother Afet Akahiskali, my parents Ayfer and Ertoz Vahit Suicmez, my aunt Aynur Akahiskali, and my older brother Ertoz Erke Suicmez.

Vural Sander Suicmez

September, 2006
London, England
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Chapter 1

Introduction

Even though petroleum and natural gas resources are finite, they remain among the most important sources of energy in the world. With the decline of hydrocarbon reserves, improved recovery of these resources to boost production is becoming increasingly important. Most improved oil recovery projects involve the flow of three phases, where a gas, which could be air, natural gas, carbon dioxide (CO₂) or steam, is injected into a reservoir containing oil and water (Lake, 1989). In particular, the use of CO₂ injection into mature oil fields is likely to become increasingly common not only to enhance oil recovery but for storage of CO₂ emitted from power stations and other large point sources (Jessen et al., 2005). To predict recovery and to design an improved oil recovery scheme, one needs to input the constitutive relationships between macroscopic properties such as relative permeability, capillary pressure and phase saturations into the simulation model. These relationships are used in partial differential equations to describe the transport of fluids at the large scale. However determination of these constitutive relationships is complicated as they are dependent of the fluid properties, the pore space of the rock and the system’s saturation history.

Experimental measurements of three-phase flow are extremely difficult to perform and the results are frequently not reliable at low saturations (Oak, 1991). In addition to the measurement of saturations, pressure drops, and fluxes in three flowing phases, there are an infinite number of different displacement paths. Thus it is impractical to measure relative permeability for all possible three-phase displacements that may occur in reservoir. As a result, the universal practice in reservoir simulation studies is to estimate three-phase relative permeabilities using empirical correlations, which usually have very little or no physical basis (Stone, 1970; Stone, 1973; Baker, 1988; Blunt, 2000). Moreover, recent studies suggest that currently used empirical models fail to predict the relative permeabilities accurately (Element et al., 2003; Spiteri and Juanes, 2004).

An alternative approach is to represent the pore space of a piece of rock just a few mm across as a network of pores and throats through which we simulate the
movement of oil, water and gas. Fatt (1956a,b,c) initiated this approach by using a regular two-dimensional network to find capillary pressure and relative permeability. Since then, the capabilities of pore-network modelling increased enormously and have been applied to many different processes – see, for instance, Blunt et al. (2002) for a review.

Water alternating gas (WAG) injection is one of the many improved oil recovery methods that involve three-phase fluid flow. It was originally proposed as a method to improve the sweep efficiency of gas by injecting water to control the mobility ratio and to stabilize the displacement front (Caudle and Dyes, 1958; Christensen et al., 1998). Although WAG flooding has been successfully applied to more than 60 oilfields worldwide (Christensen et al., 1998), there is still an incomplete understanding of the pore-scale physics of the process and how it leads to improved oil recovery, especially in systems with non-uniform wettability (van Dijke et al., 2004a). The major problems in evaluation of WAG behaviour are uncertainties regarding the prediction of the wettability and spreading conditions that have a significant impact on the relative permeabilities of the phases for different injection cycles.

The use of physically-based properties – such as relative permeability and capillary pressure – that properly capture the pore structure and wettability variations in the reservoir may give very different predictions than using empirical correlations (Stone, 1970; Stone, 1973; Baker, 1988). It has been proposed that the relative permeability is a unique function of the flowing (non-trapped) fluid saturation (Carlson 1981; Blunt, 2000). Therefore predictions of the trapped fluid saturations are particularly important.

Land (1968) developed an empirical expression in the context of two-phase flow that relates trapped non-wetting phase saturation to the initial and maximum non-wetting phase saturations in the system. This model embodies the idea that the maximum non-wetting phase saturation determines the amount of trapping.

Using experimentally obtained data from Prudhoe Bay sandstone core samples, Jerauld (1997a) suggested that pore structure may also play an important role in determining the trapped gas saturation. He showed that the trapped gas saturation decreases with increasing porosity for sandstones. He proposed that lower porosity samples have larger pore-throat aspect ratios which in turn results in more snap-off
displacements disconnecting gas clusters. Jerauld (1997b) also suggested that the total hydrocarbon (oil and gas) trapped in a three-phase system would be up to 20% greater than the waterflood residual oil saturation during two-phase flow. He supported this hypothesis by showing experimental data from a wide variety of oil fields including Prudhoe Bay. He concluded that unless the system is strongly water-wet, the trapped gas and residual oil saturation should be approximately independent since they are not necessarily competing to occupy the same pores.

Blunt (2000) developed a three-phase trapping model by extending Land’s (1968) model to three-phase systems. He assumed that total trapped hydrocarbon saturation in a strongly water-wet system can be estimated by using a similar approach as Land did. According to this model, the total trapped hydrocarbon (both oil and gas) saturation in a three-phase system should be same as the trapped non-wetting phase saturation in a two-phase system.

Skauge and Larsen (1994) also studied trapping in three-phase flow with reference to WAG flooding and proposed an empirical model that matched their experimental data. They proposed that the gas relative permeability decreases with repeated flooding cycles.

Kralik et al., (2000) studied a comprehensive set of experimental data obtained from an oil-wet sandstone reservoir. They suggested that gas trapping not only depends on its own saturation but also on wettability and the relative amounts of the other two phases. It was shown that in oil-wet reservoirs trapped gas saturation can be significantly lower during waterflooding since gas may become the intermediate-wet phase which inhibits the water to gas snap-off displacements during water invasion. This explanation is similar to that for water-wet systems in which residual oil saturation is lower for intermediate-wet systems than water-wet systems (Jadhunandan and Morrow, 1995).

In this work, we apply pore-network modelling as a tool to predict three-phase relative permeabilities during cyclic injection of water and gas as well as to estimate the trapped hydrocarbon saturation. Using our network model, we will compute the trapped oil and gas saturations separately and relate it to the initial gas saturation and wettability of the system for a particular saturation path (gas injection followed by waterflooding). Before discussing our results in detail, we will review the previously
conducted two- and three-phase network modelling studies and the fundamentals of physics of three-phase flow at the pore-level.
Chapter 2

Literature Review

One of the key uncertainties in reservoir characterisation and simulation is the assignment of multiphase flow properties. Relative permeabilities are measured on only a few core samples and then assigned in reservoir simulation to large heterogeneous grid blocks that may contain many rock types. As a consequence, relative permeabilities are rarely considered to be reliable and are often modified with no physical justification during history matching. However, to predict recovery and to design an improved oil recovery scheme, one needs to input the constitutive relationships between relative permeability and saturation during multiphase fluid flow in porous media. Therefore the prediction of relative permeability and saturation has been the subject of many studies in the past years using pore-scale modelling.

Modelling flow behaviour using network models was pioneered by Fatt (1956a,b,c). Fatt computed the flow properties using an equivalent physical network of electrical resistors, since at this time, numerical solution of the flow/conductance equations was not readily available. Since then many authors have developed pore scale network models to simulate single and multi-phase fluid flow in porous media. However, further advances for network modelling was only possible after the late 70s when computer processing power became more readily available. In the course of this study, we will give a brief introduction to the recently developed two-phase network models which incorporate the impacts of wettability. Then we will give a detailed review of previously developed three-phase network models.

2.1 Two-Phase Flow

The impact of wettability on relative permeability has been previously studied using network modelling. McDougall and Sorbie (1995; 1997) developed a network model to investigate trends in oil recovery with wettability. They used a regular cubic lattice and did not explicitly include the wetting layers. However, they were able to predict hitherto puzzling trends in oil recovery. They concluded that optimum
recovery would be reached with about the half the pore space is water-wet and other half oil-wet, in accord with experimental measurements (Janahundran and Morrow, 1995).

Blunt (1997; 1998) developed a network model, also using a cubic lattice, but where the pores and throats had square cross-sections. Using angular elements enabled him to include flow through the wetting layers in his model. In each element, multiple wetting conditions were allowed, with corners remaining water-wet and the centres becoming oil-wet. The main conclusions of the work, particularly the non-monotonic trend of recovery with wettability index, were similar that those of McDougall and Sorbie (1995; 1997).

Using pore-throat networks reconstructed from thin section images of reservoir rocks (the process-based technique), Øren et al., (1998), Øren and Bakke (2002; 2003) and Valvatne and Blunt (2004) were able to predict two-phase relative permeabilities and waterflood oil recovery for sandstones of arbitrary wettability. The basic pore-scale physics used was similar to that presented by the authors mentioned above, but in combination with a representative model of the pore space, quantitative predictions could be made. In this thesis we extend this work to three-phase flow.

2.2 Three-Phase Flow

Heiba et al. (1984) extended a previously developed two-phase network model (Heiba et al. 1983) to three-phase flow. This was the first three-phase network simulator. A Bethe lattice was used to represent the porous medium. Only single phase occupancy was allowed in the pore elements. All of the six possible displacements (gas into oil, gas into water, oil into gas, oil into water, water into gas and water into oil) were modelled and local entry capillary pressures were calculated to control the displacements. The results suggested that the gas and water relative permeabilities are functions of their own saturations but otherwise independent of saturation path. Oil isoperm curves were obtained and found to be strongly curved, meaning that oil relative permeability was not only a function of its own saturation. These results corresponded qualitatively with the assumptions of empirical three-phase relative permeability models (Stone, 1970; Stone, 1973) and experimental measurements on water-wet systems (Leverett and Lewis, 1941; Corey et al., 1956;
Saraf and Fatt, 1967). The authors also suggested that three phase relative permeabilities are not only dependent on the saturation but also the saturation history of the system.

Soll and Celia (1993) developed a two-dimensional capillary-dominated network model in order to simulate two- and three-phase flow in micromodels. The model was used to predict capillary pressure – saturation relationships in a water-wet medium. Hysteresis was modelled using different advancing and receding contact angle values. Every pore was allowed to accommodate one fluid at a time as well as wetting layers. The results were compared against micromodel experiments (Soll et al. 1993). Predicted two-phase results were in good agreement with the experiments although the model did not successfully match three-phase data. The model was not used to calculate three-phase relative permeabilities.

Øren et al. (1994) developed a two-dimensional strongly water-wet square-lattice network model with rectangular links and spherical pores in order to compute oil recovery for spreading and non-spreading systems. They studied immiscible gas injection into waterflood residual oil (tertiary gas injection). Simulated recoveries compared very well with micromodel experiments (Øren and Pinczewski, 1991; Øren et al., 1992). The authors defined a double displacement mechanism where gas displaces trapped oil and trapped oil displaces continuous water allowing immobile oil to become connected boosting oil recovery. Oil recovery decreased significantly for non-spreading systems without layers to provide continuity of the oil phase. In spreading systems oil recovery was more effective and double displacement played an important role to recover more oil. In this work relative permeability was not computed.

Pereira et al. (1996; 1999) developed a dynamic two-dimensional network model in order to simulate the pore-scale movement of three phases in strongly water- and oil-wet systems when viscous forces are significant. Both pores and throats were assumed to be lenticular in cross-section allowing wetting and spreading layers to be present. The authors compared the recoveries for spreading and non-spreading conditions. The simulated recoveries were compared against previously conducted micromodel experiments (Øren et al., 1992). A large difference was observed for spreading and non-spreading systems. The oil recovery was the lowest for a water-wet and non-spreading system due to the absence of oil layers that resulted in trapping of
oil clusters. Even when system is spreading, oil recovery was lower for a water-wet case. This is because although layers do form in a spreading system, they may more easily collapse compared to an oil-wet case. This will be discussed further in Chapter 5 of this thesis where trapping is studied. Again relative permeability was not computed.

Mani and Mohanty (1997; 1998) developed a pore scale network model to study the effects of spreading coefficient in three-phase flow. The system was considered to be water-wet and the shapes of pores and throats were spherical and cylindrical respectively. The throat size distribution in the network was obtained by tuning it to match the mercury-air capillary pressure data for Berea sandstone (Mohanty and Salter, 1982). Immiscible gas injection into a porous medium which was initially saturated with water and oil was studied. Three displacement events were involved; direct water drainage (gas displacing water), direct oil drainage (gas displacing oil), and double drainage (gas displacing oil and displaced oil displacing water). In non-spreading systems, residual oil saturation increases as the magnitude of the spreading coefficient increases. They computed and compared three-phase relative permeabilities for different saturation paths and spreading coefficients. It was observed that water relative permeability is a function of its own saturation for three-phase systems. It has no dependence on saturation history or spreading coefficient of the system. Gas relative permeabilities were found to be strongly dependent on the spreading coefficient of the system. Trapping of the oil blobs in systems with negative spreading coefficients led to different gas relative permeability curves. Connected oil paths always existed for spreading systems and hence the oil relative permeability never dropped to zero. However, for a non-spreading system, while oil was being displaced by gas, the oil relative permeability dropped to zero at a finite oil saturation when no more connected oil paths existed. The effect of spreading coefficient on oil trapping and layer stability will be discussed in more detail in Chapter 4.

Fenwick and Blunt (1998a; 1998b) developed a three-phase network model for a strongly water-wet system (oil/water contact angle assumed to be zero). A regular cubic network of angular pores and throats was used. Two- and three-phase displacement mechanisms including oil layer flow observed in micromodel experiments were incorporated in the model. All of the six possible double displacement processes (this will be discussed in more detail in Chapter 3) were
introduced in the model. The model was able to simulate any sequence of fluid injection. A finite capillary-pressure dependent conductance of oil layers was considered and oil relative permeabilities were calculated. It was shown that at low oil saturation values oil relative permeability varies quadratically with oil saturation due to oil layer drainage consistent with experimental observations (Grader and O'Meara, 1988; Goodyear and Jones, 1993; Sahni et al., 1998). The authors also showed that three-phase relative permeabilities have a strong dependence on system’s saturation history. They introduced an iterative methodology in order to obtain self consistent relative permeability values (see Figure 2.1). A physically-based network model coupled with a one-dimensional Buckley-Leverett simulator was used to find the correct saturation path for a predetermined process with an initial condition and known injection fluid.

Figure 2.1 Schematic diagram of iterative procedure to obtain self consistent relative permeability values. (1) A saturation path through the three-phase region is guessed and followed with network model. (2) During the displacement three-phase relative permeabilities are calculated. (3) These relative permeabilities are inputted into one-dimensional numerical simulator with selected initial conditions, injection conditions and fluid properties. (4) The simulator generates another saturation path. (5) This path is compared with the proposed path with the network model. (6) If the paths do not coincide, repeat the procedure starting from step 4. From Fenwick and Blunt (1998a).

Laroche et al. (1999) conducted a series of three-phase experiments on glass micro-models. They studied the effects of wettability heterogeneities for gas injection
into oil and water. They then developed a two-dimensional network model and compared the results against the experimentally obtained data. n-Dodecane, water and nitrogen were used as the three phases during the experiments. All two-phase interfacial tensions, densities, viscosities and contact angles were measured. The initial spreading coefficient was 7.3 mN/m and hence oil was assumed to be spreading. During the simulations, throats had triangular cross-sections and pores were circular cylinders. The fluid distributions were in good qualitative agreement with those obtained experimentally.

Hui and Blunt (2000) analyzed ten different fluid configurations in a single pore for a three-phase system. The capillary pressure for all possible displacements was calculated. Oil and water layer formation and stability were analyzed. Wettability alteration was modelled by altering the wettability of the solid surface which comes into direct contact with oil phase. In order to illustrate the effects of wettability in three-phase flow, relative permeabilities were calculated. The network was bundle of capillary tubes of different size with equilateral triangular cross-sections. The displacement sequence was primary oil drainage, followed by waterflooding and gas injection. The authors concluded that the relative permeability of the intermediate wet phase, which is oil in water-wet media, water in weakly oil-wet media and gas in strongly oil-wet media, depends both its own saturation and initial oil saturation.

Lerdahl et al. (2000) used a process-based construction technique (Bakke and Øren, 1997) to obtain a network of pores and throats which was representative of the pore space of a core sample taken from an oil reservoir. They studied drainage-dominated three-phase flow in a water-wet system. They compared the simulation results against experimental data obtained by Oak (1990). In our work, we extend this study for different wettability and injection conditions.

Larsen et al. (2000) used the network model developed by Fenwick and Blunt (1998a,b) to obtain self-consistent relative permeability values for a one-dimensional field-scale simulation model of WAG flooding cycles. This study was a good example for the practical applicability of three-phase pore-scale network modelling.

Van Dijke and Sorbie (2002) and Van Dijke et al. (2004a) developed a regular three-dimensional network model for systems with different wettabilities by extending their previous studies using a bundle of capillary tubes assumption (Van Dijke et al., 2000; Van Dijke et al., 2001). Larger pores were considered to be oil-wet while
smaller ones were assumed to be water-wet. The coordination number could be changed by removing throats from the network. A large number of simulations were performed to study the behaviour for different wettabilities and saturation paths. As the coordination number was reduced, connectivity was impaired and trapping became significant. For media with such low connectivity double and multiple displacements – described below – played an important role. They also performed a visual comparison between the network estimated and experimentally obtained (Sohrabi et al., 2000; Sohrabi et al., 2001) fluid distributions following certain displacement sequences. Figure 2.2 compares the simulated and experimental fluid configuration after the first gas flood and first water flood (van Dijke et al., 2004a).

Double displacement, involving a single trapped cluster, has been observed in micromodel experiments (Øren et al., 1992; Keller et al., 1997; Feng et al., 2004) and has been coded into network models (Øren et al., 1994; Fenwick and Blunt, 1998b; Mani and Mohanty, 1998; Piri and Blunt, 2005a). Van Dijke et al. (2004a) demonstrated using a combination of pore-scale simulation and micromodel experiments (Sohrabi et al., 2000) that for media with low phase connectivity, multiple displacements, involving trapped clusters of more than one phase, need to be considered, since repeated water and gas cycles increase the number of trapped clusters significantly.

Van Dijke and Sorbie (2003) investigated the occurrence and impact of multiple displacements during WAG injection. They concluded that multiple displacement is an important mechanism for the trapping and remobilization of gas and oil, especially in media with a low coordination number and poor connectivity of wetting and spreading layers. Svirsky et al. (2004) extended the work of van Dijke and Sorbie (2003) by predicting three-phase relative permeability using a network model anchored to two-phase data. They first matched experimental two-phase data (Oak, 1990) using several free parameters such as volume and conductance exponents, pore-throat size distribution, coordination number and contact angles. Then they predicted the three-phase relative permeabilities, which were in good agreement with the experimental data. The authors then used same parameters for conducting generic WAG simulations with different spreading and wettability conditions. It was shown that there is a significant decrease in gas relative permeability with subsequent injection cycles for water-wet and mixed-wet systems in accordance with
experimental measurements (Skauge and Larsen, 1994; Larsen and Skauge, 1998; Oak, 1990; Element et al., 2003).

Figure 2.2 Simulated (van Dijke et al., 2004a) and experimental (Sohrabi et al., 2000) fluid configurations after (a) first gas flooding (b) first water flooding. Gas was coloured white during the simulations and yellow during the experiments.

Al-Futaisi and Patzek (2006) developed a predictive three-phase network model to simulate secondary and tertiary gas injection into water-wet and partially spreading systems. The model incorporates the current state-of-art pore-scale displacement mechanisms and wettability hysteresis. A realistic representation of a sample of Bentheimer sandstone (Al-Futaisi and Patzek, 2003) was used during the simulations. The calculations demonstrated that saturation paths were strongly dependent on the initial conditions. Oil saturation after gas injection was found to be very low (around 1%), consistent with the assumption that a single intermediate oil layer in a duct is sufficient to maintain the oil connectivity. All three iso-perm curves were drawn and authors suggested that only water relative permeability is a function of its own saturation. Both gas and oil relative permeabilities may be dependent on the two other saturations during gas drainage into oil and water.
van Dijke and Sorbie (2006) and van Dijke et al., (2006) derived a thermodynamic pressure criterion for formation and removal of fluid layers during three-phase flow in angular pores of non-uniform wettability using the Mayer-Stowe-Princen (MSP) theory (Mayer and Stowe, 1965; Princen, 1969a; Princen, 1969b; Princen, 1970). In all current three-phase network models, we use a rather simpler approach, using semi-empirical two-phase expressions. Layer stability during the displacements is assessed by using a simple geometrical layer collapse criterion (Hui and Blunt, 2000). However, van Dijke et al. suggest that using two-phase expressions in a three-phase flow context may lead to serious inconsistencies in the relation between pressures and pore occupancies for angular pore and throat elements.

Piri and Blunt (2005a,b) presented a three-dimensional mixed-wet network model in order to simulate two- and three-phase fluid flow. A random network, generated by using process-based techniques (Øren and Bakke, 2002), was used to represent the pore space in Berea sandstone. The model simulated any sequence of oil, water and gas injection. Threshold capillary pressures for all possible displacements were computed for 30 different phase configurations. Two- and three-phase relative permeabilities were successfully predicted and compared with the steady state experiments conducted by Oak (1990). Results from this study will be discussed in more detail in the following chapter. An extension of this model will be used in this thesis.
Chapter 3

Network Modelling of Three-Phase Flow

Before describing the Berea sandstone network used as the pore space in this study and before discussing the details of network modelling, we need to briefly review the physics of three-phase flow at the pore-level. When only one fluid exists in the pore space, there is only one set of forces to consider, the attraction between the rock and the fluid (Amyx et al., 1960). In a three-phase system, there are six sets of active forces affecting capillary pressure and wettability. Three of them act between the rock and each fluid phase; others act between two fluids at the interface.

3.1 Interfacial Tensions and Spreading Coefficients

In dealing with multiphase systems, it is necessary to consider the effect of the forces acting at the interface when two immiscible fluids are in contact. Considering water, oil and gas, fluids commonly found in oil reservoirs, it is found that an interfacial tension always exists between them (Amyx et al., 1960). 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 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 the initial spreading coefficient and defined by Adamson and Gast (1997):

\[ C_s^i = \sigma_{gw} - \sigma_{go} - \sigma_{ow} \quad (3.1) \]

where \( \sigma \) is an interfacial tension between two phases labelled \( o, w, \) 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 (Zhou and Blunt, 1997). 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 the equilibrium spreading coefficient (Adamson and Gast, 1997):
If $C_s^i$ is negative then the system is non-spreading, if $C_s^i$ is positive and $C_s^{eq}$ is negative then the system is partially spreading, if $C_s^i$ is positive and $C_s^{eq}$ is close to zero then system is spreading. To be able to model the three-phase fluid flow appropriately, it is essential to input correct values for interfacial tensions since flow of three phases and hence the residual oil saturation is strongly dependent on the spreading coefficient of the system (Mani and Mohanty, 1997). For instance, in thermodynamic equilibrium conditions, the spreading coefficient, $C_s^{eq}$, must be either zero or negative (Adamson and Gast, 1997). The difference between initial and equilibrium conditions is normally achieved through a reduction in the gas-water interfacial tension due to the presence of a molecular film of oil on the interface.

In the rest of this thesis we will always consider that the three phases are in mutual equilibrium and so all interfacial tensions will be assumed to be at equilibrium conditions. For simplicity though, we will drop the superscript $eq$.

### 3.2 Bartell-Osterhof (1927) Constraint

The angle between the two-phase line and the solid surface, measured through the denser phase, is called the contact angle. For each of the three pairs of fluids (oil-water, gas-water, and gas-oil) residing on a solid surface (Figure 3.1), a horizontal force balance can be obtained.

\[
\begin{align*}
\sigma_{os} &= \sigma_{ws} + \sigma_{ow} \cos \theta_{ow} \\
\sigma_{gs} &= \sigma_{ws} + \sigma_{gw} \cos \theta_{gw} \\
\sigma_{gs} &= \sigma_{os} + \sigma_{go} \cos \theta_{go}
\end{align*}
\]  

where the subscript $s$ refers to solid/fluid surface tensions.
A constraint on the three-phase contact angles and interfacial tensions in mutual equilibrium conditions was derived by Bartell and Osterhof (1927) by manipulation of Eq (3.3) – (3.5). According to this constraint, as long as two of the contact angles and three interfacial tensions are defined independently, we can calculate the third contact angle using the equation below.

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

(3.6)

This constraint has many implications for three-phase flow. For instance, consider a three-phase strongly oil-wet system; i.e. \( \theta_{ow} = \pi \). At ambient conditions, typical interfacial tensions for water/n-alkane systems are \( \sigma_{go} = 20mN/m \) and \( \sigma_{ow} = 50mN/m \) (Adamson and Gast, 1997). This means \( \sigma_{gw} \cos \theta_{gw} < 0 \) which in turn implies that \( \theta_{gw} > \frac{\pi}{2} \). This analysis indicates that gas may not be the most non-wetting phase in a strongly oil-wet medium.
Blunt (2001) showed in an $n$-phase system there are $\frac{n(n-1)}{2}$ contact angles, $\frac{(n-1)(n-2)}{2}$ constraints and $(n-1)$ independent contact angles. Therefore, in a three-phase system, only two of the contact angles need to be defined independently.

### 3.3 Contact Angle Hysteresis and Wettability Alteration

Wettability is the ability of one fluid to spread on a solid and form a wetting film (Laroche et al., 1999). The wetting condition of the porous medium is of great importance in defining the flow characteristics. Three broad classifications can be identified for oil-water systems – water-wet, oil-wet and neutrally-wet, where oil-water contact angles are less than 90°, greater than 90° or close to 90°, respectively. Based on the distribution of contact angle values, porous media can be water-wet (containing only pores and throats with contact angles less than 90°), mixed-wet (containing pores and throats with contact angles both less than and greater than 90°), or oil-wet (containing pores and throats with contact angles greater than 90°).

In three-phase flow we can define wetting, intermediate and non-wetting phases. If we define contact angle as measured through the phase of interest, the wetting phase has a contact angle less than 90° in contact with the other two phases; the intermediate-wet phase has a contact angle greater than 90° in contact with the wetting phase and more than 90° with the other (non-wetting phase); and the non-wetting phase has a contact angle greater than 90° with the other two phases. For a water-wet system, water is the wetting phase, oil is intermediate-wet and gas is non-wetting. As discussed after Equation (3.6), in an oil-wet system, oil is wetting, gas is intermediate-wet and water is non-wetting.

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 the direct contact of oil with the solid surface which changes the wettability by adsorption of the polar components of the crude or the presence of naturally oil-wet minerals within the rock (Lake, 1989).

Kovscek et al. (1993) developed a model where the wettability of the rock surface was assumed to be altered by direct contact of oil. Before primary oil invasion,
the system is assumed to be saturated with only water and strongly water-wet. Once oil invades into the system, it collapses water films coating the solid surfaces at a threshold capillary pressure, contacts the solid surface and changes its wettability (Kovscek et al. (1993); Blunt (1997)). Thus it is possible to have any oil-water contact angle values in a three-phase system.

The contact angle also depends on the direction of the displacement. During a displacement process where the denser phase (water for oil-water or gas-water displacements, or oil for gas-oil) is receding (that is the denser phase is displaced by the less dense phase: oil displacing water, for instance) the contact angle is called the receding contact angle, whereas during invasion of the denser phase it is called the advancing contact angle (such as water displacing oil). The difference between the advancing and receding contact angle values is called contact angle hysteresis and might be significant depending on the surface roughness and surface heterogeneity (Amyx et al., 1960; Dullien, 1992, Morrow, 1975). Figure 3.2 shows the hysteresis model suggested by Morrow (1975) for oil-water systems.

In order to obtain good predictions of multiphase flow behaviour, representative oil/water, gas/water and gas/oil contact angle values need to be inputted into the simulation model (Valvatne and Blunt, 2004; Piri and Blunt, 2005a).

![Figure 3.2 Relationship between receding/advancing and intrinsic contact angles on a rough surface as a function of intrinsic contact angle measured at rest on a smooth surface for oil-water systems (Morrow, 1975).]
Valvatne and Blunt (2004) showed that contact angle values may play an important role while estimating the experimentally measured two-phase relative permeabilities. By modifying the oil-water contact angles to match the experimentally-determined residual non-wetting phase saturation, they obtained good predictions of experimentally measured relative permeability data (Oak, 1991).

For three-phase flow there is an issue associated with the use of the Bartell-Osterhof equation (3.6) to find the gas-water contact angle. The relation is derived for static contacts in equilibrium. However, in our simulations we are concerned with displacement where the fluid-fluid-solid contact is moving. In this thesis we compute the gas-water contact angle twice: first we use receding values of the oil-water and gas-oil contact angles and then we use advancing values for these two contact angles. The smaller computed gas-water contact angle is chosen to be the receding value, while the larger is the advancing value. While there is no direct experimental verification of this approach, it does have a physical justification. Imagine a spreading system, there is normally oil sandwiched between gas and water. Hence a gas-water displacement is similar to a combination of gas-oil and oil-water. For gas displacing water (receding gas-water contact angle) we should therefore use receding gas-oil and oil-water contact angles, and for water displacing gas (advancing gas-water contact angle) we should use advancing gas-oil and oil-water values.

3.4 Description of the Pore Space

Pore scale network modelling of three-phase flow not only requires a detailed understanding of the multiphase displacement mechanisms at the pore-level but also an accurate and realistic characterization of the porous media in which we can perform our simulations (Pereira et al., 1996). It is essential to have a reliable physically-based network that can provide plausible estimates of macroscopic properties. Arns et al. (2004) investigated the effect of topology on relative permeabilities and underlined the importance of incorporating realistic three-dimensional topologies in network models for predicting multiphase flow properties. They compared the relative permeability curves computed on a geologically realistic rock network and on a regular lattice. Although the rock network and the lattice had identical geometric characteristics (pore and throat size distribution) and similar
average coordination number, the results showed poor agreement. It was only when the coordination number distribution was matched were the relative permeabilities in reasonable agreement. This work suggests that to make good predictions of multiphase flow properties, the network has to have a structure very close to that of the real rock sample.

The construction of realistic three-dimensional representations of porous media has been the subject of several studies in the recent years (Delerue et al., 1999; Øren et al., 1998; Delerue and Perrier, 2002; Silin and Patzek, 2003; Al-Kharusi and Blunt, 2006; Jiang et al., 2006). Different methods have been introduced in the last decade, including direct imaging of the pore space at a resolution of a few microns using micro CT scanning (Arns et al., 2005; Olafuyi et al., 2006), and statistical reconstruction from high-resolution two-dimensional thin section images (Adler et al., 1990; Okabe and Blunt, 2004; Okabe and Blunt, 2005). Another approach, the process-based technique, generates a model porous medium by simulating the packing of grains (Øren et al., 1998). Although it is a challenge to simulate the geological processes for carbonate rock samples due to their complex geological histories, some very encouraging results were obtained for sandstones (Øren and Bakke, 2002). These methods, however, are limited by the resolution of the image – this is particularly important for carbonates that may have sub-micron-scale features, the statistical validity of the reconstruction process and/or the geological realism in the process-based approach.

A three-dimensional voxel representation of Berea sandstone generated using the process-based technique is the basis for the network used in this work, Figure 3.3. A topologically equivalent network of pores and throats (Figure 3.4) is then extracted from the pore-space image (Øren and Bakke, 2002). Table 3.1 lists some of the important features of the Berea sandstone network while Figure 3.5 shows pore and throat size distributions.

For the Berea sandstone network used in this work, each pore or throat is assigned a total volume, an inscribed radius and a shape factor. The inscribed radius is used to assign a capillary entry pressure during multiphase fluid flow. Cross-sections of the pores and throats are regular and irregular triangles, rectangles and circles (Figure 3.6). The cross-section has the same shape factor $G$ (ratio of cross-sectional
area, $A$, to perimeter, $P$, squared), as the real system from which the network is derived.

\[
G = \frac{A}{P^2}
\]  

(3.7)

Therefore, the shape factor for a circular cross-section is $\pi/4$, for a square cross-section $1/16$, and for an equilateral triangle 0.04811. If the shape factor ranges from zero to 0.04811, then it represents an element with a cross-section that is an irregular triangle. As can be seen from the Table 3.1, most of the elements (98.8 %) have angular cross-sections which allows wetting phase to occupy the corners while non-wetting phase fills the centre. From the shape factor we model the pore or throat as a circle, square or triangle using the method described previously (Valvatne and Blunt, 2004; Patzek, 2001). This enables us to capture the physics of wetting layer flow which is vitally important, especially in the low saturation region (Blunt, 2000). We assume that this characterisation of the shape is sufficient to model multiphase flow accurately, although the proper description of pores and throats remains an open question.

A clay volume is also associated with the network (see Appendix for more detail). This represents an immobile volume that remains water saturated throughout all displacements. It can be adjusted to match the observed connate water saturation (Bakke and Øren, 1997; Øren and Bakke, 2002).
Figure 3.3 The void space of a sandstone produced by process-based simulation (Øren and Bakke, 2002).
Figure 3.4 A topologically equivalent network representation (Øren and Bakke, 2002). Figure taken from Piri and Blunt (2005a).
Table 3.1 Properties of the Berea sandstone network.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-dimension (mm)</td>
<td>3</td>
</tr>
<tr>
<td>Y-dimension (mm)</td>
<td>3</td>
</tr>
<tr>
<td>Z-dimension (mm)</td>
<td>3</td>
</tr>
<tr>
<td>Absolute permeability (md)</td>
<td>3055</td>
</tr>
<tr>
<td>Porosity (%)</td>
<td>18.309</td>
</tr>
<tr>
<td>Clay volume (%)</td>
<td>5.715</td>
</tr>
<tr>
<td>Average pore size (micron)</td>
<td>19.167</td>
</tr>
<tr>
<td>Average throat size (micron)</td>
<td>10.970</td>
</tr>
<tr>
<td>Average coordination number</td>
<td>4.192</td>
</tr>
<tr>
<td>Triangular elements (%)</td>
<td>92.261</td>
</tr>
<tr>
<td>Square elements (%)</td>
<td>6.510</td>
</tr>
<tr>
<td>Circular elements (%)</td>
<td>1.229</td>
</tr>
</tbody>
</table>

Figure 3.5 Pore and Throat size distribution for the Berea sandstone network (Øren and Bakke, 2002) used in this study.
3.5 Network Modelling

The fluids used in this work are assumed to be Newtonian, incompressible, and immiscible. The displacements at the pore scale are assumed to be quasi-static and capillary dominated. A displacement is defined as a change in the configuration of an element (pore or throat) in order to satisfy capillary equilibrium conditions. This can either be a displacement of a phase by another in the centre of an element or layer collapse/formation in a single corner. Each displacement has a threshold capillary pressure associated with it. In other words, displacement is carried out only if the invading phase reaches the required (threshold) phase pressure. At a certain phase pressure, all possible displacements take place until there is no more available displacements, which means system is relaxed and capillary equilibrium conditions are satisfied. The analytical computations of the threshold pressures have already been discussed in the literature (Øren et al., 1998; Hui and Blunt, 2000; Piri and Blunt, 2005a). We are not going to present all these equations here in this thesis: however two- and three-phase fluid configurations and available displacement mechanisms do deserve a brief introduction.

3.5.1 Generic Fluid Configurations

For elements with circular cross-section, only one phase can occupy the pore or throat element. For the vast majority of elements that are angular, one or more phases may reside in them simultaneously. It is assumed that connectivity of the phases is dependent on the stability of layers and their ability to transport the fluids in the pore space, especially in the low saturation region (Fenwick and Blunt, 1998; Hui and Blunt, 2000; Blunt, 2000). Depending on the capillary pressure, spreading coefficient,
contact angle and corner half angle values, it is possible to accommodate fluids in the
corners of the angular pore and throat elements with different configurations. Generic
two- and three-phase fluid configurations are shown in Figures 3.7 and 3.8. These are
all of the configurations implemented in our model. However, multi-phase fluid
occupancy in the real pore space is quite complicated and with the development of
better visualisation techniques and further understanding of fluid and rock properties
there might be future extensions to currently implemented fluid configurations.

In all our simulations, we assume the system is initially 100% saturated with
water and strongly water-wet. Once non-wetting phase (oil) migrates into the system
during primary drainage, it invades the centre of the element and changes the
wettability of the central portion of the pore/throat. Depending on the magnitude of
the new contact angles, each pore or throat can become water-wet, oil-wet or
intermediate-wet (see section 3.3). The new configuration of the phases in the pore or
throat element is dependent on the wettability of the system and geometry of the
element. For subsequent displacements we assume that the non-wetting phase
capillary pressures are never sufficiently high that any interface penetrates further into
the corners of the pore space than during primary drainage.

For instance, we can explain how we can reach configuration F-1 (Figure 3.8). As
discussed above, we assume the system is initially saturated with water and the
initial configuration is A-1 (Figure 3.7). Then if oil invades into the water-filled pore,
it changes the wettability of the oil-occupied region and the new configuration will be
B1 (note that we assume system is still water-wet as θ_{ow} < 90°). Then, once we inject
gas into the system, gas occupies the centre of the pore and forms an oil layer in
between the water in the corner and the oil in the centre – as long as pore geometry
and θ_{og} allows (this will be discussed in more detail in section 3.5.4) – and we end up
with configuration F-1.

Configurations B-4, C-4, D-2, E-2, F-4 and G-4 all involve configurations
with a pinned interface where the wettability has been altered. This is associated
where secondary injection of a non-wetting phase does not reach the same location as
during primary drainage. Then, due to contact angle hysteresis, this interface may
hinge during subsequent displacement of these phases.
In all these configurations, each phase may either be trapped or continuous depending on its connectivity to the inlet and outlet. One of the difficulties associated with three-phase network modelling is the determination of whether a phase is trapped or not and updating this information during different displacement processes. Piri and Blunt (2005a) solved this problem by using an extension of the Hoshen and Kopelman algorithm (1976) which will be discussed in more detail in the next section.
Figure 3.7 One- and two-phase fluid configurations for a single corner. The bold solid line indicates the regions of the surface with altered wettability. From Piri and Blunt (2005a).
Figure 3.8 Three-phase fluid configurations for a single corner. From Piri and Blunt (2005a).
3.5.2 Continuity and Clustering

In pore network modelling of multiphase fluid 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. A phase location is the presence of a phase in any of the corners of an element (pore or throat) or in the centre of the element. This is vitally important because for every displacement continuity of both displacing and displaced phase locations have to be known \textit{a priori}. Also while computing the relative permeabilities, the conductance of the phases is calculated only for continuous phase clusters (Piri and Blunt, 2005a).

Piri and Blunt (2005a) presented an algorithm which is applicable to any two- and three-dimensional regular and random network with any number of phases residing in pore and throat elements. First, the network at its original condition is scanned to determine continuity of all its present phase locations. Flags are assigned to every phase location indicating if it is continuous or trapped. A cluster number is also assigned for every trapped cluster. A cluster is a collection of phase locations that are connected to each other. One should note that we assume that corners of the neighbouring elements are connected and so are the layers and centres holding the same phase. Once the scan of the network is completed, the injection of different phases and thus different displacements may start. New displacements may create new phase locations that result in trapping and/or reconnection events. This means that the old flags of the phase locations may not be valid anymore and must be kept updated. However, after the very first scan of the network, we do not scan the entire network anymore. Instead, we start from the phase location where the displacement takes place and try to reach the inlet and outlet. If we can reach to both the inlet and outlet then the cluster is considered to be continuous and contributes to the relative permeability of the phase; otherwise if we can reach to either inlet or outlet but not both, then cluster is still considered continuous, which allows direct, single displacement of elements in the cluster, but will not contribute to the conductance and relative permeability. If we can reach neither inlet nor outlet then the cluster is considered to be trapped. This means that single displacement is not allowed, although, as
discussed later, elements in the cluster may move through multiple displacement processes.

3.5.3 Order of Displacements

Based on which phase displaces which phase, there are six possible direct two-phase displacement processes: oil displacing water, water displacing oil, oil displacing gas, gas displacing oil, water displacing gas and gas displacing water. Every displacement belongs to one of these six processes.

A process can be carried out either by increasing the pressure of the displacing fluid or decreasing the pressure of the displaced fluid. In two-phase flow, both methods produce the same results but the situation might be more complicated for three-phase systems since each continuous phase has two capillary pressures associated with two other phases. Therefore in this work, we model all the processes by increasing the pressure of the displacing phase only. For example, during gas injection process, displacements are carried out by increasing the phase pressure of gas, not by decreasing the pressures of oil or water.

For every single displacement, a threshold capillary pressure is calculated (Piri and Blunt, 2005a) which might depend on the relevant contact angles, corner half angles and inscribed radius of the element of interest. Threshold pressures for all possible displacements are calculated, ranked and a sorted list is formed for each phase injection process. In three-phase systems there will be three main sorted lists for gas, oil and water injection processes.

By knowing the injection fluid, the relevant main sorted list is selected. The list is sorted in ascending order beginning with the most favourable (displacement which requires the lowest threshold pressure) and ends up with the least favourable displacement (with the highest threshold pressure).

3.5.4 Displacement Mechanisms

A displacement is valid when the displacing and displaced phase locations are present and their continuity status flags are consistent. Depending on the continuity status, a
displacement might be either a single displacement (a continuous phase displaces another continuous phase) or a double displacement (continuous phase displaces a trapped intermediate phase and displaced trapped phase displaces another continuous phase).

In this section we will only give a brief description of the principal processes we consider in our model. More detail will be provided for cases where a thorough understanding is necessary to understand the results presented in the later chapters.

We apply fixed pressures for connected phases across the whole network. We then increase the pressure of the phase that is being injected. A displacement event occurs when the pressure difference between the injected phase and one of the continuous phases reaches a threshold value. This is a network-wide event that is made up of local configuration changes in individual pores and throats. For single displacements, this involves a change in configuration of any or all of the corners, or the centre, of a single element. For double displacement, this involves two separate configuration changes in two different elements and so is a non-local process.

**Single Displacements.** If a continuous phase is displaced by another continuous phase, then displacement is called a single displacement. For every single displacement, there is a displacing phase and a displaced phase. Each displacement is either drainage or imbibition. If a wetting phase is displaced by a non-wetting phase, the displacement is called drainage; if non-wetting phase is displaced by the wetting phase then the displacement is imbibition. A displacement occurs at the threshold absolute pressure of the displacing phase. However, due to the invasion-percolation nature of the displacements there might be more than one available displacement. In that case, the displacement with the lowest threshold pressure will be performed first.

A single displacement involves one of four sub-groups of local configuration change: piston-like, pore-body filling, snap-off, and layer collapse and formation. Piston-like refers to the displacement of one phase by another through the centre of a throat. Due to contact angle hysteresis, the threshold capillary pressure for piston-like displacement can be different for drainage and imbibition events. Pore-body filling refers to the displacement of one phase in the centre of a pore by the displacing phase located in the centres of adjoining throats. For a drainage event, the threshold capillary pressure is given by similar expressions for piston-like advance. However the
imbibition threshold capillary pressure for the displacement depends on the number of neighbouring throats that hold the invading phase and are able to contribute to the displacement (Lenormand et al., 1983).

Snap-off corresponds to an imbibition event where the non-wetting phase located at the centre of the element is displaced by the wetting phase, which is located either in the corners or in the layers of the element. During waterflooding, spontaneous snap-off only occurs when $\theta_{ow} + \alpha < \pi/2$. Snap-off is not favoured over a piston-like or pore-body filling event when there is a neighbouring element with the invading phase in the centre that is able to carry out the displacement. For spontaneous snap-off the arc menisci in the corners (AM’s) meet each other when they reach halfway along the sides of the element (Figure 3.9).

The threshold capillary pressure for spontaneous snap-off event for an n-sided regular pore or throat can be found by equating the half length of one side of the element to the meniscus-apex distance of the moving AM’s and is given as (Hui and Blunt, 2000):

$$P_{cow} = \frac{\sigma_{ow} (\cos \theta_{ow} - \sin \theta_{ow} \tan \alpha)}{R}$$  \hspace{1cm} (3.8)

where $R$ is the inscribed radius of the element and $\alpha$ is the corner half angle of the element. $P_c$ is a capillary pressure – that is a pressure difference between phases. The threshold water pressure at which this event occurs is the oil pressure minus $P_{cow}$. Note that as the contact angle increases, snap-off becomes less favoured. As a consequence, significant amounts of snap-off are normally only seen in strongly wetting systems.

Snap-off can also occur in gas-water systems; this will be discussed in Chapter 5. In this case we require $\theta_{gw} + \alpha < \pi/2$ and the threshold capillary pressure is:

$$P_{cgw} = \frac{\sigma_{gw} (\cos \theta_{gw} - \sin \theta_{gw} \tan \alpha)}{R}$$  \hspace{1cm} (3.9)

Again note that snap-off is favoured for low values of the gas/water contact angle.
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. From Valvatne and Blunt (2004).

Layer collapse and formation. The model developed by Piri and Blunt (2005a) considers layer collapse and formation events as separate displacements. Depending on the contact angles, capillary pressures, and corner half angles, layers may be formed through displacement from the fluids residing in the centres or the layers of the neighbouring elements. Once a layer forms, it is possible to collapse this layer with an increase in the pressure of the fluids residing on either side of the layer (corner or centre). Sometimes the same phase (water) may be residing both in the corner and centre of the element next to either a gas or an oil layer, in which case both the centre and the corner contribute to the layer collapse event if the pressure of the water phase increases.

The presence and stability of oil layers is assessed using a geometric criterion (Hui and Blunt, 2000). If, after a displacement event, a layer can be drawn in the pore space at the prevailing capillary pressures then it is assumed to be present. This approach allows displaced intermediate-wet phase to remain as layer(s) sandwiched between the fluids in the corner and in the centre of the element – if the pertinent
contact angles, corner half angles and spreading condition of the system permit. However, recently it has been shown, using Helmholtz free energy balance principles, that these layers may not be formed after a direct displacement – it is energetically more favourable for the process to occur without a layer being left behind (van Dijke et al., 2004b; Piri and Blunt, 2004; van Dijke and Sorbie, 2006; van Dijke et al., 2006). Furthermore, layers form and collapse at pressures that may be different from that derived geometrically: in brief, geometric stability is a necessary but not sufficient condition to determine the presence of a layer. It has been shown that using two-phase expressions for displacement capillary pressure combined with a geometric rule for layer stability in a three-phase flow context may lead to serious inconsistencies in the relation between pressures and pore occupancies for angular pore and throat elements. This may lead to incorrect estimations of the residual fluid saturations due to the inconsistent computation of the layer formation/collapse capillary pressure.

During both gas and water injection, oil layers may be formed and be present sandwiched between gas and water (see Figures 3.7 and 3.8 – configurations D, E, H, J, K). Having these layers is extremely important as the oil recovery is very much dependent on the stability of these layers especially in the low oil saturation region (Blunt, 2000). According to the geometrical criterion (Hui and Blunt, 2000; Piri and Blunt, 2005a), oil layers may be formed during gas injection, if

\[ \theta_{go} + \alpha < \frac{\pi}{2} \]  

where a similar equation is obeyed for \( \theta_{ow} \). Since the layer is surrounded by two different fluids, a change in the pressure of either fluid can result in layer collapse event. Depending on the magnitude of the two contact angles (\( \theta_{go} \) and \( \theta_{ow} \)), two different collapse scenarios are possible: if the gas-oil contact angle is larger than oil-water contact angle, then the layer is stable until the three-phase contact points meet each other (Figure 3.10a, where phase i is gas, j is oil and k is water); instead if the oil-water contact angle is larger, then the layer is stable until two arc menisci (AM), which is the interface at a corner of a non-circular element, meet each other at the centre (Figure 3.10b).
Imagine one case that we will study in more detail in Chapter 5, where water is injected to displace gas and oil. We assume that the gas/oil interface was established during gas injection, so the gas/oil contact angle $\theta_{go}$ is its receding value. We keep the gas/oil capillary pressure fixed and increase the water pressure (that is, decrease the oil/water and gas/water capillary pressures). The water in the corner swells until the oil/water interface contacts the gas/oil interface. If this occurs by movement of the oil/water/solid contact line moving towards the centre of the element, then the prevailing oil/water contact angle $\theta_{ow}$ is its advancing value and we compute the threshold oil/water capillary pressure as follows (Hui and Blunt, 2000):

$$p_{cow} = \frac{\sigma_{ow} p_{go}}{\sigma_{go} R_c}$$  \hfill (3.11)

for $\theta_{ow} > \theta_{go}$, the threshold ratio of curvatures is given by,

$$R_c = \frac{\sin \alpha - \cos \theta_{go}}{\sin \alpha - \cos \theta_{ow}}$$  \hfill (3.12)

while for $\theta_{ow} < \theta_{go}$,

$$R_c = \frac{\cos(\theta_{go} + \alpha)}{\cos(\theta_{ow} + \alpha)}$$  \hfill (3.13)
Figure 3.10 A layer collapse event takes place once the fluids in the corner and the centre touch each other (Piri and Blunt, 2004). (a) $\theta^*_E < \theta^*_j$ (b) $\theta^*_E > \theta^*_j$.

One should note that the layer collapse event is more favoured for strongly water-wet systems. As the value of $\theta_{ow}$ decreases, the threshold radius of curvature $R_c$ will also decrease meaning that $P_{cow}$ increases. This makes physical sense: oil layers become increasingly favoured as the system becomes more oil-wet.

Layer collapse is also more favoured for large values of the gas-oil contact angle; again this makes physical sense, as oil layers present over a wider range of pressures if it is wetting to both water (high $\theta_{ow}$) and gas (low $\theta_{go}$). Also, oil layers are only possible for low values of the gas-oil contact angle, Equation (3.10).

Furthermore, the gas-oil contact angle is related to spreading coefficient. Consider a strongly water-wet system, $\theta_{ow} = \theta_{gw} = 0$, then from the Bartell-Osterhof constraint, Equation (3.6):
\[
\sigma_{gw} = \sigma_{ow} + \sigma_{go} \cos \theta_{go}
\]  

(3.14)

from which we find, using Equation (3.2):

\[
\cos \theta_{go} = 1 + \frac{C_j}{\sigma_{go}}
\]  

(3.15)

Recall that the (equilibrium) spreading coefficient is zero or negative.

The implication of Equation (3.15) is that the gas-oil contact angle increases as the system becomes more non-spreading, leading to less stable oil layers. Again this makes sense: one would expect layers to be more favoured in spreading systems. If the system is not strongly water-wet there is a less direct relationship between gas-oil contact angle and spreading coefficient. This issue will be discussed in more detail in Chapter 4.

It is also possible that layer collapse occurs when the oil/water and gas/oil interfaces meet without any movement of the oil/water/solid contact line. During water injection, the water layer swells, but the contact line will not move until the advancing oil/water contact angle is reached. This means that the layer tends to bulge with the apparent oil/water contact angle increasing. In this case the oil/water contact angle is called a hinging angle \( \theta_h \) which increases with increasing water pressure.

Consider then a case where the interfaces meet in the middle – Figure 3.10(b). In this case the threshold capillary pressure is related to the distance of the pinned contact from the apex of the corner and the gas/oil capillary pressure. The critical ratio of curvatures is now given by:

\[
R_c = \frac{\sin \alpha - \cos \theta_{go}}{\sin \alpha - \cos \theta_h}
\]  

(3.16)

which is a special case of Equation (3.12) where the oil/water capillary pressure is found from Equation (3.11) and the hinging contact angle is defined as:
\[
\theta_h = \cos^{-1}\left(\frac{P_{\text{cow}} b \sin \alpha}{\sigma_{\text{ow}}}\right) - \alpha
\]  

(3.17)

where \(b\) is the meniscus-apex distance.

For this type of layer collapse, the threshold capillary pressure is \textit{independent} of the oil/water contact angle, as long as the hinging angle is less than the advancing oil/water contact angle. Note that Equations (3.11), (3.16) and (3.17) give an implicit equation for the threshold oil/water capillary pressure \(P_{\text{cow}}\) that has to be solved iteratively.

Note that, unlike the model developed by Hui and Blunt (2000), we assume it is also possible to form gas layers if \(\theta_{\text{gw}} + \alpha < \pi/2\) (for instance, Figure 3.7 – configuration E1 and E2). Let us take a case – as discussed later in Chapter 5, where the gas/oil contact angle is zero. Then, according to the Bartell Osterhof equation (3.6), we find:

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

(3.18)

At reservoir conditions, where the gas and oil may be close to miscibility, \(\sigma_{\text{go}}\) is typically around 1 mN/m or lower and is considerably smaller than the oil/water interfacial tension. Since gas and oil have similar properties, \(\sigma_{\text{gw}} \approx \sigma_{\text{ow}}\) and hence \(\theta_{\text{gw}} \approx \theta_{\text{ow}}\) which makes physical sense: as gas and oil become more similar then they should share the same wettability. The consequence is that in oil-wet reservoirs, we expect gas too to be wetting to water, especially close to miscibility where gas layers between oil in the corners and water in the centre of the pore space may be present.

\textbf{Double Displacements.} In two-phase static network models, a fluid phase is able to move and contribute to displacement events only if it is connected to the inlet or outlet. In three-phase flow, however, the displacement of trapped clusters is vital for predicting recovery mechanisms: for instance oil that is trapped during waterflooding becomes reconnected by gas through the pore-scale migration and coalescence of oil clusters. Our model only considers double displacement where a continuous phase displaces a trapped phase that displaces another continuous phase (Figure 3.11).
However, in principle, there may be an arbitrarily long intermediate chain of disconnected clusters displacing other disconnected clusters before displacement of a continuous phase (van Dijke and Sorbie, 2002; van Dijke et al., 2004). It is possible to activate/deactivate the double displacement processes while conducting a simulation with our model (see Appendix).

There are six possible double displacements (Table 3.2; Fenwick and Blunt, 1998b) out of which only double drainage (gas displacing oil and displaced oil displacing water) was included in the model developed by Piri and Blunt (2005a), since the authors were mainly interested in tertiary gas injection.

To simulate WAG injection appropriately, where both oil and gas are getting trapped, we extended this model by including two other double displacement processes: double imbibition (water displacing trapped oil that displaces gas) and imbibition-drainage (water displaces trapped gas that displaces oil). Since we do not consider oil injection during cyclic floods and water is almost always continuous, the three other double displacement mechanisms are ignored.

When a double displacement is carried out, the displacement can be considered as two single displacements. The first one is a continuous phase displacing a trapped phase, and the second one is displaced trapped phase displacing another continuous phase. In our model, we assume the inlet and outlet are connected to each other. In other words, a phase cluster connected to either inlet or outlet will be considered as continuous and will have exactly same phase pressure as another phase cluster connected to either inlet or outlet. For instance, if we have a gas cluster connected to inlet and another gas cluster connected to outlet, we do not threat them as two different clusters. They are considered as members of one big continuous gas cluster and have exactly the same phase pressure. However, if a phase is not connected to either inlet or outlet then it is considered as trapped and may move only through double displacement.

To perform the double displacement, we first increase the trapped phase absolute pressure to the threshold absolute pressure of the second single displacement (trapped phase displacing the continuous phase). Then, by adding this difference to the threshold pressure of the first single displacement (continuous phase displacing the trapped phase), we can calculate the threshold pressure for the double displacement event. It is given as:
where $P$ is the absolute pressure, $DD$ stands for double displacement, $first$ is the displacement of trapped phase by a continuous phase, and $second$ is the displacement of the continuous phase by the displaced trapped phase.

If a trapped cluster of some phase becomes connected to either the inlet or outlet as a result of double displacement, then we re-set the pressure of the continuous clusters of that phase to the pressure of this previously trapped cluster. This pressure of the cluster is set by the last double displacement event it was involved in: it is the pressure of the continuous displacing or displaced phase plus the capillary pressure for the single displacement in the double displacement sequence. For instance, consider gas displacing oil by double drainage. The oil pressure in the trapped cluster is equal to the gas pressure minus the gas-oil capillary pressure for the gas-oil displacement event. This will be the same as the water pressure plus the oil-water capillary pressure for the oil-water displacement. Phase pressures may change significantly due to double displacement: for instance, during gas injection into residual oil, the continuous oil pressure increases as double displacement connects hitherto trapped clusters by oil displacing water through relatively narrow throats. This has a significant impact on the water relative permeability, as discussed in Chapter 4.

Table 3.2 Possible double displacement processes for a water-wet medium (Fenwick and Blunt, 1998b). Depending on wettability, the name of the displacement may change, but the sequence of phase displacement remains same.

<table>
<thead>
<tr>
<th>Name</th>
<th>Displacement Sequence</th>
</tr>
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<tbody>
<tr>
<td>Double Drainage</td>
<td>Gas displaces oil and oil displaces water</td>
</tr>
<tr>
<td>Drainage-Imbibition</td>
<td>Gas displaces water and water displaces oil</td>
</tr>
<tr>
<td>Imbibition-Drainage</td>
<td>Water displaces gas and gas displaces oil</td>
</tr>
<tr>
<td>Double Imbibition</td>
<td>Water displaces oil and oil displaces gas</td>
</tr>
<tr>
<td>Imbibition-Drainage</td>
<td>Oil displaces gas and gas displaces water</td>
</tr>
<tr>
<td>Drainage-Imbibition</td>
<td>Oil displaces water and water displaces gas</td>
</tr>
</tbody>
</table>
Figure 3.11 Double displacement where gas displaces trapped oil and trapped oil displaces the continuous water cluster (a) resulting in a final configuration (b) (this is the double drainage mechanism for a water-wet medium). From Fenwick and Blunt (1998b).

3.5.5 Calculation of Transport Properties

The estimation of transport properties can be done at any point after a pre-determined number of displacements (see Appendix for more detail). Saturation is computed once the system is relaxed which means system is in capillary equilibrium and it is not possible to carry out any more displacements with the current phase pressure.

The absolute permeability $K$ of the network is found from Darcy’s law when the system is fully saturated with a single-phase $p$ of viscosity $\mu$.

$$K = \frac{\mu_p q_{\text{vol}} L}{A(P_{\text{in}} - P_{\text{out}})} \quad (3.20)$$

The total single-phase flow rate $q_{\text{vol}}$ through the network is found by imposing a pressure drop $(P_{\text{in}} - P_{\text{out}})$ across its length, $L$ with $A$ being the cross-sectional area of the model.
For the purpose of multiphase fluid flow, once the saturation is computed, relative permeability and capillary pressure can also be found. Since we perform the displacements by only increasing the displacing phase pressure, the differences between the phase pressures of the displacing fluid and the two displaced fluids can be used to predict the three-phase capillary pressures. To compute relative permeability, the conductance of each continuous phase location in each element is first computed. Normally an exact analytical solution is not available and empirical expressions derived from the Stoke’s equation for flow in pores of different geometries and for different fluid configurations are used. Piri and Blunt (2005a) have already discussed the details of the empirical expressions used to calculate the conductance of the phase locations. If $\theta \leq \frac{\pi}{2} - \alpha$ (for instance see configuration B-1, Figure 3.7) then conductance of a phase flowing in a corner of an element is estimated by:

$$g = \frac{A^2_c(1 - \sin \alpha)^2(\varphi_2 \cos \theta - \varphi_1)\varphi_3^2}{12\mu \sin^2 \alpha(1 - \varphi_3)(\varphi_2 + f\varphi_3)^2}$$  \hspace{1cm} (3.21)

$$\varphi_1 = \left(\frac{\pi}{2} - \alpha - \theta\right)$$  \hspace{1cm} (3.22)

$$\varphi_2 = \cot \alpha \cos \theta - \sin \theta$$  \hspace{1cm} (3.23)

$$\varphi_3 = \left(\frac{\pi}{2} - \alpha\right)\tan \alpha$$  \hspace{1cm} (3.24)

where $A_c$ is the area of the corner of an element, $\mu$ is viscosity of the fluid residing in the corner, $f = 1$ for no-flow boundary condition (suitable for oil/water interfaces) and $f = 0$ for free boundary conditions (for gas/oil or gas/water interfaces). If $\theta > \frac{\pi}{2} - \alpha$ (see configuration B-4, Figure 3.7) then corner conductance is calculated using:

$$g = \frac{A^2_c \tan \alpha(1 - \sin \alpha)^2 \varphi_3^2}{12\mu \sin^2 \alpha(1 - \varphi_3)(1 + f\varphi_3)^2}$$  \hspace{1cm} (3.25)
When there is a fluid layer sandwiched between the phases residing in the corner and centre, the conductance of the phase in the layer can be calculated as:

\[
g = \frac{A_1^3(1 - \sin \alpha)^2 \tan \alpha \varphi_1^2}{12\mu A_1 \sin^2 \alpha (1 - \varphi_1) \left[ 1 + f_1 \varphi_1 - (1 - f_2 \varphi_2) \sqrt{\frac{A_2}{A_c}} \right]^2}
\]

where \( A_1 \) is the area of the layer of interest, \( A_i \) is the summation of areas of the corner and layer(s), \( A_2 \) is the summation of the areas of the corner and the second layer, if present (see for instance configuration group J, Figure 3.7, here \( A_1 \) is the gas layer \( A_{\text{layer}} \), \( A_c = A_{\text{corner}} + A_{\text{layer}} + A_{\text{layer}} \), and \( A_2 = A_{\text{corner}} + A_{\text{layer}} \)).

### 3.6 Previous Three-Phase Predictions (Piri & Blunt, 2005)

Piri and Blunt (2005b) studied secondary and tertiary gas injection into media of different wettability and initial oil saturation. Figures 3.12 – 3.15 show the two-phase relative permeability predictions performed by Piri and Blunt (2005b). The results were compared with experiments conducted by Oak (1990) on water-wet Berea sandstone. During primary drainage, the system was assumed to be initially saturated with the wetting phase and contact angles were taken to be zero. Figure 3.12 shows that this was a valid assumption as the predictions were excellent. During imbibition of water into oil and oil into gas, the authors adjusted the range of contact angle to match the trapped non-wetting phase saturation. The residual non-wetting phase saturation is higher for gas-oil systems than for oil-water. Hence the gas-oil contact angle is smaller, giving more snap-off and trapping than in the oil-water case – Table 3.3. Contact angle was assigned at random to pores and throats according to a uniform distribution with specified minimum and maximum values.

Figures 3.13 – 3.15 compare the experimentally obtained and network estimated relative permeabilities for oil-water, gas-oil and gas-water imbibition displacements. The predictions are very good.
Note, however, that although a spreading system is assumed, the advancing gas-oil contact angle is not zero: to match the measured trapped oil saturation a finite value of the gas-oil contact angle is used – Table 3.1.

For the gas-water experiment, the contact angles were found using the Bartell-Osterhof equation (3.6), and so there were no adjustable parameters in the prediction.

Figure 3.12 Comparison of experimental (Oak, 1990) and predicted (Piri and Blunt, 2005b) relative permeabilities during primary drainage. The connate water saturation has been matched by altering the clay content (see Appendix) in the network.

Figure 3.13 Comparison of experimental (Oak, 1990) and predicted (Piri and Blunt, 2005b) oil-water relative permeabilities for imbibition in Berea sandstone.
They then predicted three-phase relative permeabilities for tertiary gas injection after waterflooding into different initial oil saturations and compared the predictions with the experimental data. They used the same advancing oil-water and gas-oil contact angles as for two phase imbibition studies. They assumed that the receding
contact angles are 20° lower than the advancing values, which is typical amount of hysteresis for water-wet media (Dullien, 1992). Again the gas-water contact angle was then predicted by using Bartell Osterhof equation (3.6). Table 3.3 shows the interfacial tensions and three-phase contact angles used during the simulations performed by Piri and Blunt (2005b). The comparison of measured and predicted three-phase relative permeabilities (Figures 3.16 – 3.18) shows good agreement.

Table 3.3 The interfacial tension and contact angle values used by Piri and Blunt (2005b) in order to predict Oak’s experiments (1990).

<p>| | |</p>
<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>$\sigma_{gw}$(mN/m)</td>
<td>67</td>
</tr>
<tr>
<td>$\sigma_{go}$(mN/m)</td>
<td>19</td>
</tr>
<tr>
<td>$\sigma_{ow}$(mN/m)</td>
<td>48</td>
</tr>
<tr>
<td>$\theta^r_{gw}$(degrees)</td>
<td>36.6 – 57.3</td>
</tr>
<tr>
<td>$\theta^r_{go}$(degrees)</td>
<td>10 – 50</td>
</tr>
<tr>
<td>$\theta^r_{ow}$(degrees)</td>
<td>43 – 60</td>
</tr>
<tr>
<td>$\theta^a_{gw}$(degrees)</td>
<td>55.2 – 77.2</td>
</tr>
<tr>
<td>$\theta^a_{go}$(degrees)</td>
<td>30 – 70</td>
</tr>
<tr>
<td>$\theta^a_{ow}$(degrees)</td>
<td>63 – 80</td>
</tr>
</tbody>
</table>
Figure 3.16 Comparison of experimentally measured (Oak, 1990) and predicted (Piri and Blunt, 2005b) set of three-phase oil relative permeability data for tertiary gas injection into different initial oil saturations.

Figure 3.17 Comparison of experimentally measured (Oak, 1990) and predicted (Piri and Blunt, 2005b) set of three-phase gas relative permeability data for tertiary gas injection into different initial oil saturations.
Figure 3.18 Comparison of experimentally measured (Oak, 1990) and predicted (Piri and Blunt, 2005b) set of three-phase water relative permeability data for gas injection into different initial oil saturations.

In this study, we extend the work of Piri and Blunt (2005a,b) by adding two new double displacement processes that involve trapped gas. The only multiple displacement process considered by Piri and Blunt (2005a) was double drainage where gas displaces trapped oil that displaces water. However, in WAG flooding, double and multiple displacement processes involving trapped gas will also be important. We also corrected a number of bugs that prevented the proper simulation of repeated flooding cycles in the original code. In the previous sections we described this model and introduced the new displacement mechanisms. We will now compare our predictions with additional experimental data for cyclic and simultaneous water and gas injection as well as conducting sensitivity runs for different wettability conditions. While matching the experimental data we follow similar saturation paths observed during the experiments. However for the cases that we do not match the experiments, we implement a stopping criterion to end a flood which heavily depends on the system’s wettability. For water-wet cases we perform the first water injection until we reach the residual oil saturation which may be quite high for strongly water-wet systems and decreases as the system becomes weakly water-wet or mixed-wet. However, for oil-wet cases as oil layers, lying in between water in the corner and gas
in the centre, are stable during waterflooding, we may reach almost zero residual oil if we do not stop the flood. Therefore we stop the flood at a predetermined saturation during the first water injection in an oil-wet system.

The advantage of this model over the work of Van Dijke et al. (2004a) and Svirsky et al. (2004) is that the network explicitly represents a real rock with a disordered topology. The disadvantage is that we consider only double displacement – displacements involving trapped clusters of more than one phase are ignored. In the Berea network 98.8% of the elements have angular (square or triangular) cross-sections where water is connected in corners. As a consequence only gas and oil are trapped. We study a spreading system in our experimental comparisons, which means that the oil is normally connected in the presence of gas. As a consequence, as we show later, double displacements, although important, are sometimes rare in comparison with direct displacement of one connected phase by another and we suggest that in many of the cases we study higher order displacements are uncommon.

We will use our network model to investigate the pore scale physics of several processes; simultaneous water and gas injection, cyclic water and gas injection and hydrocarbon trapping.
Chapter 4

Predictions of WAG Flooding

We will use the network model to predict three experimental datasets: Oak (1990), Egermann et al. (2000) and Element et al. (2003) before using the model to predict trends in fluid flow behaviour with wettability and spreading coefficient.

4.1 Oak data

Piri and Blunt (2005b) successfully predicted the relative permeabilities of tertiary gas injection experiments conducted by Oak (1990), as discussed in the previous chapter. They showed that double drainage allows oil to become reconnected when gas is injected, discussed the differences in oil relative permeability as a function of water and gas saturations and demonstrated that the oil relative permeability for secondary gas injection is proportional to the square of the oil saturation. We extend this work by simulating both simultaneous and cyclic gas/water injection experiments conducted by Oak (1990). Current empirical relative permeability models are unable to predict this data accurately (Element et al., 2003; Spiteri and Juanes, 2004). Although the wettability and the spreading conditions of the medium are not clearly presented in the experimental work, we assume a water-wet and spreading oil system (Table 3.3). The same properties have been used to predict successfully Oak’s two-phase data and three-phase gas injection relative permeability – again see the previous chapter (Valvatne and Blunt, 2004; Piri and Blunt, 2005b). The success of these studies suggests that the fluid properties are representative of the experiments and that the Berea network is an adequate description of the Berea cores studied by Oak.

The network model considers a sequence of water and gas displacements that track the experimental displacement path (Piri and Blunt, 2005a) – see Appendix for more detail. Tracked and measured saturation paths as well as the comparison of predicted and measured three-phase relative permeabilities are shown in Figures 4.1 to 4.8. The results show that the relative permeability predictions are good for both simultaneous (Figures 4.1 – 4.4) and cyclic (Figures 4.5 – 4.8) gas/water injection.
During simultaneous gas/water injection, although we obtain excellent predictions for the water relative permeability, we underestimate oil relative permeability at low oil saturation (Figure 4.3). In this region, oil resides principally in layers in the pore space sandwiched between water in the corners and gas in the centre. The oil relative permeability is controlled by layer drainage. It is possible that we underestimate the conductance or stability of these layers. This result though is different from that obtained by Piri and Blunt (2005b) for gas injection, where the oil relative permeability was overestimated at low saturation. This suggests that there could be errors in the experimental data as well. However, the conclusion here is that the quantitative behaviour of the oil drainage regime requires further study. In particular, the expressions we use for oil layer stability are not based on strict thermodynamic criteria (van Dijke et al., 2004b; van Dijke et al., 2006). Instead, it is based on basic geometrical criteria (Hui and Blunt, 2000).

We overestimate the saturation at which gas breakthrough occurs (Figure 4.4). This is a finite size effect, since our network represents a considerably smaller system than the cores studied experimentally. Using percolation theory it is possible to demonstrate that the gas saturation at breakthrough will tend to zero as an increasingly large system size is considered (Wilkinson and Willemsen, 1983; Blunt et al., 1992).
Figure 4.1 Comparison of measured and tracked saturation paths for simultaneous water and gas injection. Experiment 14 – Sample 13 of Oak experiments (Oak, 1990).

Figure 4.2 Comparison of measured and predicted water relative permeabilities for the saturation path shown in Figure 4.1.
Figure 4.3 Comparison of measured and predicted oil relative permeabilities for the saturation path shown in Figure 4.1.

Figure 4.4 Comparison of measured and predicted gas relative permeabilities for the saturation path shown in Figure 4.1.
Figure 4.5 shows the experimental displacement path for a case where there are cycles of water and gas injection. Gas injection is performed into water and residual oil and then water is injected again until both gas and oil are trapped. The match to the saturation path using network modelling is good as are the predictions of relative permeability (Figures 4.6 – 4.8). Gas is the most non-wetting phase and a significant decrease in the gas relative permeability is observed during secondary water injection (Figure 4.6). The reason for this is that water traps gas, principally through snap-off, which is predicted accurately by the pore-scale model confirming other experimental and numerical studies (Skauge and Larsen, 1994; Svirsky et al., 2004). As can be seen from Table 4.1, there is a significant number of water to gas snap-off displacements during secondary water injection, although the most common mechanism is piston-like advance.

An unexpected observation is the noticeable water relative permeability hysteresis (Figure 4.7) evident in both the experiments and the predictions. Since water is the most wetting phase, it is not trapped and resides in the smallest elements of the pore space. The traditional thinking is that as a consequence the water relative permeability is a function of its own saturation only and does not display any hysteresis (Stone, 1970). However, we find that the water relative permeability is lower for the second water injection (water injected into a high gas saturation) than for the first (water displacing oil with no gas present). Figure 4.9 shows the gas and oil pore occupancies after the first and second water injection processes. Once we introduce gas into the system, oil no longer occupies the biggest pore and throat elements. Instead gas, which is the most non-wetting phase in a water-wet system, moves oil into smaller pores and throats by single and double displacements. Most of this oil is trapped. In the network model, as discussed in the previous Chapter, if trapped clusters become reconnected, the continuous phase pressure is increased to that of the trapped phase (Piri and Blunt, 2005a). This approach allows the oil/water capillary pressure to increase during gas injection through the reconnection of previously trapped oil, as evident in Figure 4.10 and observed in micromodel experiments (Sohrabi et al., 2000). When water re-injection commences, the oil/water capillary pressure increases sharply. This counter-intuitive result – in two-phase flow the capillary pressure decreases when imbibition starts – is due to the reconnection of some trapped oil in the smallest pores and throats through single and multiple
displacements. The magnitude of the capillary pressure is consistent with the reconnection of oil that was displaced into elements of radius 2-3 µm by double drainage during gas injection. This increase in capillary pressure means that oil pushes water further into the corners of the pore space: the occupancy of water-filled elements is the same, but water is pushed further into the corners of elements whose centres are filled with non-wetting phase. The water relative permeability at low mobile water saturation is controlled by the conductance of water in the corners of elements whose centres are oil or gas filled (Valvatne and Blunt, 2004). This is the case even at relatively higher saturations, around 50%. One reason for this behaviour is our assigned clay-bound irreducible water saturation of around 25%, so the mobile water saturation is actually much lower. As water is pushed into the corners, its conductance decreases sharply, causing the observed decrease in water relative permeability. While the predictions of relative permeability agree with the experimental measurements, it is not certain that our assumption of assigning the trapped phase pressure to the continuous phase on reconnection correctly represents the pore-scale processes occurring in the experiments. Moreover, we do not have the experimentally measured oil-water capillary pressure data to confirm this finding.

After the first water injection, oil is disconnected and has a zero relative permeability. During gas injection the oil is reconnected due to double drainage when gas pushes oil into smaller elements. Since volume is conserved, the oil now occupies more pores and throats and quickly fills a sufficient fraction of the network to become connected. In addition, due to spreading layers, oil remains connected in elements that contain gas. The oil relative permeability is then finite but decreases as further gas invasion displaces oil. At the end of gas invasion, the oil relative permeability is close to zero, as connected oil resides in only a few smaller elements and in oil layers. There are also trapped clusters of oil in elements where no layers are present. As shown in Figure 4.8, when water is re-injected, the oil relative permeability again increases slightly, as double imbibition allows trapped oil clusters to reconnect. Because the oil is becoming connected and disconnected through repeated flooding cycles, both the experimental and numerical data are noisy, but we predict the experimental trend in behaviour.
Table 4.2 shows displacement statistics for the first gas injection and secondary water flooding cycles. While direct gas-water and water-gas displacements are most common, there are a significant number of double displacements.

![Diagram showing saturation paths](image)

**Figure 4.5** Comparison of measured and tracked saturation paths for cyclic gas and water injection. Experiment 4 – Sample 6 of Oak experiments (Oak, 1990).
Figure 4.6 Comparison of measured and predicted gas relative permeabilities for the saturation path shown in Figure 4.5.

Figure 4.7 Comparison of measured and predicted water relative permeabilities for the saturation path shown in Figure 4.5.
Figure 4.8 Comparison of measured and predicted oil relative permeabilities for gas1 and water2 cycles shown in Figure 4.5.

Figure 4.9 Bulk pore occupancies for the first and second water injection cycles for the saturation path shown in Figure 4.5.
Figure 4.10 Oil-water capillary pressure for the first water, first gas, and second water injection cycles for the saturation path shown in Figure 4.5.

Table 4.1 Statistics for water to gas displacements during the secondary water injection process for the saturation path shown in Figure 4.5.

<table>
<thead>
<tr>
<th>Piston-like</th>
<th>Snap-Off</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number</td>
<td>13041</td>
</tr>
<tr>
<td>Percentage (%)</td>
<td>92.6</td>
</tr>
</tbody>
</table>

Table 4.2 Displacement statistics for the first gas injection and secondary water injection cycles for the saturation path shown in Figure 4.5.

<table>
<thead>
<tr>
<th>Type/Cycle</th>
<th>1st gas cycle (%)</th>
<th>2nd water cycle (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas-oil-water</td>
<td>14.4</td>
<td>-</td>
</tr>
<tr>
<td>Gas-oil</td>
<td>27.4</td>
<td>-</td>
</tr>
<tr>
<td>Gas-water</td>
<td>58.2</td>
<td>-</td>
</tr>
<tr>
<td>Water-oil-gas</td>
<td>-</td>
<td>10.3</td>
</tr>
<tr>
<td>Water-gas-oil</td>
<td>-</td>
<td>8.4</td>
</tr>
<tr>
<td>Water-oil</td>
<td>-</td>
<td>16.0</td>
</tr>
<tr>
<td>Water-gas</td>
<td>-</td>
<td>65.4</td>
</tr>
</tbody>
</table>
4.2 Egermann et al’s Data

Egermann et al. (2000) conducted WAG experiments on a water-wet Estaillades limestone core sample. Although carbonate samples usually have very complex pore structures, the inferred pore size distribution for this core is fairly close to that of our Berea sandstone network (Egermann et al., 2000). Experimental gas and water relative permeabilities were obtained by history matching the production curves. Our estimated contact angles and the interfacial tensions measured in the experiments are given in Table 4.3. The system was assumed to be weakly water-wet in order to match the waterflood residual oil saturation (Figure 4.11).

Measured and tracked saturation paths as well as the predicted versus experimental gas and water relative permeabilities are given in Figures 4.11 – 4.13. The oil relative permeability was not measured in these experiments. The network model was unable to reproduce exactly the observed saturation path. This could be due to finite size effects in addition to having different pore structures for the Berea network and the limestone core samples.

The predictions of gas relative permeability are good. Again we see that during water injection subsequent to gas injection, the gas relative permeability is lower due to gas trapping. This agrees with Oak’s observations. For the water relative permeability, we see a similar hysteresis trend as in the Oak data, for the same reason, although the displacement cycles are not identical. Both the gas and water relative permeabilities decrease for repeated cycles of gas and water injection: for the gas relative permeability this is due to trapping, while for water the conductance of water layers decreases.
Table 4.3 The interfacial tension and contact angle values used in our model to predict the experiments performed by Egermann et al. (2000).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{gw}$ (mN/m)</td>
<td>72.1</td>
</tr>
<tr>
<td>$\sigma_{go}$ (mN/m)</td>
<td>27</td>
</tr>
<tr>
<td>$\sigma_{ow}$ (mN/m)</td>
<td>40.3</td>
</tr>
<tr>
<td>$\theta^r_{gw}$ (degrees)</td>
<td>33 – 50</td>
</tr>
<tr>
<td>$\theta^r_{go}$ (degrees)</td>
<td>0</td>
</tr>
<tr>
<td>$\theta^r_{ow}$ (degrees)</td>
<td>40 – 60</td>
</tr>
<tr>
<td>$\theta^a_{gw}$ (degrees)</td>
<td>50 – 66</td>
</tr>
<tr>
<td>$\theta^a_{go}$ (degrees)</td>
<td>0</td>
</tr>
<tr>
<td>$\theta^a_{ow}$ (degrees)</td>
<td>60 – 80</td>
</tr>
</tbody>
</table>

Figure 4.11 Comparison of measured (Egermann et al., 2000) and tracked saturation paths.
Figure 4.12 Comparison of measured (Egermann et al., 2000) and predicted gas relative permeabilities for the saturation path shown in Figure 4.11.

Figure 4.13 Comparison of measured (Egermann et al., 2000) and predicted water relative permeabilities for the saturation path shown in Figure 4.11.
4.3 Element et al’s Data

Element et al. (2003) performed WAG experiments on water-wet Berea sandstone cores. The contact angles and spreading conditions of the experimental system were not measured. However, the high residual oil saturation after the first water injection suggests a strongly water-wet system. Estimated contact angles and interfacial tensions are given in Table 4.4. We assume a spreading system.

Experimentally observed and tracked saturation trajectories and predicted versus measured gas relative permeabilities are shown in Figure 4.14 and 4.15 respectively. As can be seen from Figure 4.14, after the primary oil drainage, waterflooding is followed by gas injection, water re-injection and one more gas flood. Only the gas relative permeability was measured.

We observe late gas breakthrough for our predictions due to the finite size of our network (Figure 4.15). However, the overall prediction of gas relative permeability is good. Again we see that the gas relative permeability is lower for the second cycle than for the first due to the trapping of gas. This again confirms the hysteresis trends observed and predicted for the previous two experiments. During both the first and second water injection processes we obtain many snap-off displacements (Table 4.5), which trap both oil and gas phases. This also results in more double displacements during subsequent gas/water injection cycles (Table 4.6).
Table 4.4 The interfacial tension and contact angle values used in our model to predict the experiments performed by Element et al. (2003).

<table>
<thead>
<tr>
<th></th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{gw}$ (mN/m)</td>
<td>67</td>
</tr>
<tr>
<td>$\sigma_{go}$ (mN/m)</td>
<td>19</td>
</tr>
<tr>
<td>$\sigma_{ow}$ (mN/m)</td>
<td>48</td>
</tr>
<tr>
<td>$\theta^r_{gw}$ (degrees)</td>
<td>4.4 – 16.9</td>
</tr>
<tr>
<td>$\theta^r_{go}$ (degrees)</td>
<td>0</td>
</tr>
<tr>
<td>$\theta^r_{ow}$ (degrees)</td>
<td>0 – 20</td>
</tr>
<tr>
<td>$\theta^a_{gw}$ (degrees)</td>
<td>16.9 – 33.7</td>
</tr>
<tr>
<td>$\theta^a_{go}$ (degrees)</td>
<td>0</td>
</tr>
<tr>
<td>$\theta^a_{ow}$ (degrees)</td>
<td>20 – 40</td>
</tr>
</tbody>
</table>

Figure 4.14 Comparison of measured (Element et al., 2003) and tracked saturation paths.
Figure 4.15 Comparison of measured (Element et al., 2003) and predicted gas relative permeabilities for the saturation path shown in Figure 4.14.

Table 4.5 Statistics describing the type of displacement mechanism for the first and second water injection cycles for the saturation path shown in Figure 4.14.

<table>
<thead>
<tr>
<th></th>
<th>Piston-like (water-oil)</th>
<th>Snap-Off (water-oil)</th>
<th>Layer Collapse (water-oil)</th>
<th>Piston-like (water-gas)</th>
<th>Snap-Off (water-gas)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st cycle</td>
<td>20858</td>
<td>5874</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>1st cycle (%)</td>
<td>78</td>
<td>22</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2nd cycle</td>
<td>1375</td>
<td>47</td>
<td>4557</td>
<td>4227</td>
<td>616</td>
</tr>
<tr>
<td>2nd cycle (%)</td>
<td>12.7</td>
<td>.43</td>
<td>42.1</td>
<td>39.1</td>
<td>5.7</td>
</tr>
</tbody>
</table>

Table 4.6 Displacement statistics of subsequent injection cycles for the saturation path shown in Figure 4.14.

<table>
<thead>
<tr>
<th>Type/Cycle</th>
<th>1st gas cycle (%)</th>
<th>2nd water cycle (%)</th>
<th>2nd gas cycle (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas-oil-water</td>
<td>8.8</td>
<td>-</td>
<td>49.2</td>
</tr>
<tr>
<td>Gas-oil</td>
<td>74.8</td>
<td>-</td>
<td>3.2</td>
</tr>
<tr>
<td>Gas-water</td>
<td>16.4</td>
<td>-</td>
<td>47.6</td>
</tr>
<tr>
<td>water-oil-gas</td>
<td>-</td>
<td>12.8</td>
<td>-</td>
</tr>
<tr>
<td>water-gas-oil</td>
<td>-</td>
<td>14.1</td>
<td>-</td>
</tr>
<tr>
<td>Water-oil</td>
<td>-</td>
<td>38.3</td>
<td>-</td>
</tr>
<tr>
<td>Water-gas</td>
<td>-</td>
<td>34.9</td>
<td>-</td>
</tr>
</tbody>
</table>
4.4 Effects of Wettability

After validating our model with the available experimental data, we performed two additional WAG simulations for different wettability conditions and saturation paths. We first conducted a simulation for a water-wet system. We used same contact angles and interfacial tensions to predict Oak’s experiments (Oak, 1990) (Table 3.3). The saturation path is shown in Figure 4.16 and the predicted three-phase relative permeabilities are shown in Figures 4.17 to 4.19. We inject water after primary oil drainage until we reach a residual oil saturation of 28%. Then we perform a gas cycle until the oil saturation drops to about 7%. We continue with two more subsequent water and gas cycles. As expected, we reach very low residual oil saturation, around 3%, since the system is spreading and oil remains connected in layers.

An increase in the gas relative permeability at high gas saturations is observed after the first gas injection (Figure 4.17). This is because pore filling by water is favoured in so-called dead-end pores that have only one connected throat that is water filled (Lenormand et al., 1983). During the first gas injection, gas invades the pore space by an invasion percolation process, where pore filling is favoured over piston-like advance in (smaller) throats (Wilkinson and Willemsen, 1983). At the end of gas injection the gas occupies a single connected cluster with many dead-end pores. These dead-end pores may contain a large volume, but do not contribute to the gas relative permeability. Hence filling these pores with water will change the saturation without altering the gas relative permeability making the waterflood gas relative permeability higher than for first gas invasion at high gas saturation (Figure 4.17). This effect has been discussed in the context of oil/water flow by Blunt (1997). The increase in gas relative permeability is only observed if gas is initially injected to very high saturation – in the experiments we predicted previously the maximum gas saturation reached initially was lower and this effect was not seen. This pore-filling process competes with snap-off that, as discussed before, causes disconnection of gas and a rapid drop in relative permeability. Snap-off is favoured if the throats are much smaller than the pores and has a dramatic effect on the gas phase connectivity at low gas saturation. There is only a slight decrease in relative permeability after repeated cycles of injection due to continued trapping of gas. However, Skauge and Larsen (1994) suggest that the gas relative permeability continues to decrease significantly.
with repeated flooding cycles. In our simulations gas reaches very high saturation values and displaces most of the oil in the system during the first cycle. During the subsequent water and gas injection cycles, we obtain almost identical saturation paths (Figure 4.16) and displacement processes. As can be seen from Tables 4.7 and 4.8, the displacement statistics are very similar for subsequent water and gas injection cycles with little continued trapping of oil and gas. As we reach significantly low oil saturation at the end of the first gas injection cycle, most displacements are gas displacing water and water displacing gas for the subsequent water/gas injection cycles. Figures 4.18 and 4.19 show that the water and oil relative are similar to those presented for the prediction of the Oak data (Figures 4.7 and 4.8). We observe a similar hysteresis trend in water relative permeability which can be explained by studying the oil-water capillary pressure curve (Figure 4.20). The decrease in the water relative permeability is due to the increase in the oil-water capillary pressure, however as the double displacements are no more significant in the subsequent injection cycles there is a decrease in the oil-water capillary pressure and increase in the water relative permeability in the third water injection cycle. Figure 4.19 suggests the importance of double displacement mechanisms and their effect on remobilising the trapped oil clusters.

![Figure 4.16 WAG saturation path for a water-wet system.](image)

Figure 4.16 WAG saturation path for a water-wet system.
Figure 4.17 Predicted gas relative permeabilities for the saturation path shown in Figure 4.16.

Figure 4.18 Predicted water relative permeabilities for the saturation path shown in Figure 4.16.
Figure 4.19 Remobilisation of oil due to the double displacement mechanisms. Predicted oil relative permeabilities are for the subsequent injection cycles after the first waterflooding where oil saturation reaches 28% shown in Figure 4.16.

Figure 4.20 Predicted oil/water capillary pressures for the water injection cycles for the saturation path shown in Figure 4.16.
We now simulate WAG for an oil-wet system. The contact angles and interfacial tensions are given in Table 4.9. Valvatne and Blunt (2004) used similar oil-water contact angles to predict two-phase relative permeabilities. Note that the gas/water contact angles are greater than 90°, indicating that water is now the most non-wetting phase and gas is intermediate wet. The saturation path – gas injection after waterflooding followed by a subsequent cycle of water and then gas injection – is shown in Figure 4.21. Predicted oil, gas and water relative permeabilities are shown in Figures 4.22 – 4.24. In an oil-wet medium, oil layers are very stable and do not easily collapse, which enables low residual oil saturations to be reached, as is evident in Figure 4.22. Unlike a water-wet medium, double displacement does not lead to a dramatic change in gas/oil or oil/water capillary pressure. We have fewer double displacements in an oil-wet system since there is very little trapped oil. Oil layers are stable and only collapse at low saturation values during the secondary water injection process (Table 4.10): during gas injection there is only piston-like gas displacing water and gas displacing oil events.

Although gas trapping is not as significant as in water-wet media, we do see a large decrease in gas relative permeability during the second injection cycle (Figure 4.23). During the first gas injection cycle, gas displaces principally oil as a non-

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Table 4.7 Statistics describing the displacement mechanisms for the secondary and tertiary water injection cycles for the saturation path shown in Figure 4.16.

<table>
<thead>
<tr>
<th></th>
<th>Piston-like (water-oil)</th>
<th>Snap-Off (water-oil)</th>
<th>Layer Collapse (water-oil)</th>
<th>Piston-like (water-gas)</th>
<th>Snap-Off (water-gas)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water 2</td>
<td>62</td>
<td>83</td>
<td>1876</td>
<td>23674</td>
<td>2673</td>
</tr>
<tr>
<td>Fraction (%)</td>
<td>.22</td>
<td>.29</td>
<td>6.6</td>
<td>83.4</td>
<td>9.4</td>
</tr>
<tr>
<td>Water 3</td>
<td>33</td>
<td>45</td>
<td>137</td>
<td>23472</td>
<td>3658</td>
</tr>
<tr>
<td>Fraction (%)</td>
<td>.12</td>
<td>.16</td>
<td>.50</td>
<td>85.8</td>
<td>13.3</td>
</tr>
</tbody>
</table>

Table 4.8 Statistics of the displacement mechanisms for the secondary and tertiary gas injection cycles for the saturation path shown in Figure 4.16.

<table>
<thead>
<tr>
<th></th>
<th>Piston-like (gas-oil)</th>
<th>Layer Collapse (gas-oil)</th>
<th>Piston-like (gas-water)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas 2</td>
<td>65</td>
<td>1436</td>
<td>27093</td>
</tr>
<tr>
<td>Fraction (%)</td>
<td>.22</td>
<td>5.0</td>
<td>94.7</td>
</tr>
<tr>
<td>Gas 3</td>
<td>1093</td>
<td>1065</td>
<td>27293</td>
</tr>
<tr>
<td>Fraction (%)</td>
<td>3.7</td>
<td>3.6</td>
<td>92.7</td>
</tr>
</tbody>
</table>
wetting phase and occupies the larger pores and throats. For subsequent gas injection, gas displaces both oil and water, which is now the wetting phase to water, and occupies smaller elements – see Figure 4.25. As a consequence the relative permeability is substantially lower. This decrease in gas relative permeability for gas invading water in an oil-wet medium has been observed experimentally (DiCarlo et al., 2000a,b).

A surprising observation is that the water relative permeability – Figure 4.24 – is very low, except at high saturation, even though water is the most non-wetting phase. This has already been discussed in the context of two-phase flow by Valvatne and Blunt (2004). Water is connected in the corners of the pore space, but these water layers have a very low conductance giving relative permeabilities of order $10^{-6}$. During water injection, water fills the larger pores and throats in clusters seeded from elements that remain water filled after primary drainage. Until these clusters connect, the water relative permeability remains very low. Only at intermediate saturation – around 0.5 – do the water clusters connect and the relative permeability increases rapidly.

Table 4.9 Interfacial tensions and contact angles used for WAG cycles into a strongly oil-wet system.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{gw}$ (mN/m)</td>
<td>67</td>
</tr>
<tr>
<td>$\sigma_{go}$ (mN/m)</td>
<td>19</td>
</tr>
<tr>
<td>$\sigma_{ow}$ (mN/m)</td>
<td>48</td>
</tr>
<tr>
<td>$\theta_{gw}$ (degrees)</td>
<td>99 – 124</td>
</tr>
<tr>
<td>$\theta_{go}$ (degrees)</td>
<td>45 – 65</td>
</tr>
<tr>
<td>$\theta_{ow}$ (degrees)</td>
<td>120 – 160</td>
</tr>
<tr>
<td>$\theta^4_{gw}$ (degrees)</td>
<td>115 – 134</td>
</tr>
<tr>
<td>$\theta^4_{go}$ (degrees)</td>
<td>65 – 85</td>
</tr>
<tr>
<td>$\theta^4_{ow}$ (degrees)</td>
<td>140 – 180</td>
</tr>
</tbody>
</table>
Figure 4.21 WAG saturation path for a strongly oil-wet system.

Figure 4.22 Predicted oil relative permeability for a strongly oil-wet system for the saturation path shown in Figure 4.21.
Figure 4.23 Predicted gas relative permeabilities for a strongly oil-wet system for the saturation path shown in Figure 4.21.

Figure 4.24 Predicted water relative permeabilities for a strongly oil-wet system for the saturation path shown in Figure 4.21.
Figure 4.25 Bulk pore occupancies for first and second gas injection cycles in a strongly oil-wet medium for the saturation path shown in Figure 4.21.

Table 4.10 Statistics of the displacement mechanisms for the first and second water injection cycles for the saturation path shown in Figure 4.21.

<table>
<thead>
<tr>
<th>Water</th>
<th>Piston-like (water-oil)</th>
<th>Snap-Off (water-oil)</th>
<th>Layer Collapse (water-oil)</th>
<th>Piston-like (water-gas)</th>
<th>Snap-Off (water-gas)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water 1</td>
<td>6314</td>
<td>0</td>
<td>24</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Fraction (%)</td>
<td>99.7</td>
<td>0</td>
<td>.3</td>
<td>16.0</td>
<td>6</td>
</tr>
<tr>
<td>Water 2</td>
<td>2923</td>
<td>0</td>
<td>12763</td>
<td>2594</td>
<td>6</td>
</tr>
<tr>
<td>Fraction (%)</td>
<td>16.0</td>
<td>0</td>
<td>69.8</td>
<td>14.2</td>
<td>.03</td>
</tr>
</tbody>
</table>

4.5 Effects of Spreading Coefficient and Gas-Oil Contact Angle

In this section we will investigate the effect of changing the gas-oil contact angle and gas-water interfacial tension for water-wet and oil-wet systems. Indirectly this will be a study of the effect of spreading coefficient on oil recovery. We will show that the stability of oil layers and consequently the trapping of oil is controlled by the gas-oil contact angle and the spreading coefficient for a water-wet system. However, in a strongly oil-wet case, the effect is much less since oil layers are stable throughout the displacement.

Water-wet system. We will compare the results of three simulations for different gas-oil contact angles and gas-water interfacial tensions. Using the Bartell-Osterhof
constraint, see Equation (3.6), we calculate the third (gas-water) contact angle as long as two of the contact angles and three interfacial tensions are defined independently. In our first simulation, we use exactly the same interfacial tensions and contact angles used while matching Oak’s experiments – Tables 3.3 and 4.11 (Note that these are the same parameters used by Piri and Blunt, 2005b). This is a spreading system – the equilibrium spreading coefficient is zero – but the gas-oil contact angle is finite. The reason for this choice of parameters is to find a contact angle that would give a trapped gas saturation for oil flooding that matched Oak’s experiments (see Chapter 3).

In the second case, we retain a spreading system but assume a zero gas-oil contact angle and keep all other parameters same (however, note that this also alters the gas-water contact angle slightly, see Equation (3.6)).

In the final case, we keep the same gas-oil contact angle as in Tables 3.3 and 4.11, but this time assume a non-spreading system (negative spreading coefficient) by decreasing the gas-water interfacial tension according to Equation (3.15). We find a value of 64 mN/m. The spreading coefficient is thus -3 mN/m. All other parameters are kept constant. Table 4.11 shows the contact angles and interfacial tensions used for our simulations.

Table 4.11 Contact angles and interfacial tensions used in our simulations for a water-wet system. Case 3 has a spreading coefficient of -3 mN/m.

<table>
<thead>
<tr>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{gw}$ (mN/m)</td>
<td>67</td>
<td>67</td>
</tr>
<tr>
<td>$\sigma_{go}$ (mN/m)</td>
<td>19</td>
<td>19</td>
</tr>
<tr>
<td>$\sigma_{ow}$ (mN/m)</td>
<td>48</td>
<td>48</td>
</tr>
<tr>
<td>$\theta^r_{gw}$ (degrees)</td>
<td>36.6 – 57.3</td>
<td>36.1 – 50.1</td>
</tr>
<tr>
<td>$\theta^r_{go}$ (degrees)</td>
<td>10 – 50</td>
<td>0</td>
</tr>
<tr>
<td>$\theta^r_{ow}$ (degrees)</td>
<td>43 – 60</td>
<td>43 – 60</td>
</tr>
<tr>
<td>$\theta^a_{gw}$ (degrees)</td>
<td>55.2 – 77.2</td>
<td>52.5 – 65.9</td>
</tr>
<tr>
<td>$\theta^a_{go}$ (degrees)</td>
<td>30 – 70</td>
<td>0</td>
</tr>
<tr>
<td>$\theta^a_{ow}$ (degrees)</td>
<td>63 – 80</td>
<td>63 – 80</td>
</tr>
</tbody>
</table>

We then conduct gas injection after waterflooding to low oil saturation in all three cases. Due to the reconnection of oil clusters with double displacement, we are able to reach very low residual oil saturations during gas injection (Figure 4.26). We
stop the simulation once oil relative permeability goes below $10^{-4}$. This corresponds physically to the lower limit of oil relative permeability probed experimentally that is often considered the residual oil saturation (Oak, 1990; Jerauld, 1997a,b).

For both the high gas-oil contact angle and negative spreading coefficient, we obtain a slightly higher remaining oil saturation than we do for the simulation with a zero gas-oil contact angle (around 6% for case1 and case3, and 2% for case 2). This is expected as the oil layers become less stable. This behaviour was also observed and discussed in the previously conducted experimental and numerical studies (Sohrabi et al., 2000; van Dijke et al., 2004a).

Figure 4.27 compares the oil relative permeabilities for the three simulations. As expected during the waterflood to residual oil ($S_{or} = 0.28$, see Figure 4.26), the oil relative permeabilities are exactly same. The reason is we use exactly same oil-water interfacial tensions and oil-water contact angles in all three simulations (Table 4.11). However, during gas injection ($S_o$ below 0.28, see Figure 4.27), a slight difference is observed in the oil relative permeability especially for case2. For case2, oil relative permeability is higher than for case1 and case3. Assuming a non-zero gas-oil contact angle (case1) and negative spreading coefficient (case3) make oil layers less stable and increase the number of trapped oil clusters. Therefore, oil relative permeability for case2 is slightly higher than that of case1 and case3.

Traditionally authors have discussed oil recovery in terms of the spreading coefficient, Equation (3.2), since this affects, in a strongly water-wet medium, the gas-oil contact angle, Equation (3.15), that in turn controls oil layer stability, Equation (3.10) (see, for instance, Mani and Mohamty, 1998; Fenwick and Blunt, 1998a,b). In a medium that is not strongly water-wet, there is no longer a direct relationship between spreading coefficient and gas-oil contact angle. In our simulations we have used values of the contact angles chosen to match the measured two-phase residual non-wetting phase saturations for Berea sandstone (Oak, 1990). Our simulations demonstrate that it is the gas-oil contact angle and not the spreading coefficient itself that controls layer stability and oil recovery during gas injection. We see similar recoveries for the same gas-oil contact angle for both a spreading and non-spreading system, but higher recoveries for a spreading system with a zero gas-oil contact angle.

We might expect that there is a relationship between gas-oil contact angle and spreading coefficient even in systems that are not strongly water-wet, with the gas-oil
contact angle increasing for more negative spreading coefficient. While this is plausible, there is no direct experimental evidence of this relationship. Our studies simply suggest that the gas-oil contact angle is an important parameter determining oil layer stability and oil recovery.

![Saturation paths shown for gas injection after waterflooding to residual oil for water-wet conditions. Note that simulations were stopped once oil relative permeability reaches $10^{-4}$.](image)

**Figure 4.26** Saturation paths shown for gas injection after waterflooding to residual oil for water-wet conditions. Note that simulations were stopped once oil relative permeability reaches $10^{-4}$. 
Figure 4.27 Comparison of oil relative permeabilities for gas injection after waterflooding for water-wet conditions. Note that, the results are exactly same during two-phase water injection until we reach residual oil ($S_{or} = 0.28$). The effect of varying simulation parameters is observed during gas injection process ($S_o < 0.28$).

We now study a different saturation path where a secondary water injection follows gas invasion. Gas is injected after waterflooding until the gas saturation reaches 0.3. We continue waterflooding until all gas and oil clusters get trapped. We use same contact angles and interfacial tensions shown in Table 4.11. Figure 4.28 compares the saturation paths for the three simulations. Although the paths are similar, we obtain a slightly lower residual oil saturation for case2. Relative permeability predictions confirm this result as the oil relative permeabilities for subsequent gas and water injection cycles are highest for case2 (Figure 4.29).

We also compare the displacement statistics for all three cases (Table 4.12). We obtain significantly fewer double displacements for case2: the zero gas-oil contact angle makes oil layers significantly more stable compared to the two other cases. These results again confirm that oil layer stability is heavily determined by the gas-oil contact angles and not by the spreading coefficient alone. Although we obtain more double displacements in case3 (negative spreading coefficient and a finite gas-oil contact angle) as the layers are the least stable in this case, the difference with case 1 (zero spreading coefficient and the same gas-oil contact angles as case3) is not that
significant. These results also underline the importance of double displacement mechanisms during WAG injection cycles in a water-wet medium.

If there was no double displacement then there would be no additional oil recovery after waterflooding; gas injection can only boost recovery if double displacements are allowed regardless of the gas-oil contact angle or spreading coefficient.

![Diagram showing saturation paths](image)

**Figure 4.28** Saturation paths shown for gas injection to a gas saturation of 0.3 after waterflooding followed by a subsequent waterflooding for water-wet conditions.
Figure 4.29 Comparison for oil relative permeabilities for gas injection after waterflooding followed by a subsequent water injection cycle for water-wet conditions.

Table 4.12 Comparison of the double displacement occurrences for the saturation paths shown in Figure 4.28. Both number of double displacements and their fractions to the total number of displacements are given.

<table>
<thead>
<tr>
<th></th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas-oil-water/</td>
<td>4159/26%</td>
<td>3514/25%</td>
<td>4102/27%</td>
</tr>
<tr>
<td>fraction (%)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water-oil-gas/</td>
<td>1539/27%</td>
<td>586/13%</td>
<td>1656/29%</td>
</tr>
<tr>
<td>fraction (%)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water-gas-oil/</td>
<td>578/10%</td>
<td>309/7%</td>
<td>602/11%</td>
</tr>
<tr>
<td>fraction (%)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Oil-wet system.** As for the water-wet case, we conduct three simulations by altering the gas-oil contact angle and gas-water interfacial tension. The parameters used during these simulations are shown in Table 4.13. In an oil-wet system, we can displace almost all oil with the first waterflood, as oil clusters form stable layers in between water in the centres and the corners of the pores and throats. Therefore, we continue each flood until we reach a predetermined phase saturation. For these three simulations we start with waterflooding until the water saturation reaches 50%, then gas injection until the gas saturation reaches 35%, and one more water injection until the water saturation reaches 60% (note that we also put an error margin of 2% while
stopping a flood, which means the floods may stop slightly earlier than the specified
saturation points, Figure 4.30).

Results for all three simulations are similar: oil layers are stable for all cases
and the behaviour is relatively insensitive to the gas-oil contact angle. Figure 4.31
compares the oil relative permeabilities for the three cases. As expected the results are
broadly the same in all cases since oil layers are stable in an oil-wet medium.

The conclusion of this Chapter is that our network model can make accurate
predictions of relative permeability for cycles of water and gas injection. Our
introductory sensitivity study illustrates how the three-phase flow behaviour is a
function of wettability and gas-oil contact angle.

One of the key issues that we would like to study is oil and gas trapping and
this is discussed in the next Chapter. We will show that the stability of oil layers has a
major impact on the amount of trapping and that saturation path – even for oil-wet
systems – has a significant impact on residual saturations.

| Table 4.13 Contact angles and interfacial tensions used during our simulations for an oil-wet system. |
|---------------------------------|--------|--------|--------|
| \(\sigma_{gw}\) (mN/m) | 67 | 67 | 64 |
| \(\sigma_{go}\) (mN/m) | 19 | 19 | 19 |
| \(\sigma_{ow}\) (mN/m) | 48 | 48 | 48 |
| \(\theta^r_{gw}\) (degrees) | 99.1 – 123.6 | 94.3 – 112.9 | 99.5 – 125.4 |
| \(\theta^r_{go}\) (degrees) | 45 – 65 | 0 | 45 – 65 |
| \(\theta^r_{ow}\) (degrees) | 120 – 160 | 120 – 160 | 120 – 160 |
| \(\theta^a_{gw}\) (degrees) | 115.4 – 133.8 | 105.4 – 115.6 | 116.7 – 136.4 |
| \(\theta^a_{go}\) (degrees) | 65 – 85 | 0 | 65 – 85 |
| \(\theta^a_{ow}\) (degrees) | 140 – 180 | 140 – 180 | 140 – 180 |
Figure 4.30 Saturation paths shown for water-gas-water injection cycles for oil-wet conditions. Note that the paths are almost same. However, during gas injection in case2, gas prefers to displace more water, as decreasing gas-oil contact angles to zero significantly increases the gas-oil capillary pressure.
Figure 4.31 Comparison for oil relative permeabilities in an oil-wet system. The results are similar. This is expected since oil layers are stable in an oil-wet medium regardless of the oil spreading coefficient and gas-water interfacial tension. Note that, unlike the water-wet case, we do not observe noise (fluctuations) in the data at the end of the floods since oil is connected during each injection cycle.
Chapter 5

Hydrocarbon Trapping

Geological storage of carbon dioxide (CO$_2$) is one way to mitigate atmospheric emissions of greenhouse gas. The estimated storage capacity worldwide in depleted oil and gas fields and saline aquifers is able to accommodate current levels of CO$_2$ emissions for many decades (Holloway and Savage, 1993). CO$_2$ can be captured from fossil-fuel burning power stations, compressed, piped and then injected into mature oil fields. Some of the costs of the process could be off-set by enhanced oil recovery (Jessen et al., 2005). Key parameters while conducting simulations of CO$_2$ injection are three-phase relative permeabilities.

The most rapid mechanism by which CO$_2$ can be rendered immobile after the initial injection phase is trapping as the CO$_2$ rises upwards under gravitational forces or because of water displacement due to a regional groundwater flow (Spiteri et al., 2005). Hence predictions of the trapped fluid saturations are particularly important.

The major advantage of network modelling is that once validated we can predict flow and transport properties for any given wettability and sequence of saturation changes. In this chapter we will use the network model as a first step towards developing an empirical model to predict three-phase relative permeability with an emphasis on considerations of how much oil and gas is trapped for different displacement paths.

5.1 Oil Isoperm Curves

We will study oil isoperm curves and both oil and gas trapping for four different wettability conditions. We use same interfacial tensions (oil spreading system) used during the predictions of Oak’s experiments (Table 3.3). The contact angles used to represent water-wet, weakly water-wet, weakly oil-wet and strongly oil-wet systems are shown in Table 5.1.
Based on two-phase relative permeability data obtained from Oak’s (1990) experiments, Spiteri and Juanes (2004) predicted oil isoperm curves using Stone I (1970) and Stone II (1973) models (Figures 5.1 and 5.2). Although the two sets of curves are different, in both cases a convex behaviour is observed especially in the low oil saturation region.

Figure 5.3 shows oil isoperm curves computed using our network model for a water-wet system for two different saturation paths (path 1 stands for gas injection after waterflooding and path 2 stands for waterflooding after gas injection). The isoperm curves predicted by our network model for a water-wet system are significantly different from the curves predicted by Stone’s models – Figures 5.1 and 5.2. We observe approximately linear isoperms in the low oil saturation region.

In a water-wet medium, gas injection into a three-phase system with high oil saturation results in a decrease in the oil relative permeability even if the oil saturation remains constant. Gas, as the most non-wetting phase, displaces oil from the bigger pores, pushing it into smaller elements. However, for low oil saturations, the effect is the opposite. As discussed earlier, gas injection into low oil saturation, where most of the oil is trapped, causes many double displacement events, reconnecting the trapped oil, which increases the oil relative permeability.

The isoperm curves are also quite different for two different injection paths (Figure 5.3). As we discuss below, this is principally due to different amounts of oil and gas trapping for the two displacement sequences.

<table>
<thead>
<tr>
<th></th>
<th>$\theta_{ow}$</th>
<th>$\theta_{go}$</th>
<th>$\theta_{gw}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water-wet</td>
<td>30 - 50</td>
<td>0</td>
<td>25 - 42</td>
</tr>
<tr>
<td>Weakly water-wet</td>
<td>60 - 90</td>
<td>0</td>
<td>50 - 73</td>
</tr>
<tr>
<td>Weakly oil-wet</td>
<td>100 - 150</td>
<td>0</td>
<td>80 - 110</td>
</tr>
<tr>
<td>Oil-wet</td>
<td>150 - 180</td>
<td>0</td>
<td>110 - 116</td>
</tr>
</tbody>
</table>

Table 5.1 Contact angles used to represent different wettability conditions. The ones shown in the table are the advancing values. Receding values are 20 degrees lower than the advancing ones. During primary drainage $\theta_{ow}$ is assumed to be zero.
Figure 5.1 Oil isoperm curves predicted by Stone I (Stone, 1970) model (Spiteri and Juanes, 2004).

Figure 5.2 Oil isoperm curves predicted by Stone II (Stone, 1973) model (Spiteri and Juanes, 2004).
Figure 5.3 Oil isoperm curves predicted by the network model for a water-wet system for path1 (tertiary gas injection after waterflooding) and path2 (waterflooding after gas injection).

In an oil-wet medium, the oil isoperm curves are almost straight lines which show that the oil relative permeability is approximately a function of its own saturation only (see Figure 5.4). It can also be observed that even at very low oil saturations, the oil relative permeability is non-zero. The oil clusters remain connected at very low saturations in stable layers and the relative permeability is insensitive to the relative amounts of water and gas.

The conclusion of this section is that for water-wet media it is not possible to use current empirical models to predict the oil isoperm curves accurately – the results from the network model and the work of Spiteri and Juanes (2004) are very different. Furthermore the isoperms are a function of the displacement sequence. For oil-wet media the oil isoperms are straight lines, since the oil occupies the smaller pore spaces.
5.2 Effects of Saturation Path

While three-phase relative permeabilities have a strong dependence on the saturation history of the system (Blunt, 2000; Element et al., 2003; Skauge and Larsen, 1994; Svirsky et al., 2004) it has been hypothesized that the relative permeability is independent of saturation path when plotted as a function of flowing saturation – total saturation minus the trapped saturation (Carlson, 1981). Then an empirical trapping model is used to predict the trapped saturation of each phase; from this the flowing saturations and hence relative permeabilities may be predicted for any displacement path (Blunt, 2000; Land, 1968; Jerauld, 1997b). Using network modelling it is possible to test this hypothesis by studying different fluid flow scenarios which are difficult or time consuming to perform experimentally.

Figure 5.5 shows oil isoperm curves for a water-wet medium for different injection sequences following primary drainage: water-gas (path1) and gas-water (path2). In contrast to Figure 5.3, we draw the isoperm curves with respect to the flowing fluid saturations; the curves are now approximately independent of the
saturation path. Note, however, that the oil relative permeability is still a function of two saturations – the isoperms have considerable curvature.

![Diagram of oil isoperm curves](image)

**Figure 5.5** Comparison of oil isoperm curves as a function of flowing fluid saturations for a water-wet system for different displacement sequences. Path1 stands for water-gas, path2 stands for gas-water.

### 5.3 Effects of Wettability

To predict three-phase relative permeability we need to estimate the amount of oil and gas that is trapped for any displacement sequence. Jerauld (1997b) suggested that the total hydrocarbon (oil and gas) trapped in a three-phase system would be up to 0.2 greater than the waterflood residual oil saturation during two-phase flow.

Figure 5.6 shows the trapped hydrocarbon saturation. This is computed for the following displacement sequence: primary drainage followed by gas injection to different initial gas saturations $S_{gi}$, followed by water injection until all the gas and oil is trapped in other words where the flood stops since oil and gas relative permeabilities reach zero. The contact angles used are given in Table 5.1. In oil-wet media this may give lower residual values than seen in experiments, since, as mentioned previously, an apparent measured residual is determined when the displaced relative permeability is in the range $10^{-4}$ to $10^{-3}$ (Jerauld, 1997a,b).
Figure 5.6 Comparison of total hydrocarbon trapped as function of waterflood residual oil saturation for a water-wet and a weakly water-wet system. The trapped hydrocarbon saturation is measured after waterflooding following gas injection to different initial saturations $S_{gi}$. The solid line indicates $S_{gt} = S_{orw}$, whereas the dashed line shows $S_{gt} = S_{orw} + 0.2$, as suggested by Jerauld (1997b).

For both water-wet and weakly water-wet media (Table 5.1), the trapped hydrocarbon saturation is in the range predicted, but surprisingly the amount of trapping is larger for a weakly water-wet system, where the waterflood residual oil saturation is lower. During water injection into gas, there is a competition between pore body filling and snap-off events. Table 5.2 summarises the displacement statistics for the water injection cycle for both water-wet and weakly water-wet systems. More snap-off events have taken place in a weakly water-wet medium where the gas/water contact angle – see Table 5.1 – is higher. This is a counter-intuitive result since snap-off displacement is more favoured for a strongly water-wet system. Equation (3.9) shows that decreasing the oil-water contact angle increases the displacement $P_{egw}$ meaning that a snap-off displacement requires a lower water pressure and becomes more favoured in a strongly water-wet system. How can we explain this surprising result?
Table 5.2 Statistics of the displacement mechanisms for the water injection cycle for the results shown in Figure 5.6. The initial gas saturation ($S_{gi}$) in the system is 0.5.

<table>
<thead>
<tr>
<th></th>
<th>Pore Filling (water-gas)</th>
<th>Snap-Off (water-gas)</th>
<th>Layer Collapse (water-oil)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water-wet</td>
<td>2514</td>
<td>22</td>
<td>12161</td>
</tr>
<tr>
<td>Weakly water-wet</td>
<td>1220</td>
<td>296</td>
<td>15949</td>
</tr>
</tbody>
</table>

At the beginning of water injection, the gas-filled pores and throats contain oil layers. Before water can snap-off gas in the centre, first the oil layer must collapse since these layers prevent direct contact of the gas by water. Table 5.2 shows that significantly more layer collapse events have taken place for a weakly water-wet system compared to a strongly water-wet one. However, as we discussed in Chapter 3, oil layers become more stable with a higher threshold water pressure for collapse as the oil/water contact angle increases. This is another counter-intuitive result and requires a detailed explanation.

To recap: we would expect a weakly water-wet system to see less water-gas snap-off and less oil layer collapse during water injection, resulting in a lower trapped oil and gas saturation. Instead, for a high initial gas saturation we see exactly the opposite: more snap-off and more layer collapse leading to more oil and gas trapping. How can we explain these puzzling results?

The explanation of this behaviour hinges on the nature of the oil layer collapse – indeed on the hinging contact angle. In all our simulations we assumed a zero oil/water contact angle during primary drainage and then a zero gas/oil contact angle during gas injection regardless of the wettability of the system. This means that we have exactly the same initial conditions, independent of the chosen $\theta_{ow}$ prior to waterflooding. During gas injection, gas prefers to displace oil from the bigger pores and throats. However, oil remains in these elements as layers between water and gas. During water injection, water in the corners of the pore space swells and the oil layers may collapse. As discussed in Chapter 3 there are two different ways in which this might occur. The first is due to the movement of the oil/water/solid contact line towards the centre of the element. In this case, the threshold capillary pressure decreases rapidly with oil/water contact angle, meaning that oil layers are more stable, the more oil-wet the system is. The second way is that the oil/water interface bulges with the oil/water/solid contact pinned with a steadily increasing hinging oil/water
contact angle. The layer collapses when the oil/water interfaces touches the gas/oil interface. In this case, the threshold capillary pressure does not depend on wettability.

Which process takes place? Does the contact move or is it pinned? If the initial gas saturation is large, then the final gas/oil capillary pressure is also large and hence the gas/oil interface penetrates a long way into the corner of the pore space. This means that the oil layers are relatively thin in many of the pores and throats, as illustrated in Figure 5.7. Therefore, when we inject water into the system, water may collapse these layers without moving the oil/water/solid contact. In other words, the hinging oil/water contact angle at which the water/oil interface meets the gas/oil interface is smaller than the advancing oil/water contact angle. As a consequence, the wettability of the system does not affect the threshold capillary pressure for layer collapse; for all four different wettability conditions, the displacement requires exactly same threshold pressure, see Equation (3.11).

The same layer collapse capillary pressure does not imply that layers are equally stable during a displacement, since this threshold capillary pressure has to be compared to the capillary pressures for other displacements. Water may displace oil and gas by piston-like advance, snap-off and pore filling. For all these displacements, the threshold water pressure increases with increasing oil/water contact angle. Hence, for a strongly water-wet system, water will displace oil and gas, filling pores and throats at a lower water pressure than that necessary to collapse oil layers. As a consequence, oil will remain connected and the degree of oil trapping will be small. Furthermore, since the principal mechanism for trapping of gas is snap-off by water, little gas will be trapped, since snap-off will not happen, since water will not contact gas directly due to stable oil layers.

In a weakly water-wet system, pore and throat-filling events are less favoured; as a consequence the water pressure has to increase higher for a given increase in water saturation. This means that now more layer collapse events take place, and they take place earlier in the displacement. Layer collapse helps to disconnect oil. In addition, it allows direct contact of gas by water and hence gas/water snap-off may occur, trapping gas as well. We see that the amounts of oil and gas trapped are larger than for a water-wet system.
Figure 5.7 Layer collapse after primary gas invasion. The oil/water arc meniscus adjusts its curvature as the water pressure increases with a hinging oil/water contact angle $\theta_{ow}^h$ at a pinned oil/water/solid contact. The oil layer will collapse when the oil/water and gas/oil interfaces meet. If the critical hinging angle is less than the advancing oil/water contact angle, then the threshold water pressure for oil layer collapse is independent of wettability.

Figure 5.8 shows the trapped gas saturation as a function of the initial gas saturation in the system. We obtain a reasonable match with the Land’s trapping model (1968) for a water-wet system. However, there is an increase in the trapped gas saturation once the system becomes weakly water-wet due to the fact that we obtain more water to gas snap-off displacements in a weakly water-wet system (Table 5.2), as discussed before.

Once the system becomes oil-wet, the amount of trapped gas is dependent on the ability of the gas phase to form layers in between the water clusters in the corner and water clusters in the centre of the pore and throat elements. In a weakly oil-wet medium, gas is still the most non-wetting phase and cannot form layers. The amount of trapping is similar for a weakly water-wet system. If the medium is oil-wet there are no water/gas snap-off events. However, there is even more oil layer collapse than before, since other displacement processes occur at a higher water pressure. This means that the water contacts gas directly, allowing bypassing and trapping of gas
clusters. Approximately the effects of less snap-off and more bypassing by direct water/gas displacement cancel and the overall trapped gas saturation is similar.

For a strongly oil-wet system contact angles are greater than 90° – see Table 5.1. This means that gas is not the most non-wetting phase; it is intermediate-wet and water is the most non-wetting. During water injection, as discussed above, the oil layers collapse early in the displacement, since layer collapse is favoured over any direct water/oil or water/gas displacement that requires a high water pressure, since water is the non-wetting phase. Hence most gas-filled pores and throats soon have configuration C-4 in Figure 3.7. Then, when water invades the element by piston-like advance, water occupies the centre of the pore space with a layer of gas in between – configuration E-2 in Figure 3.7. As the initial gas saturation increases, so does the final gas phase pressure. This pushes the gas/oil interface – and, after layer collapse the gas/water interface – further into the corners making the gas layers more stable and more numerous, since more elements are filled with gas. Hence the proportion of elements with gas layers after piston-like water invasion increases with increasing initial gas saturation. These layers maintain connectivity of the gas phase and result in less trapping. Hence we see a somewhat peculiar trend in trapping: the amount of trapped gas decreases with increasing initial gas saturation.

We compare the fluid configurations at the end of water injection in Table 5.3. It is observed that the number of fluid configuration E-2 (gas resides in layers between water clusters - see Figure 3.7) increases with the increase in the initial gas saturation (Table 5.3) in a strongly oil-wet medium. This confirms our explanation for the decrease in the trapped gas saturation with increasing initial gas saturation.
Figure 5.8 Comparison of trapped gas saturation as a function of initial gas saturation. Note that for a strongly oil-wet system, the amount of trapped gas decreases with increasing initial gas saturation.

Table 5.3 Percentage of elements in the E-2 fluid configuration (Figure 3.7) as a function of the initial gas saturation for a strongly oil-wet system after water injection.

<table>
<thead>
<tr>
<th>Percentage of configuration E-2 (%)</th>
<th>$S_g=0.3$</th>
<th>$S_g=0.4$</th>
<th>$S_g=0.5$</th>
<th>$S_g=0.6$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2.7</td>
<td>7.34</td>
<td>9.12</td>
<td>12.7</td>
</tr>
</tbody>
</table>

The decrease in the residual oil saturation with an increase in the initial gas saturation has already been discussed in the literature (Holmgren and Morse, 1951; Kortekaas and Poelgeest, 1991). The trend with wettability though has not been discussed before. Figure 5.9 shows that there is a crossover in the curves for a weakly water-wet and water-wet system. The amount of oil trapping is controlled by two factors: (1) how much oil is trapped for direct displacement of oil by water in elements containing no gas; and (2) the stability of oil layers in gas-filled pores and throats. As mentioned above, we obtain more layer collapse events in a weakly water-wet medium leading to more oil trapping when the initial gas saturation is high (Table 5.2). Hence the residual oil saturation in the presence of gas is higher for a weakly water-wet system. However, in the presence of water alone, the residual oil saturation is lower since there is less snap-off of oil causing trapping, since the oil/water contact...
angle is higher, as discussed in Chapter 3 (Blunt, 1997). These two effects compete and there is an initial gas saturation where the two curves cross.

For oil-wet systems, the amount of trapping at low initial gas saturation is as we expect for two-phase oil/water systems. As the oil/water contact angle increases, oil layers may form in the pore space, configurations D1 and D2 in Figure 3.7, sandwiched between water in the corner and water in the centre. These layers provide continuity of the oil and mean that little oil is trapped during waterflooding.

The unexpected observation is that as the initial gas saturation increases, implying less initial oil in the system, the trapped oil saturation increases. As mentioned before, as the systems becomes more oil-wet, layer collapse events become more common since they are favoured in comparison to direct displacement of oil and gas by water. This is confirmed in Table 5.4 that shows that for the strongly oil-wet case almost all the displacement events at high initial gas saturation are layer collapse. Once the oil layers have gone, oil is poorly connected across the system if the initial gas saturation is high – most clusters of oil-filled elements are surrounded by gas. As a consequence, direct water/oil displacement is no longer possible and the amount of oil that is trapped is quite large. Layer collapse is favoured for both weakly and strongly oil-wet systems. However, slightly less oil is trapped for the strongly oil-wet case. This is because, as with low and zero initial gas saturations, where there is water to oil displacement, oil layers form and maintain connectivity of the oil clusters, giving less trapping.

For the highest initial gas saturation considered – $S_{gi} = 0.6$ – there is only layer collapse and no direct water/oil displacement – see Table 5.4. When water is injected, the oil layers collapse and no connected oil clusters remain in the system. The initial oil saturation is approximately 16%; at the end of water injection virtually no oil has been displaced for either strongly or weakly oil-wet cases. If the initial gas saturation were to increase further, the trapped oil saturation would decrease – it would simply be close to the initial oil saturation, as the oil would become rapidly disconnected on injection of water.

Table 5.5 gives a comparison of fluid configurations for weakly and strongly oil-wet cases (for $S_{gi}=0.5$). We observe significantly more D-2 configurations (see Figure 3.7) for a strongly oil-wet system – this is where oil remains as a layer in the pore.
space. This explains the higher trapped oil saturation observed for a weakly oil-wet case.

![Figure 5.9 Comparison of trapped oil saturation as a function of initial gas saturation.](image)

**Figure 5.9 Comparison of trapped oil saturation as a function of initial gas saturation.**

Table 5.4 Fraction of the number of water collapsing oil layer displacement processes to the total number of water to oil displacements for different initial gas saturations for a strongly oil-wet system. Note that for the highest initial gas saturation the only events are layer collapse.

<table>
<thead>
<tr>
<th>$S_{gi}$</th>
<th>0.3</th>
<th>0.4</th>
<th>0.5</th>
<th>0.6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Percentage of oil layer collapse events (%)</td>
<td>73.61</td>
<td>74.64</td>
<td>87.51</td>
<td>100</td>
</tr>
</tbody>
</table>

Table 5.5 Percentage of elements in the D-2 fluid configuration (Figure 3.7) for weakly and strongly oil-wet cases. Comparison is done for $S_{gi}$=0.5.

<table>
<thead>
<tr>
<th>Strongly oil-wet</th>
<th>Weakly oil-wet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Percentage with configuration D-2 (%)</td>
<td>13</td>
</tr>
</tbody>
</table>

These results show some surprising trends with saturation history and wettability due to the complex competition between three-phase displacement processes. It is difficult and time-consuming to investigate the full range of this behaviour by conducting experiments. Pore-network modelling is a useful tool for understanding multiphase flow in porous media and, in particular, to determine sensitivities for
different displacement processes and wettabilities. From a practical perspective it is possible to study a wide range of different displacement scenarios by altering the predetermined input parameters and initial conditions and it may be possible to use the results, eventually, to propose a more physically-based model for three-phase relative permeability than the expressions currently used in the industry.

Among the puzzling results presented in this Chapter are: the increase in oil layer collapse with increasing oil/water contact angle; the increased oil and gas trapping for a weakly water-wet system compared to a weakly water-wet system; the decrease in trapped gas with increasing initial gas saturation for a strongly oil-wet system; and the increase in trapped oil with increasing initial gas saturation for weakly and strongly oil-wet systems. In all these cases a simple analysis of the problem would predict the opposite behaviour. It is only through a careful analysis of displacement statistics and fluid configurations that these results can be explained. This illustrates the need to have detailed models of the displacement process that capture the three-phase displacement physics as carefully as possible. Furthermore, all these results were obtained from just one set of simulations where water injection started from the same initial configuration in the pore space regardless of wettability; had we considered more complex saturation paths with more than one water injection cycle, the results may well have been even more bewildering and difficult to explain.

This has only been an introductory study of trapping in three-phase flow where we have only considered one network and one set of displacement paths. It is established experimentally that the amount of trapping increases as the ratio of average pore to throat size (the aspect ratio) increases and as the connectivity of the pore space decreases (Oak, 1990; Jerauld 1997a,b). This is something that could be investigated in future work when networks representing different porous media are available.

Two initial conclusions can then be made from this study. First, the complexity of three-phase flow makes it a challenge to find a simple empirical model that will be able to capture the great richness of behaviour that we have encountered. Second, most of the discussion revolves around the treatment of oil layer stability. Therefore it is vital that for future work we have as accurate a model of layers as possible. As we will discuss further in the next section, we recommend implementation of thermodynamically consistent expressions for the threshold capillary pressures,
particularly as they pertain to layer formation and collapse, before embarking on a more detailed study of oil and gas trapping. We think that the generic trends we observe will still be correct: with the same initial configuration of oil, water and gas at the beginning of waterflooding, it is likely that layer collapse will continue to occur at a capillary pressure that is largely independent of oil/water contact angle. However, we cannot be certain that all our conclusions concerning trapping will be correct if only a geometric stability criterion is used. The tendency will be to over-estimate the stability of oil and gas layers.
Chapter 6

Final Remarks

Approximately two-thirds of the world’s oil that has been discovered will be left underground using conventional extraction technologies (Lake, 1989): one reason for this is that the oil is trapped in the pore spaces of the reservoir rock. One way to improve recovery is to inject high-pressure gas, which could be air, natural gas, steam or CO₂ into a reservoir containing oil and water (Lake, 1989; Amyx et al., 1960). At the small scale, the gas can mobilize trapped oil resulting in an improved local displacement efficiency.

In this thesis we have studied the fundamental science associated with three-phase flow in oil reservoirs by predicting what will happen within the micron-sized gaps between grains in the rock through which oil, water and gas flow. We represent the pore space of a piece of rock just a few mm across as a network of pores and throats through which we simulate the movement of oil, water and gas. This is now a widely-used technique to predict transport properties at the core (mm or cm) scale from a knowledge of structure and displacement physics at the small (μm) scale (Blunt et al., 2002). Only once this small-scale behaviour is understood can we make predictions of recovery and gas storage at the field scale.

In this research we have extended an existing three-phase network model to predict three phase relative permeability and residual gas and oil saturation for WAG flooding as a function of displacement path and wettability. In the next section we highlight the main conclusions of the work.

6.1 Conclusions

We used a physically-based three-phase network model (Piri and Blunt, 2005a,b) to predict three-phase relative permeabilities for WAG flooding for different wettability conditions. We extended the model by adding two new double displacement mechanisms, double imbibition (water-oil-gas) and imbibition-drainage (water-gas-
oil). We first validated the model by accurately predicting relative permeabilities from three water-wet experimental datasets in the literature. We then performed two WAG injection studies for water-wet and oil-wet media. We also underlined the importance of interfacial tensions and contact angles by comparing the results of simulations with varying parameters for both a water-wet and an oil-wet system.

When gas is injected after waterflooding in the first WAG cycle, double displacement of residual oil is essential for recovery; without double displacement no incremental oil can be recovered. The ultimate oil recovered after subsequent cycles of water and gas injection is controlled by the stability of oil layers. Gas trapping is also controlled by oil layer stability and snap-off of gas by water. Double displacement of trapped gas is also a significant mechanism during waterflood cycles.

In water-wet media, the gas relative permeability is lower during water injection following first gas injection because of trapping. Subsequent cycles of water and gas flooding only lead to further reductions in relative permeability if the new flooding cycles reach higher gas saturations, allowing more gas to be trapped. At high gas saturation, an increase in relative permeability after the first gas injection is predicted due to cooperative pore filling. In an oil-wet system the gas relative permeability is lower for gas displacing principally water than oil, since gas is no longer the most non-wetting phase in the presence of water.

The water relative permeability in water-wet media is lower when gas is present. This surprising hysteresis trend is supported by experiment (Oak, 1990). Gas injection forces trapped oil into smaller pores and throats. During water re-injection some of this oil reconnects, which increases the oil/water capillary pressure, meaning that water layers in the corners of the pore space are thinner and have a lower conductance, resulting in a lower water relative permeability. In oil-wet media, the water relative permeability remains very low until connected clusters of water-filled elements span the system, at which point the relative permeability rises rapidly.

The oil relative permeability in water-wet media increases rapidly when gas is injected into waterflood residual oil, since oil becomes reconnected due to double drainage. The residual oil saturation can be very low if oil remains connected in spreading layers. In oil-wet media, the oil relative permeability increases monotonically with oil saturation, since oil is the most wetting phase and always
occupies the smaller elements or resides in stable layers. The residual saturation is very low due to the connectivity of wetting layers.

In a water-wet medium the stability of oil layers and hence the remaining oil saturation during gas injection is controlled by the gas-oil contact angle, with layers less stable as the gas-oil contact angle increases.

We then showed how pore-scale network modelling could be used to understand the amount of hydrocarbon getting trapped during multiphase fluid flow in porous media. Preliminary results suggested that the relative permeabilities were, approximately, independent of displacement path when plotted as a function of flowing saturation. In order to estimate the flowing saturation, it is necessary to predict the amount of oil and gas that is trapped.

We showed some surprising trends in trapping behaviour with wettability; a weakly water-wet system showed more trapping of oil and gas than a water-wet medium due to the complex competition between three-phase displacement processes. The trend in trapped oil saturation with initial gas saturation is different for water-wet and oil-wet systems. It has been shown that there would be a decrease in the trapped oil saturation with an increase in the initial gas saturation for a water-wet system. However, we observed an opposite behaviour in an oil-wet media – the trapped oil saturation did increase with an increase in the initial gas saturation.

These surprising results indicate that the degree of trapping is very sensitive to saturation path and wettability and so it may be difficult, or impossible, to formulate a simple empirical model to predict hydrocarbon trapping in all circumstances.

6.2 Future Directions

There is still great amount of work can be done in order to improve the capabilities of three-phase network modelling. In Chapter 5, we showed the practical usefulness of network modelling by predicting the trapped hydrocarbon saturation as a function of initial gas saturation in the system. As mentioned before, this is of great interest due to the fact that geological storage of carbon dioxide (CO$_2$) is becoming increasingly important not only to enhance oil recovery but also for storage of CO$_2$ emitted from power stations and other large point sources (Jessen et al., 2005). A physically-based numerical model combined with a realistic network topology can be very helpful to
understand and study the degree of oil and gas trapping for different initial and injection conditions for systems with non-uniform wettability. The work presented here could be extended to a full range of wettability conditions and displacement paths and, possibly, an empirical equation for the degree of oil and gas trapping found that matches the network model predictions. Then, using the hypothesis that three-phase relative permeability is independent of saturation path when computed as a function of flowing saturation, the relative permeability could be parameterized as a function of wettability and flowing saturation. This then would lead to a predictive model for three-phase relative permeability in a form suitable for inclusion in field-scale numerical simulators. A similar approach could be applied for capillary pressure. However, note that the results to date show some subtle and surprising trends and it is likely that a simple closed-form expression may not be sufficient to give accurate predictions for the full range of possible conditions encountered in three-phase flow. In this case, network modelling, validated against available data, could be used to predict representative relative permeabilities and capillary pressures for cases of interest for a given field setting or dynamically coupled into a larger-scale flow simulator (Jackson and Blunt, 2000; Fenwick and Blunt, 1998).

In common with all other three-phase network models, we use a rather simple approach to compute the displacement capillary pressures: a semi-empirical two-phase expression, during both layer formation and collapse events. Layer stability during these displacements is assessed by using a simple geometrical layer collapse criterion (Hui and Blunt, 2000). Piri and Blunt (2004), van Dijke and Sorbie (2006) and van Dijke et al., (2006) suggest that using two-phase expressions in a three-phase flow context may lead to serious inconsistencies in the relation between pressures and pore occupancies for angular pore and throat elements. This may very well result in with incorrect estimations of the trapped hydrocarbon saturations. Our work tends to over-estimate the stability of oil layers and consequently is likely to under-estimate the residual oil saturation. It would certainly be useful to include thermodynamically consistent expressions for layer stability and displacement in our network model. Indeed this is a necessary first step before embarking on a more thorough examination of hydrocarbon trapping. However, this extension is not straightforward: at present the threshold displacement pressure is found as a function simply of the pressure difference between the displaced and displacing phases; using proper thermodynamic
criteria the threshold is a function of two pressure differences which means that the sorted lists for displacement have to be re-ordered after every invasion event, making the code considerably slower.

We have only studied flow in a single network representing Berea sandstone. We could also study the effect of different pore geometries by applying the model to different networks. At present we rely on a small number of networks generated using process-based techniques. In the near future we hope to be able to input representative networks from a wide variety of rock types obtained from a topological analysis of direct 3D micro-CT images of the pore space (Arns et al., 2005; Olafuyi et al., 2006) or generated via statistical techniques (Okabe and Blunt, 2005; Al-Kharusi and Blunt, 2006). Again such a study to determine the sensitivity of the results to pore structure is necessary before a three-phase relative permeability model can be proposed with confidence. Of particular interest are carbonate systems where there may be a wide range of pore size and coordination number.

For non-spreading systems with poor connectivity it is likely that single and double displacements are not sufficient to represent the full range of behaviour for WAG flooding. In such cases multiple displacement needs to be considered (Van Dijke et al., 2004a).

Once these extensions have been included into the model, other physical processes could be simulated, such as: solution gas drive, where gas evolves from solution in the pore space (Yortsos and Parlar, 1989; Bondino et al., 2003); miscible or near-miscible WAG with phase exchange between the oil and gas; gas condensates with liquid drop-out; and upscaling issues, where appropriate core-to-field-scale descriptors of three-phase flow are found. These are just a few examples of the many problems that can be addressed using pore scale network modelling.

Overall, pore-scale modelling that combines an accurate description of the pore space with a detailed analysis of pore-scale displacement physics is a useful tool for understanding multiphase flow in porous media. From a practical perspective it can be used to make predictions for situations that are difficult to study experimentally. The work in this thesis shows that even for rather complex displacements – WAG flooding – this approach is able to make accurate predictions while revealing the subtlety of the influence of pore-scale displacement on macroscopic behaviour. In contrast the use of
simple expressions or rules for determining three-phase properties is often inaccurate and fails to reveal the richness of the underlying displacement behaviour.
Bibliography


December 2006

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Appendix

DESCRIPTION OF INPUT DATA FILE

The 3-Phase pore network model is written in Fortran 90 and uses a number of data files. In order to be able to run the code, one needs to input a set of network data files (link1.dat, link2.dat, node1.dat, and node2.dat) in a specified format. In addition to these files, an input data file, called ‘data.dat’ should also be included. Below we are giving the definitions for the keywords used in the input data file.

Required keywords

1. **READ_BACK_UP**

Depending on the displacement sequence, running the three-phase code may be computationally costly. In order to decrease this cost, we introduce a so-called back-up (back_up.dat) data file. We can store all the necessary information from the previous floods in this data file. Each flood is called a process. Using **READ_BACK_UP** keyword we can either begin with a new process (different phase invasion) or continue with the previous one. There are two strings associated with this keyword. The first one is the answer for the question “Would you like to use a back_up file?” If the answer is yes (“Y”), this means we would like to use a previously saved back_up file. The second one is the answer for “Would you like to continue with the last process?” If the answer is yes (“Y”), then this means we want to continue with the last process. This would actually be useful, if we apply saturation path tracking algorithm and enables us to continue from the exact same saturation point we stopped before. Otherwise, if we put no (“N”), then this means, we would like to start a new process and inject a different fluid phase.

```
READ_BACK_UP
Y N
```

2. **WRITE_BACK_UP**

Due to the time limitations, during our simulations we may want to store the information from the previous floods. This enables us to continue our simulation at the same saturation point where we have stopped flooding in a previous study. There are two strings associated with this keyword. First one answers if we would like to generate a back up file (back_up.dat). If we input yes (“Y”), then it means we would like to generate a data file storing the information from the current simulation. Then we would also need to provide information on how frequently this file should be updated. We need to assign a number which is basically number of displacements before the so-called “back_up.dat” data file is updated.

```
WRITE_BACK_UP
Y 30
```
3. NETWORK_STATISTICS

3-Phase network model was developed in a way that flow simulation can be carried out in different rock networks. NETWORK_STATISTICS keyword is used to display the important features of the rock network used during the simulation. If we choose “Y” as the first string, this means yes we would like to generate a data file (results_network_statistics.dat) which displays all the necessary statistical information for the particular network used during the simulation. The other two numbers associated with this keyword are some dummy initial values for pore/throat radius and shape factor (G) which will then be used while computing the statistical distributions for these parameters. One should note that these values should be in the range of minimum and maximum values of radius and shape factor respectively.

<table>
<thead>
<tr>
<th>NETWORK_STATISTICS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Y</td>
</tr>
<tr>
<td>5 0.0079577</td>
</tr>
</tbody>
</table>

4. CLAY_VOLUME

Every pore/throat element of Berea sandstone network is assigned a clay volume. This represents an immobile volume that remains water saturated throughout all displacements. It can be adjusted to match the observed connate water saturation (Bakke and Øren, 1997; Øren and Bakke, 2002). Therefore during our simulations we need to assign a value which will give the fraction of the clay volume in our network.

<table>
<thead>
<tr>
<th>CLAY_VOLUME</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
</tr>
</tbody>
</table>

5. VISCOSITY

We should assign viscosity values for all three phases during our simulations. The values are water, oil and gas viscosity values ($c_p$) respectively.

<table>
<thead>
<tr>
<th>VISCOSITY</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 0.75 0.2</td>
</tr>
</tbody>
</table>

6. DENSITY

We should assign densities for all three phases during our simulations. The values are water, oil and gas density values ($kg.m^{-3}$) respectively.

<table>
<thead>
<tr>
<th>DENSITY</th>
</tr>
</thead>
<tbody>
<tr>
<td>1018 600 3.57e-3</td>
</tr>
</tbody>
</table>
7. **INTERFACIAL_TENSION**

We should assign interfacial tensions between the phases. The values are oil-water, gas-water and gas-oil interfacial tensions \((mN.m^{-1})\) respectively.

```
INTERFACIAL_TENSION
48 67 19
```

8. **REL_PERM**

This keyword is used to indicate whether we would like to calculate the relative permeabilities or not. And if yes (“Y”), then we will have to specify a region in the network for the relative permeability calculations. In order to avoid boundary effects we usually use only a fraction of the network away from the inlet and outlet. We are able to choose any region by inputting dimensionless locations representing inlet and outlet.

```
REL_PERM
Y
0.05 0.95
```

9. **ABS_PERM**

Similarly, this keyword is used to indicate whether we want to calculate the absolute permeability of the network or not. Again we are able to choose a certain region for our calculations.

```
ABS_PERM
Y
0.05 0.95
```

10. **SEED**

This is the seed to the random number generator, which should be a large positive integer.

```
SEED
12357
```

11. **MAX_NO_ITERATIONS**

While performing our simulations we compute a number of parameters using iterative processes. This keyword specifies the maximum number of iterations allowed during our calculations.

```
MAX_NO_ITERATIONS
300000
```
12. CONVERGENCE

This is the convergence criterion we have while solving an implicit equation. Note that for smaller values, more iterations will be required.

```
CONVERGENCE
5.0e-6
```

13. PORE_BODY_FILLING_MODEL

During spontaneous invasion, the capillary entry pressure for pore bodies will depend on the number of adjacent throats filled with the non-wetting phase. Several different models have been proposed in the literature. We can choose any one of the four models proposed before (blunt_1, blunt_2, oeren_1 and oeren_2). The details of these models and governing equations can be found at Blunt (1997; 1998), and Øren et al. (1998). The numbers next to the model are predefined parameters used for calculating the capillary pressure (Piri and Blunt, 2005a).

```
PORE_BODY_FILLING_MODEL
blunt_2   0.0   30000   30000   30000   30000
```

14. SATURATION_PATH_TRACKING

It is a well known fact that three-phase relative permeabilities have strong dependence on the system’s saturation history. Piri and Blunt (2005a) developed an algorithm, which is called saturation path tracking, enabling one to point by point track the experimentally observed saturation path. This algorithm is very useful, while comparing the results with experimental counterparts. In order to activate this algorithm, one needs to choose yes “Y” which means yes I would like to use the algorithm. However, if one chooses “N”, then it is necessary to specify the process(es) to simulate. For the latter, it is required to input the number of fluid injection processes and name of the injected phase. One can decide to inject a phase until either all available displacements are performed (shown by “complete”) or up to a certain saturation region (shown by “phase_saturation”). The first number is the proposed saturation point, second one is the error margin and the last one is the number of displacements after which relative permeabilities would be calculated.

```
SATURATION_PATH_TRACKING
N
3
  oil complete 0.0 0.0 500
  gas gas_saturation 0.63 0.03 500
  water complete 0.0 0.0 500
```
15. **DOUBLE_DISPLACEMENT**

This keyword is used to activate (“Y”) or deactivate (“N”) the available double displacement mechanisms during our simulations.

```
DOUBLE_DISPLACEMENT
Y
```

16. **NEGATIVE_AREA_CORRECTION**

We have a subroutine (area_check) which is used to check whether we calculate any negative area/volume values or not. By activating (“Y”) the keyword NEGATIVE_AREA_CORRECTION, errors associated with the negative area calculations are fixed.

```
NEGATIVE_AREA_CORRECTION
Y
```

17. **IMEDIATE_INTERFACE_UPDATE**

In our model, the displacements are carried out by increasing the invading phase pressure. It is possible to update the fluid interfaces after each displacement as the invading phase pressure increases. However, note that this might be computationally very expensive.

```
IMEDIATE_INTERFACE_UPDATE
N
```

18. **REL_PERM_TEST**

This keyword is used to conduct a test on the computed relative permeabilities. One could activate or deactivate the test by choosing yes (“Y”) or no (“N”).

```
REL_PERM_TEST
Y
```

19. **PRESSURE_DIST**

We can calculate the pore pressure distributions for each phase during our simulations. The 3 letters represent the water, oil and gas pressure distributions respectively. By choosing yes (“Y”), we can calculate the pressure distributions for each phase. A new data file will be created for each phase (called “phase_P_dist.dat”), if the keyword is activated.

```
PRESSURE_DIST
N N N
```
20. INITIAL_PHASES
This keyword is used to present the number and the names of the phases initially in the system. However, note that it is currently possible to accommodate only one phase initially in the system (therefore number of phases should always be 1), which could be water, oil or gas.

```
INITIAL_PHASES
  1 water
```

21. INITIAL_CONFIGS
This keyword is used to present the initial phase configurations in each pore/throat element. If it is set as “fixed” then it means all the configurations are fixed and same all over the network. However, if it is set as “not_fixed”, then one needs to assign corner configurations for each pore/throat element.

```
INITIAL_CONFIGS
  fixed
  1
```

22. INJECTION_FACES
In our model, we assume the inlet and outlet are connected to each other. A cluster of a phase connected to either inlet or outlet will be considered as continuous and will have exactly same phase pressure with another cluster of the same phase connected to either inlet or outlet. This makes it possible to perform injection from either inlet or outlet or even both. Using the keyword INJECTION_FACES, we are able to decide from which face we would like to perform the injection. We can choose “inlet”, “outlet” or “both”.

```
INJECTION_FACES
  inlet
```

23. ZERO_PC_REPLACEMENT
During our calculations, in some certain cases (for example contact angles close to 90 degrees) we may obtain unrealistic capillary pressure values. Therefore, we define a tolerance value and if the calculated capillary pressure is less than this value, we would replace it with a replacement value. The keyword ZERO_PC_REPLACEMENT is used to specify a tolerance and a replacement capillary pressure values respectively.

```
ZERO_PC_REPLACEMENT
  0.01 1
```
24. **CA_90_AMEND**

This keyword is used to change the contact angles that are too close to 90 degrees. This is done since 90 degrees contact angles may lead to infinite radius when capillary pressure approaches to zero. In order to activate this feature, we need to choose “Y” which stands for yes, and we also need to define a tolerance value which will either be added or subtracted from the old contact angle value (if old contact angle is less than 90 degrees, then the tolerance value will be subtracted otherwise it will be added) in order to obtain the new contact angle.

```
CA_90_AMEND
Y
0.5
```

25. **PORE_THROAT_CA**

In our model, it is possible to assign contact angles to pore and throat elements either separately or together. This can be done by inputting either “separate” or “together” in the keyword PORE_THROAT_CA.

```
PORE_THROAT_CA
together
```

26. **PDOWCA**

This keyword is used to assign oil-water contact angles for each pore/throat element during primary oil drainage. First, we need to decide whether we would like to use a distribution of contact angles or not. If we put yes (“Y”) as the first string, this means we would like to assign a set of different contact angles for pore and throat elements. However, the model is currently able to reside one initial phase only. This means system is initially saturated with only one phase and this phase is assumed to be strongly wet. Therefore during primary drainage, we do not use a distribution of contact angles; instead they are all assigned as zero. Note also that if we choose to assign contact angles for pores and throats separately, we would need to use two keywords instead of the keyword PDOWCA, namely THROATS_PDOWCA and PORES_PDOWCA.

```
PDOWCA
N N N
0.0
```

27. **ADOWCA**

This keyword is used to assign advancing oil-water contact angles. If we would like to use a distribution of contact angles we need to input yes (“Y”) as the first string. Then, if we also choose yes (“Y”) as the second string, we will need to assign contact angles for each pore/throat element independently.
However, if we choose no (“N”) as the second string, then we will have to decide whether we prefer a uniform distribution (“uniform”) or not (“weibull”). In both cases, we will need to input a minimum and a maximum values for contact angles. Note that, if we choose weibull distribution, we will also need to input two exponents in addition to the minimum and maximum values.

<table>
<thead>
<tr>
<th>ADOWCA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Y</td>
</tr>
<tr>
<td>N</td>
</tr>
<tr>
<td>uniform</td>
</tr>
<tr>
<td>60</td>
</tr>
<tr>
<td>80</td>
</tr>
</tbody>
</table>

28. **RCOWA**

This keyword is used to assign receding oil-water contact angles. We currently assume a 20 degrees difference between advancing and receding contact angles by default. However, this assumption can be (de)activated at the subroutine use_Bartell_Osterhof_Blunt. And using the keyword RCOWA, one can input receding oil-water contact angles in a similar way discussed in the previous point for keyword ADCOWA. Note that, both advancing and receding gas-oil contact angle values are also assigned at subroutine use_Bartell_Osterhof_Blunt. Using the predefined two contact angles (oil-water and gas-oil) and three interfacial tensions, we are able to calculate the third contact angle (gas-water) with Bartell-Osterhof constraint (1927).

<table>
<thead>
<tr>
<th>RCOWCA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Y</td>
</tr>
<tr>
<td>Y</td>
</tr>
<tr>
<td>N</td>
</tr>
<tr>
<td>uniform</td>
</tr>
<tr>
<td>40</td>
</tr>
<tr>
<td>60</td>
</tr>
</tbody>
</table>

29. **END_DATA**

This is the last keyword, indicating input data file is complete and all necessary information was successfully implemented in to the model. Note that no more information can be inputted once this keyword is implemented.
Abstract
We demonstrate a pore-to-reservoir simulation methodology and apply it to single-phase flow. Traditional numerical methods are based on the discretization of partial differential equations with known spatially-dependent coefficients, such as porosity and permeability. However, in porous media flow we do not know a priori what the governing transport equations are – for instance, single-phase transport cannot be accurately described by an advection-dispersion equation – nor do we know the reservoir properties everywhere.

We propose a different approach that does not pre-suppose the functional form of the upscaled transport equations and which automatically accounts for uncertainty in the reservoir description. Single-phase transport is modeled as a continuous time random walk. Particles make a series of transitions between nodes with a probability \( \psi(t)\,dt \) that a particle will first arrive at a node from a nearest neighbor in a time \( t \) to \( t+dt \). A top-down multiscale approach is used to find the flow field. At the micron scale, \( \psi(t) \) for particle transitions from pore to pore are found from modeling advection and molecular diffusion in a geologically representative network model. This \( \psi(t) \) is used to compute transport on the mm to cm scale. At larger scales, we represent the reservoir as a network of nodes connected by links. For each node-to-node transition, we compute an upscaled \( \psi(t) \) from a simulation of transport at the smaller scale. We account for small-scale uncertainty by interpreting \( \psi(t) \) probabilistically and running simulations for different possible realizations of the reservoir model. To make the number of computations manageable, \( \psi(t) \) is parameterized in terms of sub-scale heterogeneity and Peclet number, meaning that only a few representative simulations are required.
We demonstrate the methodology by finding $\psi(t)$ for pore-scale flow and using it in a million-cell reservoir model. We show that the macroscopic behavior can be very different from that predicted by assuming that the advection-dispersion equation operates at the small scale. Small-scale structure does impact macroscopic transport; increasing the pore-level heterogeneity delays breakthrough and leads to longer late-time tails of the production since the solute spends more time in slow-flowing regions of the domain. We discuss extensions to multiphase flow and the development of a novel network-based probabilistic reservoir simulation approach.

**Introduction**

The conceptual framework for reservoir simulation is borrowed from traditional fluid dynamics applications where known differential equations are solved with known – albeit complicated – boundary conditions. Current research in this field – on improved discretization of the governing conservation equations, the use of unstructured grids and parallelization – reinforces the notion that the underlying principles that we use are correct – see, for instance\(^1\). However, porous media flow presents a completely distinct set of simulation challenges that we not address appropriately. First, while we use empirical approaches to describe transport and multiphase flow at the experimental, core scale, we do not know the correct form of the constitutive relationships between pressure gradient, flux and saturation on the much larger scale at which we solve the equations. The subtle interplay of heterogeneity and the length-scale-dependent balance of capillary, diffusive, gravity and viscous forces means that our conventional dispersion-and-Darcy models of flow and transport at the field scale have a somewhat dubious foundation. Second, even if we did know the governing partial differential equations, we would not know, with any certainty, the values of the coefficients in these equations. At present, we have no automatic way to incorporate our uncertainty in the description of the reservoir model into uncertainty in prediction of transport and oil recovery.

Is there a different way of looking at flow in porous media that overcomes these problems; that does not assume \textit{a priori} the form of the transport equations and which can accommodate uncertainty? The approach we propose is conceptually simple and easy to implement. In this paper we will apply it to single-phase flow. We first discuss the traditional approach to modeling transport and illustrate its limitations.
We then introduce continuous time random walks that we use to simulate particle movement. We perform a pore-to-core analysis of dispersion to put the methodology on a firm foundation. We then show how to upscale transport to the field scale and demonstrate that variability at every scale affects the macroscopic behavior even when the field-scale reservoir description is highly heterogeneous. Last we discuss possible extensions to multiphase flow.

**Advection-dispersion equation**

Traditionally the macroscopic transport of tracer had been described by the advection-dispersion equation (ADE)\(^2\):

\[
\frac{\partial c}{\partial t} + v \cdot \nabla c = \nabla \cdot D \nabla c
\]

where \(c\) is the contaminant concentration, \(v\) is the flow speed and \(D\) is the dispersion coefficient (which, in general, is a tensor). We have assumed incompressible flow with a constant porosity. In contaminant hydrology it is often presumed that the transport can be modeled by flow in a homogenous domain with some effective \(D\) assigned to accommodate the dispersion of contaminant due to small-scale heterogeneity and molecular diffusion.

Solutions to the ADE in statistically homogeneous systems produce a plume profile that is Gaussian in nature with an average displacement that scales linearly with time, \(l(t)\sim t\), and a standard deviation about the mean that scales with the square root of time, \(\sigma(t)\sim t^{1/2}\). However, in most cases, the macroscopic behavior of the transport cannot be described by a solution to the ADE, Eq. (1), without explicitly accounting for small-scale heterogeneity. This so-called non-Fickian or anomalous contaminant transport is observed from the laboratory to the field scales\(^5,6\) and is characterized by a slowly moving maximum concentration, a rapidly advancing leading front and a long tail of late arriving fluid\(^7,8\). This demonstrates that we do not know the appropriate macroscopic description for the transport and hence a numerical simulation strategy based around discretization of Eq. (1) is flawed.

**Continuous time random walks**

We will view transport as a continuous time random walk (CTRW): particles move between a series of discrete nodes or sites with a probability \(\psi(t; i, j)dt\) that a particle
that first arrives at site $i$ will move to site $j$ in a time $t$ to $t+dt$. CTRWs were first introduced in the 1970s to describe electron transport in semi-conductors; more recently they have found a particularly rich application in modeling contaminant transport. Berkowitz et al. have written an excellent, recent review.\textsuperscript{9}

CTRW does not make any assumptions about the governing transport equations; instead physical modeling of the process of interest is used to derive $\psi$ from which the resultant macroscopic behavior can be found analytically or numerically. Anomalous transport can be elegantly described in terms of CTRW. If $\psi(t)dt$ is the probability that a particle that has just arrived at a site will move to a nearest neighbor in a time $t$ to $t+dt$, then, for many systems, at late time there is a power-law dependence of the probability: $\psi(t)\sim t^{-1-\beta}$ with some exponent $\beta \leq 2$. This leads to an outlet concentration that, at late time, scales as $C(t)\sim t^{-1-\beta}$. For $1 \geq \beta \geq 0$ we find that both the average plume displacement its standard deviation scales as $l(t)\sim \sigma(t)\sim t^{\beta}$, while for $2 \geq \beta \geq 1$ the average displacement scales normally: $l(t)\sim t$, but the spread is still anomalous: $\sigma(t)\sim t^{(3-\beta)/2}$. For $\beta > 2$ the system displays Gaussian behavior.\textsuperscript{9}

Generally CTRW has been applied to find the ensemble average behavior of a plume in a macroscopically homogenous domain.\textsuperscript{9,10} However, in most reservoirs the permeability distribution is described on a scale of a few meters. What is needed is a rapid simulation technique to capture the behavior for different, explicit reservoir models while capturing the effects of uncertainty in the reservoir description at smaller – below a meter – scales. CTRW has been applied to heterogeneous media, but for relatively coarsely-gridded two-dimensional systems where the solution involves the numerical inversion of a multi-dimensional Laplace transform.\textsuperscript{11} Here we propose a simpler approach: we simply simulate particle transport from site to site with some known $\psi(t;i,j)$: in CTRW this is equivalent to solving the master equation numerically.

We employ a multiscale methodology where, at each stage, transport is considered conceptually as a series of transitions from node to node – see Fig. 1. All the physics of the process is contained in the transit time distribution $\psi(t)$. At the very smallest scales – the pore and sub-pore level – we do know how to describe transport: it is Stokes flow in a spatially varying flow field with molecular diffusion. Hence we
start at the pore scale and then describe how to upscale these results to determine transport in the field.

Fig. 1 – A schematic of the pore-to-core-to-field simulation technique proposed. At the smallest scales, advective and diffusive transport is simulated at the sub-pore level through a network representing the porous medium of interest. We consider transport as a series of transitions between discrete nodes via links with a known transit time distribution $\psi(t)$. At the small scale, this is simply transport from one pore to another via throats described by a $\psi$ that is averaged over all possible statistical realizations of the structure. At the field scale we again model transport as a series of transitions between conceptual nodes. The distribution of transition times is found from a series of core-scale simulations.
Pore-to-core simulation

Bijeljic et al.\textsuperscript{17} developed a pore-scale network model of dispersion. They represented a porous medium as a two-dimensional diamond lattice of throats connecting volumeless pores (nodes or sites). Each throat had a square cross-section and the distribution of throat radius matched that inferred for Berea sandstone. They then simulated transport as a series of advective and diffusive steps with physically-based mixing rules at pores. They accurately predicted the experimentally-measured dependence of longitudinal dispersion coefficient, $D_L$, on Peclet number, the ratio of advective to diffusive forces, $Pe=vl/D_m$, where $v$ is the average flow speed in the porous medium, $l$ is the throat length and $D_m$ is the molecular diffusion coefficient.

For moderate Peclet numbers $400>Pe>10$ there is an approximate power-law dependence of $D_L$: $D_L \propto Pe^\delta$ with $\delta \approx 1.2$. As we discuss later, Bijeljic and Blunt\textsuperscript{18} provided a physical explanation for this behavior in terms of the distribution $\psi$ of pore-to-pore transit times.

We can replace a direct simulation approach that involves sub-pore-scale transport with one where particles simply hop from pore to pore with a known transit time distribution, $\psi(t;i,j)$. There are two ways in which this can be done. The first is to have the same network and measure the transit time distribution for each pore-to-pore transition. In the large $Pe$ limit, $\psi$ will tend to delta function around the advective transit time $l/v$. The flow speed $v$, however, will be different for each throat, reflecting the heterogeneity of the network.

The second way to simulate transport is to consider $\psi$ an \textit{ensemble averaged} transit time distribution that accounts for all possible statistically equivalent realizations of the pore-scale structure. Since there are no systematic long-range correlations, the ensemble average network is homogeneous. However, now $\psi$ must accommodate a much wider range of transit times, even in the advective-dominated limit, since it accounts for the variation in flow speed between elements in each possible realization of the structure. This ensemble average $\psi$ is found by averaging the transit times over every pore-to-pore transition in the heterogeneous network. Bijeljic and Blunt\textsuperscript{18} found that $\psi$ was very well fit by a truncated power-law form over six orders of magnitude in time and $Pe$: 
where $A$ is a normalization constant, $t_1$ is an average advective transit time = $l/v$ where $l$ is the average pore-to-pore length and $v$ is the average velocity in a throat, and $t_2$ is a typical diffusive transit time = $l^2/2D_m$. This empirical form of the transit time distribution has been analyzed before in the context of CTRW and makes physical sense: we do not allow transit times longer than the time it would take a particle to diffuse through a stagnant throat, while for intermediate times $t_2>t>t_1$ we see an approximately power-law distribution of transit times that reflects the heterogeneity of the network. $\beta$ is a parameter that encapsulates this heterogeneity: more heterogeneous systems will have smaller values of $\beta$, representing a broader distribution of transit times. The best-fit value of $\beta$ for our simulations is 1.8.

We perform three simulations of pore-to-core transport. While the results of Bijeljic et al. were generated for a two-dimensional network, we are interested in three-dimensional systems. In the first simulation we use a topologically disordered network representing a sample of Berea sandstone 3 mm across with 12,349 pores and 26,146 throats. From the known hydraulic conductance of each element (pore and throat) we can compute the flow rate in the network for a given pressure drop between inlet and outlet – this is identical to what is done in conventional network modeling. We then launch 10,000 particles at the inlet face, weighted by the flux in each inlet throat and track their progress as they move in a series of discrete hops between pores. We assume that between pores the transport is represented by a one-dimensional ADE, Eq. (1), with the known velocity in the throat and where the dispersion coefficient is the molecular diffusion coefficient, $D_m = 10^{-9}$ m$^2$s$^{-1}$.

For one-dimensional solutions of the ADE we can find $\psi$ semi-analytically. We find the cumulative transit time distribution:

$$Y(t) = \int_0^t \psi(t) dt$$

where, by definition, $Y(t=\infty)=1$. For each transition, we find a random number $z$ between 0 and 1. We then invert $Y$ to find the transit time $t_z$ such that $Y(t_z)=z$. The particle is then moved to the next pore and the time counter associated with each particle is incremented by $t_z$. 

\[
\psi(t) = A \frac{e^{-t/t_1}}{(1+t/t_1)^{\beta}}
\]
When a particle reaches a pore there may be several nearest neighbor pores to which it can move next. We can also find, analytically, the probability of transitions to each neighboring pore based on the Peclet number in each connecting throat. More details on this simulation methodology are given in 19.

We know that even in a single throat, the use of the ADE is a poor representation of the transport, since, in reality, there is a variation in velocity across the element 17. However, this does give the correct advective and diffusive limits, and we will show later, gives good macroscopic predictions of transport, since this is dominated by the variation of velocity between throats, not the variation within a throat.

During the simulation we compute the mean particle location:

$$l(t) = \bar{x}(t) = \frac{1}{N_p} \sum_{k=1}^{N_p} x_k(t)$$  \hspace{1cm} (4)

where $x_k$ is the displacement of particle $k$ from where it was launched and $N_p$ is the number of particles. The variance in location is given by:

$$\sigma^2(t) = \frac{1}{N_p} \sum_{k=1}^{N_p} (x_k(t) - \bar{x}(t))^2$$  \hspace{1cm} (5)

Then we define the longitudinal dispersion coefficient as:

$$D_L = \frac{1}{2} \frac{d\sigma^2(t)}{dt}$$  \hspace{1cm} (6)

In Fig. 2 we plot the late-time dispersion coefficient, Eq. (6), as a function of Peclet number, where $Pe$ is varied by changing the pressure drop across the network. The results are compared to experimental results in the literature and the network studies of Bijleijic et al. 17,18 It is evident that both modeling approaches predict the experimental results accurately. This comparison demonstrates that it is possible to represent transport as a series of discrete hops between nodes (pores). In this case, even though the transit time distribution between pores is not accurate, we still obtain good results, since we do model the heterogeneity of the porous medium correctly – it is the consequent distribution of velocity in different throats that dominates the behavior.

For the upscaling presented later it is convenient, in this first implementation of the method, to use cubic networks. Also shown in Fig. 2 are results using a 100×100×100 cubic network but with the same Berea-derived distribution of throat radius. The
throat length is 100 µm, and so this represents a sample 1 cm across. Note that the results are similar to those obtained for the topologically disordered network, except at very large $Pe$, indicating that for single-phase transport a regular network can be used to predict the behavior accurately, as demonstrated by other authors\textsuperscript{17, 20, 21}

Our third simulation also uses a cubic network of the same size, but now we represent an ensemble averaged system that is homogeneous. Here we do not need to compute the flow field – we simply use Eq. (2) to find the transit time distribution for each pore-to-pore hop. Again this predicts the experimental data accurately. It is this approach that we will use to upscale transport later in the paper.

Note the approximate power-law behavior of the dispersion coefficient at intermediate values of $Pe$: $D_L \sim Pe^\delta$ with $\delta \approx 1.2$. It is possible to show that this exponent is related to $\beta$ by $\delta = 3 - \beta$ – the macroscopic dispersion is a direct consequence of the power-law distribution of throat velocities.\textsuperscript{18}

**Core-to-field-scale simulation**

It is not practical to simulate field-scale transport using a pore-scale network model. We propose an upscaling strategy that embraces the CTRW approach and where, at any scale, we represent transport as a series of transitions between discrete nodes. We consider that we have a field-scale reservoir description and we want to honor this heterogeneity explicitly. However, we will compute transport for all possible realizations of the reservoir below the grid-block scale. The approach we use borrows ideas from multiscale modeling.\textsuperscript{12-16}

First, we compute the flow field at the field-scale with known boundary conditions (wells) and initial distribution of fluids – for single-phase flow we assume that this is independent of the solute concentration. We then extract pairs of grid blocks, as represented in Fig. 3. We know the total flux across each face, $Q$. We then perform a sub-block simulation. Within each block, we represent the medium as a network of elements – at this scale this will be an ensemble-averaged, homogeneous, cubic pore-level model, described in the previous section. We find the flow rate in each throat by solving for the flow field with the known, Neumann, boundary conditions.
Fig. 2 – The longitudinal dispersion coefficient as a function of Peclet number, $Pe$. The points are experimental results on sand packs and sandstones in the literature collated by Bijeljic et al. The lines are predictions using different pore-scale modeling approaches. All the models assume that transport occurs between pores connected by throats. The squares show the two-dimensional network model results of Bijeljic and Blunt where advection and diffusion are modeled within throats. The asterisks represent a three-dimensional simulation on a network representing the topology of Berea sandstone, but where pore-to-pore transitions are computed semi-analytically assuming a one-dimensional advection-diffusion equation in each throat. The crosses indicate an equivalent simulation in a cubic lattice, but again with a throat size distribution representing Berea. The last – dots and line – shows a simulation on a homogeneous cubic lattice using an ensemble averaged transit time distribution, Eq. (2). In all cases the models give accurate predictions of the data.

We then launch particles at the faces of the left-hand block in proportion to the flux across that face. We move particles from pore-to-pore as before, using Eq. (2) for the transit time distribution. The difference here is that despite the homogeneity of the network, the velocity in each element is different because of the different face fluxes, and this is accounted for in Eq. (2). When a particle moves to the right-hand block we start a clock for that particle. When it exits this block, we stop the clock. The time is the transit time for the particle to cross the block. We compute the distribution of transit times for all the particles and for different pairs of blocks.

For this example, each grid block was represented by a 50×50×50 homogeneous cubic network, 5 mm across. We launched 10,000 particles into the left-hand block.

At the grid block scale, transport is advection-dominated in our examples. As a consequence, particles almost always moved macroscopically in the direction of the imposed flux. We also found that regardless of launch or exit face, or which pair of blocks we considered, the transit time distribution was exponential with the following functional form:

$$\psi_s(t) = \frac{\lambda Q}{V} e^{-\lambda Q/v}$$  \hspace{1cm} (7)
where $Q$ is the flux across the face between the two blocks of interest (with units of volume per unit time), $V$ is the block volume and $\lambda$ is a dimensionless coefficient whose value we found to be approximately 5. The subscript $g$ on $\psi$ indicates that this is the transit time distribution at the core scale, to distinguish from the pore-level $\psi$, Eq. (2).

This result is not surprising – when the average transport is advective-dominated there will be a typical transit time with some variation around the average that is well captured by an exponential. The typical transit time through a single throat is $l/v$ where $v$ is an average flow speed. $v \approx Q/\phi A$ where $A$ is the face area and $\phi$ is the porosity. If a particle traverses $n$ pores across the block, then the transit time is $nl/v = n\phi A/Q$. Now if we take $nl \approx L$, the block length in the direction of $Q$ and $AL=V$, we find a typical transit time of order $\phi V/Q$ and a coefficient $\lambda$ of order 1, which is what we find.

We demonstrate this relationship, Eq. (7), in Fig. 4 where the exponent in a best-fit to $\psi_g$ in Eq. (7) is plotted against a macroscopic Peclet number $= Q/LD_m$ which will, typically, always be much greater than 1.

In this case we did not explicitly take out pairs of blocks from the field scale model – instead we simply studied pairs of blocks in isolation with different fluxes across the faces. The reason for this is that we could find an empirical relation for the transit time distribution without having to perform a pore-scale simulation for each macroscopic block.
Fig. 3 – The upscaling methodology. From a larger-scale simulation the flow field is computed and so the fluxes $Q$ across each block face are known. Pairs of grid blocks are extracted from the model. Then a simulation is performed within these blocks. In this example, the sub-grid scale is a pore-level network model. As an ensemble average, the sub-grid is homogeneous. The flow rate in each element is computed using the block face, Neumann, boundary conditions; while the network is homogeneous, there is a distribution of velocity between throats because of the different fluxes at the block faces. Transport is modeled, as before, by a series of pore-to-pore transitions using Eq. (2) with the known average velocity in each element. Particles are launched along the face of the left-hand block. When a particle first enters the neighboring, right-hand block we record the time taken before the particle first exits that block. We then find this transit time distribution for all the particles, and for different pairs of blocks. At the larger scale this transit time distribution is used to represent, conceptually, a hop between two nodes indicating the centers of the grid blocks.
Field-scale results

For our reservoir description we chose the SPE10 model based on a North Sea oil reservoir. The model contains regions of high permeability, meandering sand channels surrounded by shaley low permeability regions with permeability varying by more than four orders of magnitude\(^2\). We used a Cartesian grid containing 1,122,000 blocks with \(60 \times 220 \times 85\) blocks. The total size of the model is \(366 \times 670 \times 52\) m. We chose two different boundary conditions. In the first we completed an injector well and a producer well at opposite corners of the model. We set the control on the injector to a flux of \(800\) m\(^3\)/day and the producer to a bottomhole pressure of \(27\times 10^3\) kPa. In the second, we injected across one face of the model and produced from the opposite face with no flow across the other faces. With these boundary conditions we first solved for the flow field and found the fluxes \(Q\) at each block face.

![Graph](image)

**Fig. 4** – Tests of the empirical core-scale transit-time distribution, Eq. (7). The exponent \(\alpha = LQ/V\) in the exponential relation is plotted against the macroscopic Peclet number, \(Pe_m = Q/LD_m\). The linear relation demonstrates that a simple transit time distribution can be used for larger-scale simulation. The upper line through the crosses is the base case for sub-scale transport in a network representing Berea sandstone (\(\beta = 1.8\) in Eq. (2)). We find \(\alpha = 2\times 10^{-4} Pe_m s^{-1}\). Since we perform the simulations for blocks 50 pores across, \(L = 5\) mm and \(V = 1.25 \times 10^{-7}\) m\(^3\), \(D_m = 10^{-9}\) m\(^2\) s\(^{-1}\) and so the dimensionless constant \(\lambda = 5.0\). The middle line is a parameterization of a more heterogeneous network with \(\beta = 1.1\) and \(\lambda = 1.8\). The lowest line is for a highly heterogeneous sub-grid system with \(\beta = 0.5\). In this last case the transit time exponent varies non-linearly with Peclet number, Eq. (8).

For transport, we represent the field scale as a cubic network of links (equivalent to throats) joining neighboring nodes (pores). The links join centers of adjoining blocks and the face flux \(Q\) is associated with the link, as shown in Fig. 3. We then launched 10,000 particles along the injector by a flux-weighted scheme and monitored the time taken for each to reach the producer. In the second simulation we injected particles along one face of the model and produced from the opposite face with no flow on the
other faces. We compute transport as before, as a series of transitions between nodes using Eq. (7) for the transit time distribution.

While conceptually transport is node-to-node, the upscaling methodology does account for the average behavior of particles traversing the blocks through all possible paths. Furthermore, while the transit time is counted for transport across a block and the macroscopic simulation is, conceptually, from block center to block center, the methodology does correctly track typical transit times, since we consider movement block-to-block across specified faces.

It is remarkable to note how simple the macroscopic transit time distribution is. In theory, an ensemble-averaged macroscopic transport algorithm needs to consider a convolution integral in time that accounts for the probability of particles arriving after sampling different paths. Of course, this subtlety is blithely ignored in all petroleum upscaling applications – fortunately without significant error for single-phase flow at least.

**Fig. 5** shows the macroscopic mean particle location and standard deviation at early time for the two different boundary conditions. The mean $l(t)$ scales linearly with time, while the standard deviation $\sigma(t)$ of the particle location scales as a power-law, indicative of anomalous transport with an exponent $\beta_m \approx 1.7$. The subscript $m$ is to indicate that this macroscopic exponent can, and indeed is, different for that used to model pore-scale transport. While the boundary conditions alter the time-scale of the displacement, the scaling behavior is broadly similar for both well and face-to-face transport.
Fig. 5 – The early-time mean particle location \( \langle l(t) \rangle \) and standard deviation \( \sigma(t) \) of the particle location for macroscopic transport with two different boundary conditions. The upper curves are for well boundary conditions while the lower curves are for face-to-face transport. The mean and standard deviation scale as linearly and as a power-law with time respectively. The solid lines are best-fits indicating linear scaling for \( \langle l(t) \rangle \) and an exponent \((3-\beta_m)/2\) of approximately 0.66±0.02 and 0.64±0.04 for \( \sigma(t) \), indicative of anomalous transport with \( \beta_m = 1.68\pm0.04 \) and \( 1.72\pm0.08 \) for face-to-face and well boundary conditions respectively.

Fig. 6 shows the corresponding concentration at the producer where we find \( C(t) \sim t^{-\langle 1/\beta_m \rangle} \) but this time the apparent exponent is \( \beta_m = 1.2\pm0.1 \). The inconsistency with the exponent from the early-time behavior indicates long-range spatial correlation in the transport; the simple characterization with a single exponent assumes statistical homogeneity in the system, which is not appropriate for this highly structured reservoir description.\(^{23}\)

The macroscopic boundary conditions do not affect the late-time behavior of the plume and so the power-law scaling is not due to near-well radial flow. Also note the highly heterogeneous nature of the field leads to breakthrough in around 100 days, while it takes over 100,000 days for all the particles to traverse the system.
Fig. 6 – Breakthrough curves for macroscopic solute transport. The late-time behavior is matched by an approximate power-law $C(t) \sim t^{-1/\beta_m}$ with $\beta_m = 1.2 \pm 0.1$. The same late-time behavior is observed for two different boundary conditions (triangles are for wells and squares are for face-to-face transport) and when the ADE is assumed in each link (crosses for wells and asterisks for face-to-face). However, note that the ADE solution under-predicts the breakthrough time, particularly for face-to-face transport since it does not capture the transport of solute through slow-flowing domains.

**What affects field-scale recovery: small or large-scale heterogeneity?**

Traditionally transport would be simulated directly on the field-scale model without any upscaling with some dispersion coefficient used to represent sub-grid-block heterogeneity. In this section we test to see if the proper incorporation of small-scale transport affects the large-scale results.

In Fig. 6 we also show the breakthrough curves where we use a $\psi$ assuming a one-dimensional ADE in each link with $D = D_m$. This is equivalent to a traditional simulation with an infinitely-resolved discretization between nodes. The late-time results are similar to those obtained using Eq. (7) for $\psi$, indicating that the large-scale heterogeneity dominates the overall behavior. This is to be expected, since the pore-scale representation of the field as a relatively homogeneous Berea sandstone contrasts with the extreme variability in the large-scale permeability. Streamline-based simulation, again assuming advective transport on the same reservoir model also gave the same macroscopic behavior with $\beta_m = 1.2 \pm 0.1$.

However, assuming the ADE at the small scale under-predicts the breakthrough time, particularly for face-to-face transport. This is because it does not account for the fact that particles will, occasionally, encounter stagnant regions across which transport occurs only slowly by diffusion. This tends to slow down the solute as shown in previous CTRW simulations in macroscopically heterogeneous media.
We ran one further suite of tests, where we assumed more pore-scale heterogeneity. At the pore scale we used Eq. (2) for transport in an ensemble-averaged (homogeneous) network, but now with $\beta=1.1$ and $\beta=0.5$. We re-ran the upscaling step to find an empirical form for the transit time distribution, Eq. (7). For $\beta=1.1$ Eq. (7), is still valid – see Fig. 4 – but with $\lambda=1.8$, indicating slower transport. This is to be expected: as the medium becomes more heterogeneous, particles will encounter more slow-flowing domains and this will, on average, increase the transit times.

For the most heterogeneous pore-scale network (representing, for instance, a vuggy carbonate) with $\beta=0.5$, we can no longer use Eq. (7). Instead we find, Fig. 4:

$$\psi_t(t) = \frac{\lambda Q \rho^{-\gamma} e^{-\lambda t \rho t / V}}{V} e^{-\lambda t \rho t / V}$$

(8)

with an exponent $\gamma=0.8$ and constant $\lambda=1.6$

Fig. 7 shows the breakthrough curves for macroscopic face-to-face transport with differing amounts of pore-scale heterogeneity. Even through the macroscopic reservoir description, captured at the meter scale with over a million grid blocks, is the same, the macroscopic behavior is very different, with breakthrough times that vary by a factor of around 4 and slightly different late-time exponents, decreasing from an apparent $\beta_m$ of 1.2 to around 1.1 as the pore-scale $\beta$ decreases. Increasing the pore-scale heterogeneity forces the solute to sample stagnant regions of the pore space more frequently. This slows down the overall transport and also leads to a very long tail in the breakthrough curve.$^{11}$ Heterogeneity at all scales affects the macroscopic behavior. It is not correct to presume that simply because the meter-scale reservoir description is highly structured with more than four orders of magnitude variation in permeability it will dominate over any smaller-scale variability. Hitherto there has been no tool to see this phenomenon: a direct simulation of this pore-to-field transport would require of order a trillion cells, and using fewer cells and some effective ADE, is, as we have shown, inadequate.
Fig. 7 – Breakthrough curves for macroscopic particle transport for with different degrees of pore-scale heterogeneity. As the pore-scale exponent decreases, indicating more heterogeneity at the pore scale, the breakthrough curves are shifted to later times and have a shallower late-time tail $C(t) \sim t^{(-1/\beta_m)}$, with a macroscopic exponent $\beta_m$ that varies from around 1.2 to 1.1.

$C(t)$ is a first travel-time distribution and so can be viewed as a field-scale transit-time probability $\psi(t)$. This concept can be used to define intermediate upscaling steps as described in the next section.

**Further refinements: the missing scale**

There are a number of ways in which the current methodology could be refined. The most glaring problem with the results presented here is that the pore-to-core simulations represent a sample around 1 cm across, while the field-scale grid-blocks are meter-sized. We need to include a third, intermediate core-to-grid-block upscaling step. This would involve modeling typical sub-meter-block heterogeneity at the cm scale. Then the transit time distribution across a heterogeneous representation of a meter-scale block at the core, node-to-node scale is found; it may be matched to Eq. (8), or a truncated power-law, Eq. (2), or some other functional form. To find an ensemble average, different macroscopic flux boundary conditions and small-scale realizations need to be considered. Then the field-scale simulation is performed as before. It is likely that with significant, correlated heterogeneity, the transit time distribution used at the meter (grid-block) scale would not be a simple exponential.

Another limitation of the current work is that we only consider homogeneous pore-scale networks. Ideally we would consider different networks that properly represent the differences in pore structure between blocks of different macroscopic permeability and porosity.
Extensions to multiphase flow

The current approach relies on using a particle tracking approach where the flux is linearly related to the solute concentration. This allows us to treat each particle independently and makes ensemble averaging easy. In multiphase flow, however, the flux from node to node is non-linearly dependent on saturation making particle tracking and ensemble averaging problematic. While it is possible to extend particle tracking to multiphase flow, this method has yet to be fully developed. Instead, we propose that the node-to-node transport of saturation is treated as in single-point upstream weighting, but with a probabilistic distribution of putative fractional flows, representing different possible smaller-scale structure.

The advantage of this approach for general petroleum reservoir simulation is that the logic of the nodal structure does not have to be ordered and so it is easy to deal with unstructured grids representing large-scale geological features, such as faults, and to couple the reservoir transport with flow in wells and facilities.

Conclusions

We have proposed a pore-to-field transport simulation approach and applied it to single-phase flow accounting for advection and diffusion. We assume that transport occurs as a series of transitions between discrete sites governed by a transit time distribution.

We can predict the Peclet number dependence of dispersion coefficient at the core scale by modeling transport as a series of pore-to-pore hops. This can be done by either explicitly representing the pore-scale heterogeneity of Berea sandstone, or by using a homogeneous network with an ensemble-averaged transit time distribution that is given by a truncated power-law.

We developed a multiscale upscaling methodology to simulate transport. We showed how to find the transit time distribution at the core scale and how to use this in macroscale simulation.

For advective-dominated transport the transit time distribution at the core scale is exponential in time, with a time-scale related to the time for a particle to advect across the block with a typical velocity.
At the field scale, with a finely-resolved highly-heterogeneous reservoir model, the overall transport behavior is anomalous with power-law scaling of the mean plume location, its standard deviation and the breakthrough curves.

The macroscopic behavior is affected by the small-scale transport even when a very heterogeneous field-scale reservoir description is used. Increasing the pore-level heterogeneity delays the particle transport, since advective trapping in slow-flowing regions becomes more common with significantly increased tailing of the breakthrough curves. It is erroneous to assume that small-scale heterogeneity is, in some mysterious way, only controlled by larger-scale geology; we are now able to perform rigorous pore-to-field simulation and it is evident that such an assumption cannot be sustained.

Future work will refine the methodology to account for cm to m scale heterogeneity and to extend it to multiphase flow.

**Acknowledgements**

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**References**


Abstract
We use X-ray microtomography (micro-CT) to image rock cuttings of poorly consolidated sandstone and vuggy carbonate from Saudi Arabian oil and gas fields. The cuttings are a few mm across and are imaged to a resolution between 3 and 12 microns. The details of the three-dimensional pore space can be clearly seen. A maximal ball algorithm is used to extract a topologically equivalent pore network: the largest inscribed spheres in the pore space represent pores, with throats representing the connections between them. The results are validated through comparison with networks derived by a different method from idealized sphere packings and Fontainebleau sandstone.

The aim of this work is to input the models into pore-scale network models to predict macroscopic properties such as relative permeability and capillary pressure. This acts as a valuable complement to special core analysis, enabling predictions of properties – such as three-phase relative permeabilities and the impact of wettability trends – outside the range of parameters probed experimentally. Furthermore, using microtomography, rock cuttings can be analyzed that are too small for conventional core flood experiments.

Introduction
Pore-scale network modeling can now be used to predict multiphase flow properties as a complementary tool to special core analysis\(^1\text{-}^5\). However, the pore structure of the rock and its wettability needs to be determined.
It is possible to image the three-dimensional pore space directly using micro-CT scanning that has a resolution of a few microns\textsuperscript{6,7}. However, it is difficult to simulate quasi-static multiphase flow directly through these images. Instead a topologically equivalent network of pores and throats is extracted through which flow is computed. This paper uses a novel method for this network extraction using maximal balls\textsuperscript{8}, validates it against other methods and applies it to a series of Saudi Arabian reservoir rocks.

At present the networks that are used for predictions are derived from an analysis of two-dimensional thin section images of sandstones\textsuperscript{2,9}. From these the grain size distribution is determined. Then packings of these grains with subsequent compaction and diagenesis is simulated. Since the locations of the grain centers is known it is possible to find pores and throats in the void space and from this to extract a topologically equivalent network.\textsuperscript{2,9} However, this process-based method is restricted to granular media and does not make use of three-dimensional images if they are available.

**Micro-CT imaging**

We extract pore networks from micro-CT images. A micro-CT scanner at Imperial College London, \textbf{Fig. 1}, and a synchrotron tomographic scanner at ELETTRA in Italy have been used to image sandstone and carbonate samples. The best spatial resolution obtained so far in our series of experiments is 2.9 µm on a carbonate sample with a diameter of 2 mm.

**Fig. 1.** The left picture shows the micro-CT scanner at Imperial College London. The right picture shows the X-ray tube in this scanner and the sample stage.

The micro-CT scanners output three-dimensional (3D) arrays of reconstructed linear X-ray attenuation coefficient values (CT numbers), which can be viewed as gray scales in image processing software. The raw images are filtered to smooth the image, reduce noise and improve the contrast between grain and
void. We use the median filter which replaces the gray scale value of a voxel by the median value of the nearest 26 surrounding cells. Then a threshold value is chosen to binarize or segment the gray scales into two phases: solid and void. The effect of image processing is seen in Fig. 2.

![Image of cross sections and histograms](image)

**Fig. 2.** (a) A cross section of the raw image of a sandstone; (b) is the segmented image of (a); (c) is the median filtered image of (a); (d) is the segmented image of (c). Comparing (b) and (d), we find the median filter preserves the integrity of the grains and the pore space. The side length of the four cross section images is 0.75mm; (e) shows the effect of median filtering on the gray scale histogram and where the threshold value is set. The two peaks representing two phases (void and solid) are more distinguished after the filtering.

**Pore network extraction**

Binarized micro-CT images preserve the morphology and topology of the pore space. However, these images cannot be input into pore scale simulators directly. A topologically equivalent network of pores and throats has to be extracted. Then using a series of rules to determine fluid displacements in pores and throats, multiphase flow can be simulated and predictions made.\(^1\)\(^5\).
Two principal approaches have been used to extract a topologically equivalent network from 3D micro-CT images: medial axis analysis and maximal balls. These will be discussed in turn.

**Medial axis algorithms** use thinning\(^{10,11}\) to erode the pore space from grain surfaces until the medial axis – lines with branches denoting the centers of the pore space – is found. Pores are located at branches in the medial axis, while throats connect pores. The size of the pores and throats can be determined by the number of steps of erosion from the surface of the grains. The medial axis mathematically preserves the topology of the pore space. However, the intrinsic sensitivity to the irregularity of pore space makes the unambiguous identification of pores, that may encompass several branches of the medial axis, difficult\(^{11}\). Generally, medial axis based algorithms readily capture the interconnectivity of the pore space but pore identification is a problem.

**Maximal ball algorithms** construct the largest spheres centered on each void voxel that just fits in the pore space. A maximal ball is one of these spheres that is not completely enclosed by another. The concept of maximal balls was used by Sillin et al.\(^8\) to study the morphology of 3D pore-space images for the identification of pores and throats. A maximal ball that does not overlap any larger sphere defines a pore. Throats are defined as chains of smaller balls that connect pores. The maximal ball method easily and unambiguously identifies pores, but the construction of throats is difficult, since there may be many ways to connect pores by overlapping smaller spheres.

**Algorithm validation**
In this paper we will apply the maximal ball method to extract a network. The key statistical parameters of the pore networks will be compared with the results of the process-based method\(^1,2,9\). Then the algorithm will be applied to images of Saudi Arabian sandstones.
We test the algorithm on a series of standard, idealized granular systems where it is possible to determine the network using the processed-based method. **Fig. 3** compares the number of pores found for a series of simple packings; it can be seen that the maximal ball and process-based algorithms give similar results.
Fig. 3. We compare the number of interior pores of designed sphere packings and simple granular rocks (generated by the process-based method), which are good prototypes for unconsolidated materials. The figure shows a good agreement of the two methods on the number of pores extracted.

We next study a more realistic case: a 3D image of a grain packing representing Fontainebleau sandstone with considerable compaction and diagenesis. The image consists of $300^3$ voxels representing a subset of the sandstone with a volume of $2.25^3$ mm$^3$. The extracted network is illustrated in Fig. 4, while Fig. 5 compares the coordination number distribution for the network with that using process-based extraction. While the distributions are similar, the maximal ball method implies a better connected network. This test is a particular challenge, since the porosity of the sample is only 13.5 % and many of the throats have been completely sealed by diagenesis. Fig. 6 compares the pore and throat size distributions. Again the agreement is good, particularly for the pores that are well captured by maximal balls. For throats some of the discrepancy is due to a random assignment of throat radius about discrete values in the process-based approach.

Fig. 4. The pore network generated from a reconstructed Fontainebleau sandstone image using a modified maximal ball algorithm.
Fig. 5. The coordination number is the number of links connected to one pore, which reflects the spatial connectivity of the pore space. Both the methods find that the distribution peaks at 3. The average coordination number of the network from the maximal ball method is 3.75 while that from the process based method is 3.19.

Fig. 6. Comparison of pore and throat size distributions. The size distributions are in good agreement especially for large pores and throats. Some of the differences are due to dissimilar considerations of boundary pores and the random assignment of radius about discrete values in the process-based method.
Analysis of Arabian rock samples

Ten Arabian samples provided by Saudi Aramco have been scanned and fourteen images have been obtained using industrial and synchrotron micro-CT scanners. To obtain suitable samples for imaging, we drilled cylindrical specimens out of the larger samples before scanning. The resolution of the 3D images varies from 3 to 12 µm corresponding to specimen diameters ranging from 2 to 8 mm. Cross-sections of the images for all the samples are shown in Fig. 7.
Pore networks have been extracted from two sandstones and one carbonate (the first three samples in Fig. 7.) The sandstone sample SA1 has a porosity of 16.4% and a measured permeability of 906 mD. We drilled a 10 mm long, 8 mm diameter...
cylindrical specimen from the core plug and used a subset of the image (1.73 mm$^3$) for our pore network analysis. The image resolution is 8µm. The porosity measured on the image is 16.8% and the permeability computed using lattice Boltzmann simulation is 1400 mD. The subset of the image can be considered a representative elementary volume (REV) of the sandstone.

The second sample is sandstone E3. The image has a resolution of 5.0µm and consists of $150^3$ voxels representing a volume of 0.42 mm$^3$. The last sample is a limestone L1. The 3D image has a resolution of 3µm. The volume is 0.1 mm$^3$. The 3D images of these samples are shown in Fig. 8.

![Fig. 8. Transparent view (left) and the cutaway view (right) of the 3D micro-CT images. (a) SA1, (b) E3, (c) L1.](image)

We extracted pore networks from these three samples, see Fig. 9, and we list the properties of the networks in Table 1. Since the minimum size of pores and throats is always the resolution value of the image, we don’t list them in the table. We find that the sandstones have average coordination numbers between 4 and 5, which is in agreement with other analyses of granular media.$^2$ The vuggy carbonate has higher coordination numbers and a wider distribution of pore and throat size than the sandstones.
Fig. 9. Pore networks generated from micro-CT images using the maximal ball algorithm. From left to right, these are networks of SA1, E3 and L1 respectively.

Table 1 - Properties of the pore networks extracted from Arabian reservoir samples

<table>
<thead>
<tr>
<th>Properties</th>
<th>SA1</th>
<th>E3</th>
<th>L1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity (%)</td>
<td>16.8</td>
<td>25.2</td>
<td>29.8</td>
</tr>
<tr>
<td>Number of pores</td>
<td>442</td>
<td>279</td>
<td>347</td>
</tr>
<tr>
<td>Number of throats</td>
<td>1018</td>
<td>631</td>
<td>1265</td>
</tr>
<tr>
<td>Ave. coordination Number</td>
<td>4.71</td>
<td>4.59</td>
<td>8.6</td>
</tr>
<tr>
<td>Max. coordination number</td>
<td>14</td>
<td>12</td>
<td>32</td>
</tr>
<tr>
<td>Ave. pore radius(µm)</td>
<td>25.0</td>
<td>19.0</td>
<td>22.3</td>
</tr>
<tr>
<td>Max. pore radius(µm)</td>
<td>87.7</td>
<td>59.7</td>
<td>117</td>
</tr>
<tr>
<td>Ave. throat radius(µm)</td>
<td>19.2</td>
<td>13.1</td>
<td>19.3</td>
</tr>
<tr>
<td>Max. throat radius(µm)</td>
<td>78.5</td>
<td>37.2</td>
<td>88.9</td>
</tr>
</tbody>
</table>

Conclusions

Micro-CT scanners provide sufficient spatial resolution to image the pore space of sandstones and some granular carbonates. Other carbonate samples may require sub-micron resolution to image intragranular porosity, which is beyond the capability of current instruments.

We have extracted topologically equivalent networks from 3D micro-CT images. The maximal ball algorithm used was validated by comparing the results with the process-based method for idealized sphere packs and a Fontainebleau sandstone.

The two poorly consolidated sandstone samples had average coordination numbers of around 4.5, representing good connectivity. For the carbonate sample, however, the average coordination was considerably higher – it was more than 8. This is because there is an exceptionally variable pore size distribution with some large pores (vugs) with a very high connectivity.

Future work will focus on using the extracted networks to predict multiphase flow properties, such as relative permeability and capillary pressure.
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