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Two-Phase Flow at the Pore-Scale Using the Volume of Fluid Method

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Two-Phase Flow at the Pore-Scale Using the Volume of Fluid Method

by

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A THESIS
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ABSTRACT

The aim of this thesis is to use digital rock physics for understanding flow through porous media. Pore-scale simulations were conducted using the Finite Volume method to solve the Navier-Stokes equations, and the Volume of Fluid method for capturing interface.

A workflow is provided, in which primary drainage simulations are performed in order to establish initial water saturation. Then, secondary imbibition simulations are performed mimicking viscosity ratios found in thermal recovery processes involving hot water and heavy oil.

Through these simulations, pore-scale events such as Haines jumps, oil ganglia mobilization, fingering and oil stripping in high shear flows are identified.

This research discusses the capabilities and limitations of the Volume of Fluid method, and through the simulation results, important insights are provided in regards to the mechanisms of oil recovery through steam or hot water injection and on the balance of viscous and capillary forces in immiscible displacements.
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TABLE OF CONTENTS

ABSTRACT ............................................................................................................................... ii
ACKNOWLEDGEMENTS........................................................................................................ iii
LIST OF TABLES ....................................................................................................................... vi
LIST OF FIGURES ..................................................................................................................... vii
NOMENCLATURE .................................................................................................................... xi

CHAPTER 1. INTRODUCTION ................................................................................................. 1
  1.1. Background .................................................................................................................... 1
  1.2. Objective ....................................................................................................................... 3
  1.3. Organization of the Thesis ............................................................................................ 4

CHAPTER 2. THE GOVERNING EQUATIONS AND NUMERICAL METHOD ........ 6
  2.1. Physical Description of the Problem ........................................................................... 6
  2.2. Governing Equations ................................................................................................... 14
  2.3. Numerical Method ....................................................................................................... 25

CHAPTER 3. NUMERICAL SETUP AND MODEL VERIFICATION ..................... 33
  3.1. Software Structure and Setup ..................................................................................... 33
  3.2. Static Droplet Numerical Experiments ...................................................................... 38
  3.3. Capillary Tube Numerical Experiments ..................................................................... 45
  3.4. The Digital Porous Media Patterns ............................................................................ 51
  3.5. Summary and Conclusions ......................................................................................... 56

CHAPTER 4. PRIMARY DRAINAGE SIMULATIONS ........................................ 58
  4.1. Primary Drainage in Geometry 1 ............................................................................... 58
  4.2. Primary Drainage in Geometry 2 ............................................................................... 66
  4.3. Summary and Conclusions ......................................................................................... 75

CHAPTER 5. SECONDARY IMBIBITION SIMULATIONS .................................... 77
  5.1. Secondary Imbibition Results .................................................................................... 80
  5.2. Low Capillary Number: Viscous Fingering vs. Capillary Imbibition ....................... 85
  5.3. High Capillary Number: High Shear Flow ................................................................. 89
  5.4. Considerations about the geometry ............................................................................ 94
  5.5. Summary and Conclusions ......................................................................................... 97

CHAPTER 6. CONCLUSIONS AND FUTURE WORK ..................................... 99
  6.1. Final Conclusions ....................................................................................................... 99
  6.2. Recommendations for Future Work ........................................................................... 101

REFERENCES ...................................................................................................................... 103
APPENDIX A. POST-PROCESSING SECONDARY IMBIBITION DATA ............108
LIST OF TABLES

Table 3.1. Theoretical capillary pressure (Pc_Theo), simulated capillary pressure (Pc_Sim) and calculated error........................................................................................................................................................................45

Table 3.2. Cases set-up for capillary tube numerical experiments, two levels of viscosity were used, and the velocities were changed to keep the same Reynolds number. ................................. 47

Table 3.3. Absolute permeability and Reynolds number for 2-dimensional and 3-dimensional cases. ........................................................................................................................................................................ 55

Table 4.1. Reynolds and Capillary numbers for 2-dimensional simulations in Geometry 1....... 63

Table 4.2. Mobility ratio, Reynolds and Capillary Numbers for 2-dimensional simulations....... 67

Table 5.1. Calculated Viscosity Ratio, Capillary and Reynolds numbers for the numerical experiments ................................................................................................................................................... 79

Table 5.2. Summary of results indicating recovery, residual saturation, pressure drop and breakthrough time. .................................................................................................................................................. 81
LIST OF FIGURES

Figure 1.1. Example of a pore network model (5) (Figure A), and a 3-dimensional geometry reconstructed from glass beads (Figure B) ................................................................. 2

Figure 2.1. SAGD experiment showing three distinct zones, (9) ............................................. 7

Figure 2.2. Schematic of a steam-flooding, showing distinct flowing zones at a macro-scale (10) ...................................................................................................................... 8

Figure 2.3. Example of a temperature profile ahead of an advancing steam front. Figure A shows the extent of the heat transfer boundary layer, and Figure B shows a zoom of the first meter with the distance in logarithmic scale. ........................................................................... 13

Figure 2.4. Viscosity increase ahead of the advancing steam front due to reduction in temperature. Figure A shows the overall viscosity increase, and Figure B shows a zoom of the first meter with the distance in logarithmic scale. ................................................................. 13

Figure 2.5. Residual oil versus Capillary number curves for the case of continuous oil (waterflooding at initial oil saturation), and discontinuous oil (enhanced recovery after initial waterflooding). ........................................................................................................... 22

Figure 2.6. Representation of a computational mesh, (28). ......................................................... 27

Figure 3.1. Files structure of a case in OpenFOAM (35). ............................................................ 34

Figure 3.2. Static droplet of oil in water, at initial conditions, and after $t \sigma \mu r = 2500$ ........... 41

Figure 3.3. Droplet dimensionless velocity vs. dimensionless time for original solver (interFOAM) and modified solver (modInterFOAM) at three levels of coefficients: 0.3, 0.5 and 1.0 .......................................................................................................................... 42

Figure 3.4. Droplet dimensionless velocity vs. dimensionless time for modified solver (modInterFOAM) with coefficient of 0.5, with increased mesh refinement (40k cells) and increased oil viscosity (100 mPas) ......................................................................................... 44

Figure 3.5. Spectrum range of sizes, from molecular sizes to grain sizes, including typical pore size distributions (40) ........................................................................................................ 46

Figure 3.6. Theoretical vs. simulated capillary pressures for the two levels of viscosity evaluated in the capillary tube experiments. .............................................................................. 48

Figure 3.7. Interface sharpness of capillary tube experiments for low viscosity cases ($\mu_0 = 1$ mPas), red represents oil and blue represents water ......................................................... 49
Figure 3.8. Interface sharpness of capillary tube experiments for high viscosity cases ($\mu o = 50$ mPas), red represents oil and blue represents water. ................................................. 49

Figure 3.9. Error in the simulated capillary pressure vs. cAlpha for the case of $\mu o = 50$ mPas and capillary diameter of 10 $\mu$m. ................................................................. 50

Figure 3.10. Interface representation for the case of $\mu o = 1$ mPas and capillary diameter of 5 $\mu$m at different values of cAlpha. ................................................................. 51

Figure 3.11. Porous volume for 2-dimensional geometry with dimensions of 0.579 mm x 0.289 mm ................................................................. 52

Figure 3.12. Porous volume for 2-dimensional geometry with dimensions of 0.727 mm x 0.445 mm ................................................................. 53

Figure 4.1. Image of a pore draining event, the black arrow indicates the meniscus that jumped (44)........................................................................... 59

Figure 4.2. Velocity magnitude profile for pore drainage events (44). ......................... 59

Figure 4.3. Initial configuration for primary drainage simulation in Geometry 1. .......... 60

Figure 4.4. Pressure difference in a primary drainage simulation in Geometry 1, showing the effect of individual pore drainage events on pressure response........................................................................... 61

Figure 4.5. Pore drainage event of a large pore body (observation pore). It can be observed withdrawal of fluids in the vicinity (white arrows). ................................................. 62

Figure 4.6. Initial configuration for primary drainage case in Geometry 1 where pore-scale events in the observation pore will be investigated. ................................................. 63

Figure 4.7. Interfacial velocity for a pore drainage event at different injection rates for the cases with oil viscosity of 10 mPas and interfacial tension of 0.05 N/m. ......................... 64

Figure 4.8. Interfacial velocity for a pore drainage event at different injection rates showing the effect of interfacial tension. ................................................................. 64

Figure 4.9. Interfacial velocity for a pore drainage event at different injection rates showing the effect of oil viscosity........................................................................... 65

Figure 4.10. Flow pattern at breakthrough for case 1 (1 mPas). In this case it can be observed that large areas are by-passed, leading to a water saturation at breakthrough of 0.47........ 68

Figure 4.11. Flow pattern at breakthrough for case 4 (100 mPas). Oil phase flows into the water-wet rock in a “piston-like” fashion. Water saturation at breakthrough is 0.37 in this case........................................................................... 69
Figure 4.12. Schematic of flow regimes in two-phase flow immiscible displacements, according to viscosity ratio definition in this thesis. ................................................................. 70

Figure 4.13. Visualization of an oil finger for case 1 (1 mPas), under the capillary fingering flow regime. ........................................................................................................................................ 71

Figure 4.14. Pressure field during primary drainage of the 100 mPas oil (case 4). ......................... 72

Figure 4.15. Pressure and Saturation behavior for primary drainage (case 4). The saturation in the oil invaded zone varies between 0.05 and 0.25, due to the presence of trapped (immobile) water ......................................................................................................................... 72

Figure 4.16. Pore drainage event for lower viscosity (case 1). This event is characterized by a rapid burst of 2 to 3 milliseconds .................................................................................................................. 73

Figure 4.17. Pore draining event for higher viscosity (case 4). This event takes a longer time (15 to 16 milliseconds) due to the dampening effect of high viscosity in a Haines jump. ... 74

Figure 5.1. Porous volume for 2-dimensional geometry. The image shows the initial condition for volume fraction, with oil as red and water as blue. ............................................................................ 77

Figure 5.2. Viscosity of oil and water. The vertical (light grey) dashed lines indicate the temperatures in which the physical properties were taken for the numerical experiments (18), (53). ................................................................................................................................. 78

Figure 5.3. Density of oil and water. The vertical (light grey) dashed lines indicate the temperatures in which the physical properties were taken for the numerical experiments (52), (53). ................................................................................................................................. 78

Figure 5.4. Example of pressure profile for simulation at 220°C at 2.5 x 10^-4 m/s. The pressure over the length of the sample reduces as more water imbibition occurs. .............................. 82

Figure 5.5. Example of pressure difference and oil recovery versus time for simulation at 220°C at 2.5 x 10^-4 m/s. Water breakthrough is distinguished by the low and constant value of pressure and leveling off of oil recovery. ............................................. 83

Figure 5.6. Volume fraction field for simulation at 140°C at 2.5 x 10^-4 m/s. Several pore-scale phenomena may be observed in this sequence of images, such as choke-off (from 120 to 122 milliseconds, and from 128 to 130 milliseconds), Haines-jump (from 122 to 124 milliseconds), and oil blob mobilization (sequence from 130 to 144 milliseconds). ....... 84

Figure 5.7. High velocity pathways at water breakthrough for cases at 220°C, at velocity of 1 x 10^-3 m/s in figure A, and at velocity of 1 x 10^-4 m/s in figure B ....................................................... 86

Figure 5.8. Incremental Recovery versus Capillary number correlation by Abrams from etched glass micromodel experiments (58). ................................................................................................................................. 87
Figure 5.9. Oil recovery (\% OOIP) versus Capillary number according to Abrams correlation, results are presented for the simulations performed in this thesis ........................................... 88

Figure 5.10. Oil recovery versus pore-volumes injected for cases at velocity of $1 \times 10^{-3}$ m/s, and viscosity of 140°C and 220°C. .............................................................................................................................. 90

Figure 5.11. Sequence of time steps for the volume fraction field in a region of the geometry for case at velocity of $1 \times 10^{-3}$ m/s and viscosity of 140°C. Oil ganglia moves in a dynamic displacement mode, enhancing ganglia breakup. .................................................................................................................... 90

Figure 5.12. Sequence of oil stripping and re-mobilization after breakthrough for the case at velocity of $1 \times 10^{-3}$ m/s and viscosity of 140°C (140b). ............................................................................................................................. 92

Figure 5.13. Pressure behavior for the case at velocity of $1 \times 10^{-3}$ m/s and viscosity of 140°C (140b). .......................................................................................................................... 92

Figure 5.14. Final residual oil distribution for cases at velocity of $1 \times 10^{-3}$ m/s, and viscosity of 140°C (140b) and 220°C (220b). ......................................................................................................................... 93

Figure 5.15. Fraction of the final residual oil saturation versus the area of ganglia for cases at velocity of $1 \times 10^{-3}$ m/s, and viscosity of 140°C (140b) and 220°C (220b). ......................... 94

Figure 5.16. Oil Recovery for the three viscosity levels evaluated (140°C, 180°C and 220°C) at three different velocities, $1 \times 10^{-4}$ m/s, $2 \times 10^{-4}$ m/s and $2.5 \times 10^{-4}$ m/s. ....................... 95
NOMENCLATURE

\begin{itemize}
  \item \(A\) Area (m\(^2\))
  \item \(Ca\) Capillary number
  \item \(Co\) Courant number
  \item \(c_p\) Reservoir heat capacity (J/K)
  \item \(C_s\) Coefficient
  \item \(D\) Diameter (m)
  \item \(F_c\) Surface tension force (kg/m\(^2\).s\(^2\))
  \item \(Fr\) Froude number
  \item \(g\) Acceleration due to gravity (m/s\(^2\))
  \item \(k\) Permeability (m\(^2\))
  \item \(K\) Reservoir thermal conductivity (W/m.K)
  \item \(l_c\) Characteristic length (m)
  \item \(\dot{m}\) Mass flux (kg/s)
  \item \(n\) Normal
  \item \(\hat{n}\) Unity normal
  \item \(P\) Dynamic pressure (Pa)
  \item \(Pe_x\) Dimensionless steam interface velocity
  \item \(PV\) Pore volume (m\(^3\))
  \item \(q\) Volumetric flow rate (m\(^3\)/s)
  \item \(R\) Radius (m)
  \item \(Re\) Reynolds number
\end{itemize}
\( S \)  \hspace{1em} \text{Surface area (m}^2\text{)}

\( S_\phi \)  \hspace{1em} \text{Source term in generic transport equation}

\( t \)  \hspace{1em} \text{Time (s)}

\( T \)  \hspace{1em} \text{Temperature (K)}

\( \textbf{U}_r \)  \hspace{1em} \text{Compression velocity (m/s)}

\( \textbf{v} \)  \hspace{1em} \text{Velocity vector (m/s)}

\( v_c \)  \hspace{1em} \text{Characteristic velocity (m/s)}

\( v_x \)  \hspace{1em} \text{Velocity of steam interface (m/s)}

\( V \)  \hspace{1em} \text{Volume (m}^3\text{)}

\( We \)  \hspace{1em} \text{Weber number}

\( x \)  \hspace{1em} \text{Distance in the x direction (m)}

\( y \)  \hspace{1em} \text{Distance in the y direction (m)}

\( z \)  \hspace{1em} \text{Distance in the z direction (m)}

\textbf{Greek Letters}

\( \alpha \)  \hspace{1em} \text{Thermal diffusivity (m}^2\text{/s) or volume fraction}

\( \Gamma \)  \hspace{1em} \text{Generic diffusion coefficient (m}^2\text{/s)}

\( \delta \)  \hspace{1em} \text{Unity tensor}

\( \theta \)  \hspace{1em} \text{Contact angle (°)}

\( \kappa \)  \hspace{1em} \text{Curvature (m}^{-1}\text{)}

\( \lambda \)  \hspace{1em} \text{Dilatational viscosity (Pa.s)}

\( \mu \)  \hspace{1em} \text{Viscosity (Pa.s)}

\( \xi \)  \hspace{1em} \text{Auxiliary distance for axis transformation (m)}
\( \rho \) Density (kg/m\(^3\))

\( \sigma \) Interfacial tension (N/m)

\( \tau \) Stress tensor (kg/m.s\(^2\))

\( \phi \) Porosity or generic variable

Subscripts

\( d \) Defending phase

\( D \) Dimensionless

\( i \) Invading phase

\( l \) Interface

\( o \) Oil

\( p \) Owner cell in Finite Volume

\( r \) Reservoir

\( s \) Steam

\( t \) Tangential

\( w \) Water
CHAPTER 1. INTRODUCTION

1.1. Background

The use of digital rock physics for modelling and understanding flow through porous media has been increasing over the past decade, due to advanced imaging techniques and increasing computational power. The basic workflow of digital rock physics includes the generation of a digital porous media, which can be performed through micro-computer-tomographic (μCT) imaging or 3-dimensional reconstruction of microscopic images (1). This is followed by simulating physical processes through the digital rock to obtain properties, such as, porosity, thermal conductivity, absolute and relative permeability, resistivity, etc. (2), (3).

Traditionally, laboratory experiments and empirical correlations have been used for modelling of rock physics. Although those are useful and popular methods, they have drawbacks. Experiments can be costly, destructive and usually represent a limited range of experimental conditions. Empirical correlations, on the other hand, are approximations or they only hold for a specific set of conditions. With increasing computational power, the study of rock physics evolved from experiments and simple correlations to sophisticated and realistic computational approaches. The use of digital rock physics allows extraction of a much wider range of information when used as a complement to laboratory experiments. This is a growing field of research that started to have some commercial applications, in which the ultimate objective is digital core analysis. Through this process, one can have insights from dynamics of pore-scale phenomena to macroscopic properties, allowing us to obtain fundamental understanding of porous media flows.
The simulation of physical processes through digital porous media can be performed through direct simulations (e.g. computational fluid dynamics methods), or through pore-network modelling (4). Pore-network models are becoming popular tools to obtain macroscopic properties, such as capillary pressure and relative permeability curves. The main advantage of pore network simulations is the fact that they are less computationally expensive when compared to direct simulations. Therefore, larger pore assemblies can be analyzed in a shorter time frame. On the other hand, in pore-network models, the porous media are idealized based on pore-body and pore-throat size distributions, which is a subjective concept for a real porous media. Most of the pore-network models are based on the assumption of a capillary dominated flow, in which viscous forces are negligible. Finally, quasi-static rules that govern the flow are used to simulate the problem, which may result in an over-simplification of the physics of the flow.

Figure 1.1. Example of a pore network model (5) (Figure A), and a 3-dimensional geometry reconstructed from glass beads (Figure B)
Computational fluid dynamics (CFD) has been receiving increasing attention in the industry with regard to simulation of flows at micro-scales, particularly due to the ability to model dynamic effects that are not fully accounted for in pore network models. In the CFD approach, the main features of the porous media are preserved, providing more realistic representation of porous patterns. CFD methods are used to solve the Navier-Stokes or Stokes equations, and they have been used to evaluate single phase properties, such as absolute permeability, by averaging pressure and velocity fields obtained as a solution of the continuity and momentum equations \(^{(6)}\). CFD methods associated to capture of interface techniques allow simulation of two phase flow \(^{(7)}\), which opens a wide range of possibilities in the workflow of rock physics.

Pore-scale direct simulations of digital porous media are computationally demanding. However, they allow sensitivity on several operational conditions in a more realistic geometry. When combined with additional physics (fluid interface, reactions, heat transfer, non-Newtonian fluid flow, etc.), pore-scale direct simulations provide powerful insights in enhanced oil recovery and application of new technologies in porous media.

1.2. Objective

The objective of this thesis is to investigate pore-scale phenomena in two-phase flow in 2-dimensional digital porous media through direct simulations. In the framework of digital rock physics, this research concentrates on the investigation of the ability of a CFD model to provide useful information regarding the physics of porous media flows. A free, open-source CFD package distributed by OpenCFD Ltd. is used to perform simulations. The Finite Volume method is used to solve the Navier-Stokes equations, and the Volume of Fluid method is used for interface
capturing. This research demonstrates that CFD is a powerful tool towards digital core analysis. The ability of the model to reproduce pore-scale instabilities is evaluated. Also, the model is used to investigate the balance between capillary and viscous forces at the micro-scale, providing important insights about two-phase flows in thermal recovery process.


The simulations in regular geometries (e.g., capillary tubes) are used to evaluate the optimal numerical set-up by verifying agreement with analytical solutions. In the primary drainage simulations, the main objective is to create an initial water saturation in the medium, and to observe typical pore-scale events and its influence on final fluids configuration and pressure behavior. Finally, secondary imbibition simulations are used to evaluate characteristic pore-scale events and the balance between viscous and capillary forces in immiscible displacements. Conditions of immiscible displacements of heavy oil by hot water are reproduced, and important insights on pore-scale phenomena in this process are discussed.

1.3. Organization of the Thesis

Chapter 1 presents the background and main objectives of investigating pore-scale phenomena in the framework of digital rock physics.

In Chapter 2, the description of the problem of two-phase flow in thermal recovery methods is elaborated, the governing equations for this process are described, and a detailed explanation of the numerical approach used in this thesis is provided.
Chapter 3 provides the numerical setup used and a verification of the model with analytical solutions in simple geometries. Also, the digital porous media patterns are presented, and results from single phase flow simulations are given in order to determine absolute permeability and anisotropy.

In Chapter 4, the results of primary drainage in complex 2-dimensional patterns are presented, and a discussion about the main pore-scale events observed in this process is provided.

In Chapter 5, secondary imbibition results are given for operational conditions that represent several temperature levels in a hot-water immiscible displacement, where a temperature gradient is present.

Finally, in Chapter 6 the main conclusions from this study are provided, highlighting the main achievements and recommendations for future work.
CHAPTER 2. THE GOVERNING EQUATIONS AND NUMERICAL METHOD

2.1. Physical Description of the Problem

The study of oil recovery from reservoirs containing heavy oil is of interest in several parts of the world, including Canada, Venezuela, United States and Brazil, to name a few. In some cases, oil can flow at reservoir conditions, in spite of its higher viscosity when at the surface. In other situations, however, oil viscosity is too high (in the order of millions of mPas) under original reservoir conditions, which renders it immobile. Thermal recovery techniques are used to allow mobilization of oil in situ, such as steam flooding, cyclic steam injection, steam-assisted gravity drainage (SAGD), among others (8). This is the case of many heavy oil reservoirs in Canada, in which steam and/or solvent is used in order to allow oil mobilization and production.

In thermal methods, when steam is injected, heat exchange occurs between steam and the surroundings (cold oil region, overburden and underburden), resulting in steam condensation. In a simplified interpretation of the process, three potential flowing conditions can be identified (9):
- Two-phase flow of oil and liquid water, which occurs when steam condenses, and oil is basically displaced by hot water.
- Two-phase flow of steam and oil, which may occur in the steam zone (or chamber). The residual oil that was not displaced by the hot water front drains down, usually in a film flow regime, until a new residual oil saturation level is reached.
- Three-phase flow of oil, water and steam, in which simultaneous flow occurs, with phase change as a result of condensation (steam is converted to water condensate once it exchanges heat with the surroundings), or evaporation (when water condensate and heated oil are produced after a soak
period in cyclic injection). Liquid water is considered to be the wetting phase, and it will be covering the rock grains.

These regions are expected to develop in steam injection processes, such as steamflooding, SAGD, and cyclic steam injection. Figure 2.1 gives a graphical representation of the regions, which were identified in micromodel experiments of a SAGD process (9). In SAGD, steam is injected continuously into a horizontal well located parallel to, and closely above, a horizontal production well at the base of the reservoir. In this case, gravity drainage is the main driving force. However, according to observations in micromodel experiments (9), pore-scale immiscible displacement and invasion of both steam and water condensate into the bitumen zone were also observed.

![Image of SAGD experiment showing three distinct zones](image)

Figure 2.1. SAGD experiment showing three distinct zones, (9)

In the case of steamflooding, steam is also injected continuously, but the objective is not only to reduce oil viscosity, but also to provide a pressure drive to displace heavy oil towards the
producers. As steam condenses, a hot water bank is formed (Figure 2.2), in which two-phase flow occurs in the presence of a temperature gradient.

Figure 2.2. Schematic of a steam-flooding, showing distinct flowing zones at a macro-scale (10)

As observed above, the oil/water two-phase flow region will exist in many thermal processes in which steam or hot water is used to displace oil. In this region, a process of secondary imbibition happens, in which water condensate displaces oil. In this immiscible displacement process, oil bypassing is the main cause of residual oil saturation, due to its high viscosity.

The pore-scale mechanisms involved in heavy oil immiscible displacements are complex, even in the absence of a temperature gradient. The main recovery mechanisms involved in heavy oil waterflooding have been discussed in the literature (11). Many mechanisms can be identified in this process, such as:

1. Viscous fingering due to unstable displacement resulting in high velocity water channels;
2. Capillary imbibition from the water channels to adjacent regions;
3. Viscous drag exerted by the high velocity water;
4. Stripping of oil and blockage of water channels, diverting water to regions of un-mobilized oil.

The presence of different mechanisms leads to significant differences from immiscible displacements in conventional oil reservoirs. The high viscosity contrasts involved in heavy oil two-phase flows leads to unstable displacement fronts. However, although viscous forces are dominant, capillary forces may also contribute to recovery.

In an attempt to verify the effect of viscous forces on isothermal immiscible displacements, Vizika et al. (12) performed numerical and physical experiments in regular pore-network models. The physical experiments were performed in a range of viscosity ratios \( \mu_o/\mu_w \), as defined in the paper, from 0.66 to 3.35, and no initial water saturation was present before the start of imbibition. They concluded that at low Capillary numbers the occurrence of capillary micro-fingers (fingering that occurs in the length scale of one to a few pores) is intensified even at unfavorable viscosity ratios. They observed an increase in residual non-wetting phase saturation with viscosity ratio.

More recently, a series of sand pack experiments indicated a different trend from that observed by Vizika et al. (12). Mai et al. (13) conducted isothermal waterflooding experiments in heavy oil saturated sand packs with varying viscosity ratios and permeability to investigate the balance between viscous and capillary forces. The heavy oil samples used were in the order of thousands of mPas. The imbibition was started with an initial water saturation, at injection velocities ranging between \( 10^{-7} \) and \( 10^{-6} \) m/s. They concluded that after breakthrough the contribution of capillary forces are significant, resulting in higher ultimate recovery for the lower permeability cases. Nevertheless, they also verified that for displacement in low permeability sand packs and at lower velocity, a higher oil recovery was also observed at the point of water breakthrough. This indicated
that, although viscous forces are dominant before breakthrough, capillary forces will also play a role in oil recovery at this stage.

In another paper by the same authors (14), a description of heavy oil waterflooding performed in sand packs at similar conditions to the previously reported experiments was presented. An increase in oil recovery at breakthrough for lower injection rates was also observed. The only exception was in the case of very low injection velocity (~10^{-7} m/s), in which the recovery at breakthrough was low, but the amount of oil recovered per pore volume injected was the highest (indicating more efficient flooding).

In the case of thermal processes, as hot fluids are injected, a temperature gradient is established within the reservoir, leading to distinct fluids mobility and flowing conditions in different regions. As the distance from the steam zone (or chamber) increases in the direction of the oil zone, oil viscosity will continuously increase with decreasing temperature away of the interface. This is an important implication of thermal methods, and the details of the dynamics of pore scale flows under these conditions still needs investigation. For example, how will the viscosity ratio between hot water and bitumen influence flow patterns that lead to residual saturation? Or what kind of pore-scale events are present which contribute (or not) to residual saturations?

Although other factors are responsible for alterations in oil mobilization in the reservoir during injection of a hot fluid, viscosity reduction is the most important one. It has been discussed previously in the literature that higher initial water saturation has an impact on water breakthrough times (11). Also, an increase in temperature may result in contact angle and wettability alterations that may be positive or negative for oil mobility (15), (16). Although these factors influence the process, it is expected that the effect of reduction in oil viscosity would be more significant for
heavy oil production than other mechanisms that result from temperature increase. It is not the objective of this thesis to evaluate these parameters.

To give an idea about how temperature and viscosity changes ahead of a steam zone (or chamber), we evaluate the case of heat conduction ahead of an advancing front. The one-dimensional governing equation for this process is the following (8):

\[
\frac{1}{\alpha} \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}
\]

Eq. 2.1

Where \( T \) is temperature and \( x \) is the distance measured normal to the advancing steam interface.

The thermal diffusivity is defined as: \( \alpha = K/\rho c_p \), where \( \rho \) is the reservoir density, \( c_p \) is the reservoir heat capacity and \( K \) is reservoir thermal conductivity.

Assuming that the steam interface moves at a constant velocity, \( v_x \), during an infinitesimal time, a transformation of the coordinate system is done by considering its origin at the steam interface, rather than a fixed origin. This transformation is performed by defining an auxiliary variable, \( \xi \), so that \( \xi = x - v_x t \). If the front advances in a quasi-steady-state manner, the temperature will vary along the depth (\( \xi \)), but it will be constant over time.

By differentiating the auxiliary variable and replacing into Eq. 2.1, we obtain (8):

\[
\frac{1}{\alpha} \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial \xi^2} + \frac{v_x}{\alpha} \frac{\partial T}{\partial \xi}
\]

Eq. 2.2

In dimensionless form,
\[
\frac{\partial T_D}{\partial t_D} = \frac{\partial^2 T_D}{\partial \xi_D^2} + Pe_x \frac{\partial T_D}{\partial \xi_D}
\]  
Eq. 2.3

In the above equation, \( Pe_x \) is the dimensionless interface velocity (heat transfer Peclet number), \( Pe_x = v_x l_c / \alpha \), where \( l_c \) is a characteristic length for the reservoir (i.e., formation thickness). \( T_D \) is the dimensionless temperature \( T_D = (T - T_r) / (T_s - T_r) \), where \( T_r \) is the reservoir temperature and \( T_s \) is steam temperature. The dimensionless time is defined as the diffusive time, \( t_D = \alpha t / l_c^2 \), and the dimensionless distance is normalized to a characteristic length of the reservoir, \( \xi_D = \xi / l_c \). As the process is assumed quasi-steady-state, \( \partial T / \partial t = 0 \). For boundary conditions, at the steam interface (\( \xi = 0 \)), the temperature corresponds to the steam temperature (\( T_D = 1 \)), and far from the interface (\( \xi = \infty \)), the temperature corresponds to the original reservoir temperature (\( T_D = 0 \)). The quasi-steady-state equation can then be solved analytically, and after substituting the original dimensional variables the temperature profile can be calculated as follows:

\[
\frac{T - T_r}{T_s - T_r} = \exp(-v_x \xi / \alpha) = \exp[-(v_x / \alpha)(x - v_x t)]
\]  
Eq. 2.4

Orders of magnitude of viscosity variation with temperature in the two-phase flow zone were evaluated by using reservoir properties from an example available in the literature (17). The viscosity can be obtained by using an empirical correlation (18). For a reservoir with an original temperature of 15°C, thermal diffusivity of 7 x 10^{-7} m^2/s, where steam at 205°C is injected, and the interface is moving at 2 x 10^{-7} m/s, the temperature profile ahead of the steam zone is as follows:
Figure 2.3. Example of a temperature profile ahead of an advancing steam front. Figure A shows the extent of the heat transfer boundary layer, and Figure B shows a zoom of the first meter with the distance in logarithmic scale.

Figure 2.4. Viscosity increase ahead of the advancing steam front due to reduction in temperature. Figure A shows the overall viscosity increase, and Figure B shows a zoom of the first meter with the distance in logarithmic scale.

As it can be observed from the plots above, the heat transfer boundary layer has orders of magnitude of several meters (Figure 2.3). The steepest temperature gradient will happen in the region closest to the steam zone. In order to evaluate the balance between viscous and capillary forces at the pore level in the two-phase flow region, a “zoom” of a small element of rock is taken, in the order of micrometers. By evaluating the first 1 millimeter ahead of the steam front, where a
steep temperature gradient is present, it can be observed that variation in temperature and viscosity are negligible at this length scale when compared to the extent of the heat transfer boundary layer. To be more accurate, a piece of rock of 1 millimeter taken ahead of the steam front will have a temperature decrease from 204.89°C to 204.84°C, which results in a viscosity increase from 9.028 to 9.036 mPas.

The digital porous media used in pore scale simulation in this thesis have dimensions less than 1 millimeter, therefore, the temperature and viscosity gradients are considered negligible in such a small scale, and for the secondary imbibition cases evaluated in this thesis, the element of rock will be considered as isothermal, and the flow will be evaluated with physical properties of the fluids that correspond to specific temperature snapshots.

2.2. Governing Equations

In an immiscible displacement of heavy oil by water, the micro-scale fluid continuum is comprised of two domains, oil and water, and the solid phase is assumed to be rigid. The conservation of mass and momentum over a control volume for isothermal two phase flow at a micro-scale are as follows:

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{Eq. 2.5} \]

\[ \frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) + \nabla \cdot \mathbf{\tau} = -\nabla P + \rho \mathbf{g} \tag{Eq. 2.6} \]
The first term in the left hand side of equation Eq. 2.6 corresponds to the rate of increase of momentum per unit volume, the term $\nabla \cdot (\rho \mathbf{v} \mathbf{v})$ corresponds to the rate of momentum addition by convection, the term $\nabla \cdot \mathbf{\tau} + \nabla P$ corresponds to the rate of momentum addition due to molecular transport, and the term $\rho \mathbf{g}$ corresponds to an external force per unit volume due to the gravitational acceleration ($\rho \mathbf{g} = \rho g \nabla z$). Each of these equations are developed for each phase, for a description of two-phase flows. $\rho$ is the fluid density, $\mathbf{v}$ is the velocity vector, $P$ is the dynamic pressure.

The variable $\mathbf{\tau}$ corresponds to the viscous stress tensor, which for a Newtonian fluid, is expressed as:

$$\mathbf{\tau} = -\mu(\nabla \mathbf{v} + (\nabla \mathbf{v})^T) + \left(\frac{2}{3} \mu - \lambda\right) (\nabla \cdot \mathbf{v}) \mathbf{\delta}$$

Eq. 2.7

In this equation, $\nabla \mathbf{v}$ is the velocity gradient, and the superscript $T$ corresponds to the transpose of this tensor. $\mathbf{\delta}$ is the unity tensor, $\mu$ is the viscosity of the fluid and $\lambda$ is called the dilatational viscosity and it is more relevant to acoustical calculations (19). In the case of incompressible fluids with constant viscosity (constant $\rho$ and $\mu$), the continuity equation reduces to:

$$\nabla \cdot \mathbf{v} = 0$$

Eq. 2.8

Therefore, the second term in the right hand side of Eq. 2.7 vanishes. Also, expanding the term $\nabla \cdot (\rho \mathbf{v} \mathbf{v}) = \rho (\mathbf{v} \cdot \nabla) \mathbf{v} + \rho \mathbf{v} (\nabla \cdot \mathbf{v})$ in Eq. 2.6, and applying the continuity equation, it reduces to:

$$\nabla \cdot (\rho \mathbf{v} \mathbf{v}) = \rho (\mathbf{v} \cdot \nabla) \mathbf{v}$$

Eq. 2.9
Finally, expanding the differential operators in $\mu \nabla \cdot [(\nabla \mathbf{v} + (\nabla \mathbf{v})^T)]$, the stress tensor becomes

$$
\mu \nabla \cdot [(\nabla \mathbf{v} + (\nabla \mathbf{v})^T)] = \mu \nabla^2 \mathbf{v} \quad \text{Eq. 2.10}
$$

Substituting the above equations in the equation of motion (Eq. 2.6) and applying for each phase (with subscript “w” for water and “o” for oil), it becomes:

$$
\rho_w \frac{\partial \mathbf{v}_w}{\partial t} + \rho_w (\mathbf{v}_w \cdot \nabla) \mathbf{v}_w - \mu_w \nabla^2 \mathbf{v}_w = -\nabla P_w + \rho_w \mathbf{g} \quad \text{Eq. 2.11}
$$

$$
\rho_o \frac{\partial \mathbf{v}_o}{\partial t} + \rho_o (\mathbf{v}_o \cdot \nabla) \mathbf{v}_o - \mu_o \nabla^2 \mathbf{v}_o = -\nabla P_o + \rho_o \mathbf{g} \quad \text{Eq. 2.12}
$$

The standard boundary conditions for two-phase flows are no-slip and pressure jump boundary conditions. At the oil-solid and water-solid surfaces, the no-slip condition is:

$$
\mathbf{v}_w = 0 \text{ at rock-water interface} \quad \text{Eq. 2.13}
$$

$$
\mathbf{v}_o = 0 \text{ at rock-oil interface} \quad \text{Eq. 2.14}
$$

The mass flux of each phase at the interface can be expressed as $\dot{m}_w = \rho_w (\mathbf{v}_w - \mathbf{v}_I) \cdot \mathbf{n}_{wo}$ and $\dot{m}_o = \rho_o (\mathbf{v}_o - \mathbf{v}_I) \cdot \mathbf{n}_{ow}$, where subscript $I$ corresponds to the interface between oil and water, $\dot{m}$ is the mass flux at the interface due to phase change, $\mathbf{n}_{wo}$ is the unit vector normal to the boundary.
of the domain “w” (water), and \( \mathbf{n}_{ow} \) is the unit vector normal to the boundary of the domain “o” (oil). Note that the interface is assumed to have zero thickness and no thermomechanical properties, and therefore, \( \mathbf{n}_{ow} = -\mathbf{n}_{wo} = \mathbf{n} \).

The mass balance is then: \( \dot{m}_w + \dot{m}_o = \rho_o (v_o - v_i) \cdot \mathbf{n} - \rho_w (v_w - v_i) \cdot \mathbf{n} = 0 \). If there is no phase change at the interface, the mass flux at the interface is zero, \( \dot{m}_o = -\dot{m}_w = 0 \). This leads to the continuity boundary condition at the interfaces (20):

\[
\mathbf{v}_o = \mathbf{v}_w \text{ at oil-water interface} \quad \text{Eq. 2.15}
\]

Finally, the pressure jump condition is defined as:

\[
(P_o \mathbf{\delta} + \mathbf{\tau}_o) \cdot \mathbf{n} - (P_w \mathbf{\delta} + \mathbf{\tau}_w) \cdot \mathbf{n} = 2\kappa \sigma_{ow} \mathbf{n} + \nabla \sigma_{ow} \mathbf{t} \quad \text{Eq. 2.16}
\]

Where \( \mathbf{n} \) refers to normal direction of the interface and \( \mathbf{t} \) refers to tangential direction of the interface. The viscous stress tensor (\( \mathbf{\tau} \)) for an incompressible fluid is: \( \mathbf{\tau} = -\mu (\nabla \mathbf{v} + (\nabla \mathbf{v})^T) \), and \( \mathbf{\delta} \) is the unit tensor. The first term in right hand side refers to the normal stresses due to the curvature of the interface, \( 2\kappa = (1/R_1 + 1/R_2) \), where \( R_1 \) and \( R_2 \) are the principal radii of curvature. The last term in the right hand side refers to tangential stresses caused by Marangoni effects when a temperature or concentration gradient is present; under isothermal conditions without mass transfer, \( \nabla \sigma_{ow} = 0 \). The pressure jump condition then becomes:

\[
(P_o \mathbf{\delta} + \mathbf{\tau}_o) \cdot \mathbf{n} - (P_w \mathbf{\delta} + \mathbf{\tau}_w) \cdot \mathbf{n} = 2\kappa \sigma_{ow} \mathbf{n} \quad \text{Eq. 2.17}
\]
In the case of quasi-static conditions, the above equation reduces to the Young-Laplace equation:

\[ P_o - P_w = 2\kappa\sigma_{ow}\mathbf{n} \]  
Eq. 2.18

The dimensionless groups that help to understand the process can be extracted through Inspectional Analysis of the governing equations and boundary conditions (21). The main dimensionless variables are defined as follows (22):

Length: \( x_D = \frac{x}{l_c}; y_D = \frac{y}{l_c}; z_D = \frac{z}{l_c} \)

Velocity: \( v_D = \frac{v}{v_c} \)

Time: \( t_D = \frac{v_c t}{l_c} \)

Pressure: \( p_D = \frac{p_{lc}}{\sigma_{ow}} \)

Curvature: \( \kappa_D = \kappa l_c \)

Differential Operators: \( \nabla_D = l_c \nabla \) and \( \nabla_D^2 = l_c^2 \nabla^2 \)

In these definitions, \( l_c \) corresponds to a micro-scale characteristic length that has the order of magnitude of pore sizes. The characteristic velocity \( (v_c) \) corresponds to the magnitude of the pore velocity in porous media flows, which is on the order of \( 10^{-5} \) m/s. The expression for the dimensionless pressure will depend on the relevant physical phenomenon that governs fluid flow. In the case of immiscible displacements at pore-scales, capillary forces will be more significant.
(as it will be demonstrated in the following paragraphs), therefore, expressing the pressure in terms of interfacial tension is considered to be the most adequate representation.

By applying the dimensionless variables to the governing equations and boundary conditions, the following equations result:

\[ \nabla \cdot \mathbf{v}_{WD} = 0 \text{ and } \nabla \cdot \mathbf{v}_{oD} = 0 \quad \text{Eq. 2.19} \]

\[ Re_w \frac{\partial \mathbf{v}_{WD}}{\partial t_D} + Re_w (\mathbf{v}_{WD} \cdot \nabla_D) \mathbf{v}_{WD} - \nabla_D^2 \mathbf{v}_{WD} = - \frac{1}{Ca_w} \nabla_D P_{WD} + \frac{Re_w}{Fr^2} \nabla_D Z_D \quad \text{Eq. 2.20} \]

\[ Re_o \frac{\partial \mathbf{v}_{oD}}{\partial t_D} + Re_o (\mathbf{v}_{oD} \cdot \nabla_D) \mathbf{v}_{oD} - \nabla_D^2 \mathbf{v}_{oD} = - \frac{1}{Ca_o} \nabla_D P_{oD} + \frac{Re_o}{Fr^2} \nabla_D Z_D \quad \text{Eq. 2.21} \]

\[ \mathbf{v}_{WD} = 0 \quad \mathbf{v}_{oD} = 0 \quad \mathbf{v}_{WD} = \mathbf{v}_{oD} \quad \text{Eq. 2.22} \]

\[ (P_{oD} + P_{WD}) \mathbf{n} + \frac{1}{Ca_o} \tau_{oD} \cdot \mathbf{n} - \frac{1}{Ca_w} \tau_{WD} \cdot \mathbf{n} = 2\kappa_D \mathbf{n}, \quad \text{with} \quad \text{Eq. 2.23} \]

\[ \tau_D = -(\nabla_D \mathbf{v}_D + (\nabla_D \mathbf{v}_D)^T) \]

As demonstrated from the non-dimensional form of governing equations and boundary conditions, the most important dimensionless groups that represent immiscible and isothermal two-phase flows are the Reynolds Number (Re), Capillary Number (Ca) and the Froude number (Fr). Other dimensionless groups may be derived from them or from observations of the physical phenomenon.
The Reynolds Number \((Re)\) corresponds to the ratio between inertial and viscous forces, and is defined as:

\[
Re = \frac{\rho v c l_c}{\mu}
\quad \text{Eq. 2.24}
\]

Laminar flow regime in porous media (and therefore, Darcy’s law validity) prevails for a Reynolds number \((Re)\) below 1 (23). The order of magnitude of the characteristic length can be obtained from the absolute permeability and porosity of the medium, according to the following relationship:

\[
Re = \frac{\rho v c}{\mu} \sqrt{\frac{k}{\phi}}
\quad \text{Eq. 2.25}
\]

Typically, for pore scale flows, Reynolds numbers are much lower than 1. To give an idea of the order of magnitude of the Reynolds number in a porous media, for a medium with absolute permeability of \(0.987 \times 10^{-12} \text{ m}^2\) (1 Darcy), porosity of 30%, transporting a fluid with viscosity of 0.001 Pa.s and density of 1000 kg/m\(^3\) at an average pore velocity \((\sim 10^{-5} \text{ m/s})\), the Reynolds number would be in the order of \(1 \times 10^{-5}\). The term \(\sqrt{k/\phi}\) used as a characteristic length gives order of magnitude of pore throat sizes, which for this case was \(\sim 2 \mu\text{m}\). Looking back into Eq. 2.20 and Eq. 2.21, it can be observed that the inertial terms are negligible for typical pore-scale flow conditions. By eliminating negligible terms, one arrives to the Stokes or creeping flow equations.
Although the creeping flow assumption is valid for pore-scale flows, in Chapter 4 it is demonstrated that pore-scale instabilities that happen under certain conditions in immiscible displacements may increase the interfacial velocity to a point where inertial effects can start to become significant. This subject will be discussed in more detail later in this thesis.

Capillary number is an important dimensionless group in immiscible displacements and it corresponds to the ratio between viscous and capillary forces. It is derived from the ratio between Reynolds and Weber number.

\[
Ca = \frac{We}{Re} = \frac{\rho v_c^2 l_c}{\sigma_{ow}} \left( \frac{\rho v_c l_c}{\mu} \right)^{-1} = \frac{\mu v_c}{\sigma_{ow}} \quad \text{Eq. 2.26}
\]

In the definition above, the properties of the invading fluid are used for the calculation. Capillary number is widely used in the petroleum industry, as it is strongly correlated to residual oil saturation after immiscible displacements. As the characteristic length used in the definition of surface tension forces is a micro-scale quantity, the Capillary number is a microscopic group by definition. However, it is common to find in the literature different representations of Capillary number, including with macro-scale variables, such as Darcy velocity.

Chatzis et al. (24) investigated how different definitions of the Capillary number changes the relationship between this dimensionless group and a reduced residual saturation \((S_{or}/S_{or}^*)\). Reduced residual saturation \((S_{or}/S_{or}^*)\) is obtained when increased Capillary numbers are applied after a regular waterflooding has been performed (discontinuous oil). In their analysis, they concluded that, although different definitions of Capillary numbers are used, there is a similarity in the shape of all \(Ca\ vs S_{or}/S_{or}^*\) curves. Another important observation from their analysis is that
below a Capillary number of $10^{-6}$ to $10^{-5}$, little or no additional residual saturation reduction is obtained, which is also the case of residual oil saturation after initial waterflooding (continuous oil). Figure 2.5 shows a schematic of the correlation between Capillary number and residual oil for continuous and discontinuous oil (24).

![Figure 2.5](image)

Figure 2.5. Residual oil versus Capillary number curves for the case of continuous oil (waterflooding at initial oil saturation), and discontinuous oil (enhanced recovery after initial waterflooding).

Although Capillary numbers are important for the understanding of two-phase flows and residual saturations, it does not completely define how viscous forces will play a role in immiscible displacements. The viscosity ratio ($M$) is another important variable that will indicate if the displacement front is more likely to be stable or unstable. In this thesis, viscosity ratio ($M$) is defined as:
Subscript $d$ relates to the defending phase, and $i$ relates to the invading phase. Following the above definition, the smaller the viscosity ratio, the more stable the displacement is. As it can be observed, transport properties from both fluids need to be considered, although Capillary and Reynolds numbers are usually calculated based on the properties of the invading phase.

In order to take into account the viscosity of both phases in the definition of Capillary number, Abrams (25) suggested a modified Capillary number from curve fitting of $S_{or}$ vs. this dimensionless group for a series of waterflooding experiments performed for different rock types and viscosity ratios. In his case, the residual saturation was obtained by performing a secondary waterflood (discontinuous oil) with “enhanced water” (water with higher viscosity and/or reduced interfacial tension), and the viscosity ratios were varied by increasing the viscosity of either oil or water. The velocity was adjusted by dividing the pore velocity by the recovered oil saturation ($S_{oi} - S_{or}$), before calculating the Capillary number. The modified Capillary number reduced the scatter on the data, and it was suggested as follows:

$$ Ca_{Abrams} = \frac{\mu_i v}{\sigma_{ow}(S_{oi} - S_{or})} \left( \frac{\mu_i}{\mu_d} \right)^{0.4} $$

Although the importance of both viscosity ratio and Capillary number have been highlighted for the case of immiscible displacement, the relationship between these groups and its relative importance in the case of immiscible displacements is still under discussion, especially for the case
of immiscible displacements in heavy oil reservoirs, as will be discussed in more details in Chapter 5.

Another important dimensionless group that arrives from inspectional analysis of the governing equations is the Froude number, which is defined as:

\[ Fr = \frac{v_c^2}{\sqrt{g l_c}} \]  

Eq. 2.29

This group represents the ratio between inertial to gravitational forces. The ratio between the Weber number and the Froude number results in a dimensionless group that represents the relationship between gravity and capillary forces.

\[ \frac{We}{Fr^2} = \frac{\rho v_c^2 l_c}{\sigma_{ow} \left(v_c^2 \right)^{-1}} = \frac{\rho g l_c^2}{\sigma_{ow}} \]  

Eq. 2.30

When the density of the fluid \( \rho \) in the above equation is replaced by the density difference \( (\rho_w - \rho_o) \), it results in the known dimensionless group Bond number, which is relevant especially for gravity drainage and forced-gravity drainage displacements. By analysing the dimensionless group in Eq. 2.30 a characteristic length can be obtained, the so called capillary length:

\[ l_{cap} = \sqrt{\frac{\sigma_{ow}}{\rho g}} \]  

Eq. 2.31
In the context of pore-scale simulations, this group indicates at which dimensions gravity effects may start to influence fluids distribution. For a medium with interfacial tension of 0.05 N/m and density of 1000 kg/m³, the capillary length is ~2.2 millimeters, meaning that gravity effects may start to influence fluids distribution for a medium with height above this value. The porous media evaluated in this study is of the order of micrometers, and therefore, it is expected that capillary effects will be more significant than gravity effects at this scale.

2.3. Numerical Method

The governing equations described in the previous section are solved in order to obtain velocity, pressure and saturation distributions in porous media flow. In this thesis, the system of partial differential equations are solved numerically using a Finite Volume method in the open-source software OpenFOAM, (26). The general form of the transport equation for a variable \( \phi \) is (27):

\[
\frac{\partial (\rho \phi)}{\partial t} + \nabla \cdot (\rho \phi \mathbf{v}) = \nabla \cdot (\Gamma \nabla \phi) + S_\phi
\]

Eq. 2.32

In the left hand side of the above equation, the first term corresponds to the rate of increase of \( \phi \) in the control volume and the second term corresponds to the net rate of flow of \( \phi \) out of the control volume. In the right hand side, the first term corresponds to the rate of increase of \( \phi \) due to diffusion and the second term corresponds to the rate of increase of \( \phi \) due to sources.
The Finite Volume method is developed to solve the discretized form of the integral of the above equation over a control volume. Gauss divergence theorem is then used to convert from volume to surface integrals, by applying the concept that the divergence of \( \phi \) over a control volume \((dV)\) is equal to the flux of \( \phi \) across a surface \((S)\) that bounds the control volume. Therefore, the integral form of the general transport equation becomes:

\[
\frac{\partial}{\partial t} \left( \int_{CV} \rho \phi dV \right) + \int_{S} \mathbf{n} \cdot (\rho \phi \mathbf{v}) dS = \int_{S} \mathbf{n} \cdot (\Gamma \nabla \phi) dS + \int_{CV} S_{\phi} dV
\]

Eq. 2.33

The term \( dS \) represents an infinitesimal surface element, and \( \mathbf{n} \) is the normal vector to the surface element \( dS \). The product \( \mathbf{n} \cdot (\rho \phi \mathbf{v}) \) represents the flux component of property \( \phi \). Each term in the above equation is then discretized, and the value of the property \( \phi \) is interpolated based on nodal points adjacent to the cell.

Based on Eq. 2.33, important parameters can be extracted from the representation of the computational mesh. In Figure 2.6, an example of one computational mesh (cell) generated from the discretization of the solution domain is presented. The cell of interest is designated as “owner” \((P)\). The point in the cell center \((P)\) is chosen so that:

\[
\int_{V} (x - x_{p}) dV = 0
\]

Eq. 2.34

Each cell has several faces, but each face in the “owner” cell has only one “neighbor” \((N)\). In Figure 2.6, a face designated as \(f\) has its face area vector \((S_{f})\) pointing outwards from the owner
cell, $S_f$ is an important property used in the calculation of face fluxes, it is normal to the face and its magnitude is equal to the area of the face.

![Figure 2.6. Representation of a computational mesh, (28).](image)

Different discretization schemes with different interpolation techniques may be used. As the transport equation is second-order in space, the order of the discretization method (obtained from a truncation of a Taylor series expansion in space) needs to be second-order or higher for good accuracy (29). For more details on the discretization of each term in the above equation, the reader is referred to OpenFOAM Programmer’s guide (28).

For the Navier-Stokes equations, a special solution procedure is needed to handle the non-linear term $\nabla \cdot (\rho \mathbf{v} \mathbf{v})$. The solution algorithm requires solving both pressure and velocity fields in a coupled manner, as they are inter-dependent. In OpenFOAM, pressure-velocity coupling is handled by the use of SIMPLE loop (Semi-Implicit Method for Pressure-Linked Equations) for steady-state simulations, and PISO loop (Pressure Implicit with Splitting of Operators) for transient, two-phase flow simulations. Any additional equations that are not related to the loop are solved after pressure and velocity fields are calculated.
In the PISO loop, the momentum equation is optionally solved first using a pressure field from the previous time step (momentum predictor). A new velocity field is obtained, which does not satisfy the continuity condition. Using this velocity, the pressure equation is solved, generating a new pressure field. The new pressure field is then used to explicitly correct the velocity. This loop is repeated at a fixed time step, until a pre-determined tolerance is reached.

In the SIMPLE loop, velocity distribution is initially obtained using a pressure distribution from previous iteration (or initial guess), and pressure fields are then updated by the solution of the pressure equation. Under-relaxation factors are applied in order to obtain a better approximation of the correct pressure field (29).

A critical aspect of two-phase flow simulations is the methodology used to keep track of the position of the interface between fluids while it is advected. Several interface representation methods are available in the literature, each one with virtues and drawbacks (30).

Overall, one can use surface methods or volume methods for the computation of interfaces (7). Within each of these categories there are two general ways of representing the interface: explicit and implicit.

In explicit methods, the coordinates of each point on the interface are traced explicitly and would then depend on a parametric description of the curve or surface; thus giving rise to the term interface tracking. An implicit description of the interface invokes some auxiliary function where a discontinuous line determines the position of interface.

Examples of surface methods include front tracking methods in which the interface is represented explicitly or level set methods which represent the interface implicitly. In volume methods, examples include marker particle methods which populates the control volume of each material.
region with particles and are thus explicit methods, and volume of fluid methods in which an indicator function is used to compute the interface implicitly.

In the case of pore-scale two-phase flows simulations two important aspects need to be addressed: the complex topology of the porous media, and the ability to properly represent pore-scale mechanisms. If explicit techniques are used to track the interface in pore scale flows, the complex topology leading to breaking and merging of interfaces will result in difficult implementation and high computational time. Therefore, explicit methods such as front tracking and marker particle methods are unfeasible for this scenario. On the other hand, implicit techniques, such as the level-set method can handle the complex topology and flow characteristics.

Level-set methods are popular in the modeling of two-phase flows because it provides a sharp interface and it handles naturally complex topology and interfaces that can break and merge. In this method, a level set function (or signed distance function) is defined over the whole domain, and the function is solved for the advection of the interface, in which the interface is defined at a position of zero (zero level contour), (31). One issue of this method, however, is that, as the zero contour interface moves, a re-initialization is required in order to redefine the signed distance function, which results in loss of mass.

In the sub-pore scale regime, fluids entrapment and residual saturations are among the most important objectives of porous media two phase flow modelling, therefore, it demands strict mass conservation, in addition to handling the complex topology. This gives rise to a volume method for interface capturing used in this study, the Volume of Fluid method. This method is applied in the interFOAM solver, which uses the Finite Volume method for solving the Navier-Stokes equations.
In the Volume of Fluid method, an indicator function ($\alpha$) is used to define which fluid is occupying the cells, with a value of 1 for the wetting phase (water), and 0 for the non-wetting phase (oil). The fluid properties (density and viscosity) are assumed to vary linearly with the indicator function:

\[
\rho = \alpha \rho_w + (1 - \alpha) \rho_o \quad \text{Eq. 2.35}
\]

\[
\mu = \alpha \mu_w + (1 - \alpha) \mu_o \quad \text{Eq. 2.36}
\]

In these equations, subscript $w$ represents the wetting phase (water) and subscript $o$ represents the non-wetting phase (oil). By combining Eq. 2.35 with the continuity equation (Eq. 2.5), the equation for the advection of the interface is obtained (32):

\[
\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{v}) = 0 \quad \text{Eq. 2.37}
\]

In this approach, a single momentum equation is solved, and volume fraction will define which regions of the domain are occupied by oil or water. This significantly improves computational efficiency. As a single momentum equation is solved, surface tension needs to be included as a body force in the momentum equation. Therefore, it is necessary to express it as a pressure gradient. The term $F_c$ is then included in the momentum equation, which will correspond to the additional contribution due to surface tension forces.

\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) - \nabla \cdot [\mu (\nabla \mathbf{v} + (\nabla \mathbf{v})^T)] = -\nabla P + \rho \mathbf{g} + F_c \quad \text{Eq. 2.38}
\]
Brackbill et al. (33) introduced the Continuum Surface Model (CSF), with a derivation of the expression for the surface tension force in Eq. 2.39. In this model, the standard representation of the surface force per unit interfacial area is reformulated to be expressed as a volume force ($F_c$). The integral of the surface force per unit interfacial area is equal to the integral of this force over a volume, in which the interface is represented as a delta function. The vector normal to the interface corresponds to the gradient of the volume fraction field, $\nabla \alpha$, and, as this quantity is non-zero only at the interface between fluids, this volume force is zero outside the interfacial region.

$$F_c = \sigma \kappa \mathbf{n} = -\sigma (\nabla \cdot \hat{n}) \mathbf{n} \quad \text{Eq. 2.39}$$

In the equation above, $\sigma$ is the surface tension, $\kappa$ is the curvature of the interface and $\mathbf{n}$ is the vector normal to the interface. The unit normal to the interface $\hat{n}$ is given by:

$$\hat{n} = \frac{\nabla \alpha}{|\nabla \alpha|} \quad \text{Eq. 2.40}$$

A known issue of the Volume of Fluid method is numerical diffusion in the volume fraction field. The differences in density and viscosity across the fluids interface result in different relative velocities, leading to smearing of the interface, which has detrimental effects on the calculation of curvature and surface tension forces.

In order to overcome this problem, interface sharpening is obtained by introducing an artificial compression term in the vicinity of the interface in Eq. 2.37:
\[
\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{v}) + \nabla \cdot (\alpha(1 - \alpha)\mathbf{v}_r) = 0 \quad \text{Eq. 2.41}
\]

In the above equation, \( \mathbf{v}_r \) is the artificial compression velocity. This additional compression term is active only in the interfacial region, ensuring interface sharpness without affecting the solution of the equations in the fluid continuum. The degree of compression is dictated by a compression constant (cAlpha) that is used to obtain \( \mathbf{v}_r \) (26). When cAlpha is 0, no interface compression is applied, a value of cAlpha between 1 and 4 may be used in order to obtain enhanced interface sharpness (34).

Finally, wall adhesion is addressed by modifying the calculation of the normal to the interface close to solid boundaries, to take into account contact angle. The normal to the interface at the contact line is calculated as follows:

\[
\mathbf{n} = \mathbf{n}_w \cos \theta + \mathbf{n}_t \sin \theta \quad \text{Eq. 2.42}
\]

Where \( \mathbf{n} \) is the normal to the interface used to calculate surface tension forces, \( \mathbf{n}_w \) is the normal vector to the wall, \( \mathbf{n}_t \) is the tangent vector to the wall, and \( \theta \) is the contact angle.
CHAPTER 3. NUMERICAL SETUP AND MODEL VERIFICATION

Verifications of the Volume of Fluid method or the interFOAM solver were already explored in the literature (30), (32), (34). The main objective of this chapter is to identify the preferred numerical schemes and setup for the case of two-phase flow in digital porous media, in which capillary forces are high due to the small length scales. As capillary forces are dominant in the cases investigated in this thesis, a focus will be given to the accuracy in the determination of capillary pressure under the conditions expected in immiscible displacements involving heavy oil and water.

As a starter in the use of CFD methods in OpenFOAM, it is a good practice to copy a tutorial case with similar physics, and to adapt the case study to the physical problem in which one is interested to investigate by changing geometry, fluid properties, boundary conditions, and so forth. Therefore, the base case used to set up the problems in this thesis was an interFOAM tutorial called “damBreak”, in which two-phase flow is simulated. Several modifications were necessary, in order to properly simulate flows at length scales in the order of micrometers and to impose high viscosity ratios at these dimensions, including a widely used modification of the interFOAM solver itself. The modifications performed and a verification of the numerical setup by comparison with analytical solutions are provided below.

3.1. Software Structure and Setup

In OpenFOAM a case is organized in the following structure:
System Directory

In the *system* directory, the numerical schemes, equation solvers and run control parameters are set up. The *system* directory includes the file *controlDict*, in which the time steps are set up. Also, in the *controlDict* file a maximum Courant number is imposed. This is an important parameter to assure stability and convergence in the numerical solution of partial differential equations (PDEs), and it is defined as:

$$Co = \frac{\Delta t \ |v|}{\Delta x}$$  \hspace{1cm} \text{Eq. 3.1}
In this equation, $\Delta t$ corresponds to the time step, $|\mathbf{v}|$ is the magnitude of the velocity in a control volume and $\Delta x$ is the length of the control volume in the direction of the velocity. The time steps are adaptive, and they are calculated based on the above equation. For two-phase problems, it is recommended a $Co < 0.5$, but in this thesis a maximum $Co$ of 0.2 was imposed for all runs. This selection showed more accurate and stable simulation runs. As a result, time steps in the simulations were very small (in the order of $10^{-7}$ s), however, the use of parallel processing allowed to solve the problems in a timely manner, as it will be discussed later in this section.

The `fvSchemes` file in the `system` directory is used to define the discretization schemes to solve the terms of the PDEs. For the solution of two phase flow in this thesis, the temporal discretization is performed by using the Euler scheme, an implicit first-order method. The discretization of the convection term is performed by using a Gauss linear upwind scheme, and the advection of the volume fraction field was discretized by using a Gauss integration with van Leer limiter, both second-order schemes (35). For the interfacial compression flux, the `interfaceCompression` numerical scheme was used, along with the MULES solver (Multidimensional Universal Limiter with Explicit Solution), which reduces the numerical diffusion at the interface and reduces computational cost by applying a higher order scheme restricted to the interfacial region (refer to (32) for more details). Finally, gradient schemes are discretized by using the `pointCellsLeastSquares` method, which is suggested as a best practice for calculating the curvature in Volume of Fluid simulation techniques, and showed significant improvements on the representation of the interface and reduction of spurious currents (36). This is a second-order scheme and its main advantage is that it uses more points from neighbor cells for interpolation when compared to a Gauss linear scheme.
In the `fvSolution` file in the `system` directory, the equation solvers, numerical parameters and tolerances are set up. In this file, the interface compression factor (cAlpha) is set. Finally, the `decomposeParDict` file in the `system` directory is executed for parallel processing. Due to the complexity of the geometry and of the physical problem itself, the solution of two-phase flow simulations in digital porous media may require prohibitive running times if a single processor is used. Therefore, the simulations are set to run in a cluster of processors. The `decomposePar` command decomposes the mesh in smaller parts, and each part is solved by a single processor. The decomposition method used is the Scotch method, which decomposes the mesh in the required number of parts and minimizes the number of inter-processor boundaries (35). For the 2-dimensional porous patterns used in this thesis, actual running times varied from 15 to 20 days, using 48 to 60 processors, depending on the geometry. Before post-processing, the geometry is reconstructed by using the command `reconstructPar`.

**Constant Directory**

In the `constant` directory, the fluid’s physical properties, gravitational field and transport model (laminar or turbulent) are set up. The viscosity ratio and interfacial tension are defined in the `transportProperties` file. In the `turbulenceProperties` file, the laminar simulation type is selected. The `Polymesh` folder inside the `constant` directory contains the files that define the geometry. The folder contains the files that define the boundaries of the domain and a list of owner and neighbor cells, cell faces and points. The simple geometries used in this chapter were generated using the `blockMesh` utility, in which geometries can be generated and meshed using hexahedral cells. For the 2-dimensional porous patterns used, a figure of the pattern was imported to a software called
simpleWare (37), where the geometry was smoothed and meshed. SimpleWare is a program used for 3-dimensional data visualization, analysis and model generation (meshing), and therefore, it generates a 3-dimensional gridding. The model was converted to 2-dimensional by using the extrudeMesh utility in OpenFOAM, in which one face of the geometry is extruded preserving the mesh in this face.

**Time Directories**

The time steps that are required to be written are saved as a time directory. The time directory contains the results for pressure, velocity, volume fraction, fluxes and any other parameters that the user may want to record. The first time step (usually the time “0”) contains the initial and boundary conditions for the simulations. In a core-flooding experiment, a pressure drop may be defined between the inlet and outlet of the core, or a constant injection rate may be defined, with fixed pressure at the outlet. For the two-phase flow numerical experiments in this paper, the boundary conditions are defined as fixed velocity or fixed injection rate at the inlet (fixedValue or flowRateInletVelocity), and fixed pressure at the outlet (fixedValue). No-slip condition is defined at the solid walls by setting the velocity equal to zero at the solid boundaries. At the outlet boundary, the velocity out of the domain has a zero gradient condition, meaning that the velocity normal to the outlet is zero. Also at the outlet boundary, the velocity into the domain is set to zero to avoid backflow (inletOutlet). Finally, the boundary conditions for the volume fraction field are defined as follows: a fixed value at the inlet (injecting either water or oil), a zero gradient at the outlet and a constant contact angle at the walls (constantAlphaContactAngle). In all cases, the contact angle was set to zero, to have a strongly water-wet medium.
3.2. Static Droplet Numerical Experiments

As discussed in the previous chapter, the use of the interface compression coefficient (cAlpha) is necessary in the Volume of Fluid method in order to keep interface sharpness. Although this approach successfully compresses the interface, it may lead to inaccuracy on the computation of the curvature, which leads to the well-known problem of spurious currents. Spurious currents are numerical artifacts generated from the imbalance between the discrete representation of the curvature and the pressure jump across the interface. This results in the appearance of non-physical velocities at the interface that generates interfacial movements not associated with the physical problem.

The static droplet problem is often used to observe the effects of spurious currents. In this problem, a 2-dimensional droplet of fluid is placed in an immiscible medium with an initial squared shape. In the absence of gravity, viscous forces or any other external forces, the droplet will assume a spherical shape due to surface tension, with a zero total velocity. In some cases, the presence of unphysical velocities at the interface are so high that it may lead to a movement of the droplet, even in the absence of external forces.

Many methods are suggested in the literature for minimizing the problem of spurious currents, although there is no method to date that is able to completely eliminate it. Usually a recursive smoothing of the volume fraction field is performed before the normal to the interface is calculated. The smoothed volume fraction function used in the case studies in this thesis is calculated as follows (38), (39):
\[
\tilde{\alpha} = C_s \left[ \alpha \right]_{c \rightarrow f} \bigg|_{f \rightarrow c} + (1 - C_s)\alpha
\]

Eq. 3.2

The term \(c \rightarrow f\) corresponds to a linear interpolation of the volume fraction from cell centers to face centers. These face-centered values are then averaged back to the cell centers \((f \rightarrow c)\). \(C_s\) is a coefficient used on the smoothed volume fraction field. A value of \(C_s\) equal to 0 results in no smoothing. By using this approach it is possible to minimize the problem, as it will be demonstrated in the numerical examples in this chapter, allowing a better calculation of curvature.

This modification is performed in the source code, by modifying the interfaceProperties module in the solver. A header file “smoofilter.H” was created, as indicated below, which is then called in the interfaceProperties0.C file (#include "smoofilter.H") before the curvature is computed.

```cpp
// smoofilter.H

volScalarField alphap ("alphap", alpha1_);
const fvMesh& mesh = alphap.mesh();

// The number of times the filter is applied (filt)
scalar filt (readScalar
(mesh.solutionDict().subDict("PIMPLE").lookup("filt")));

// The coefficient (relax1)
scalar relax1 (readScalar
(mesh.solutionDict().subDict("PIMPLE").lookup("relax1")));

// The smoothing operation
for (int loopfilt=0; loopfilt<filt; loopfilt++)
{
    surfaceScalarField alphaf ("alphaf", fvc::interpolate(alphap));
    alphap = relax1*alphap+(1.0-relax1)*fvc::average(alphaf);
}
Info << " SMOOTHING " << average(alphap) << endl;
```
The problem of spurious velocity is aggravated when mesh refinement increases, for low viscosity fluids and when density ratios are high. In this thesis, the numerical experiments were performed with fluid properties similar to those used by Brackbill et al. (33), but with a diameter of the relaxed droplet in the order of micrometers to represent typical dimensions of pore-scale flows.

The results are presented in terms of normalized capillary time scale ($t\sigma/\mu r$), where $r$ corresponds to the radius of the droplet, the velocity of the droplet was normalized by the capillary velocity ($|v|\mu/\sigma$), where $|v|$ is the magnitude of the velocity of the droplet, and the final steady droplet spherical shape is achieved at $t\sigma/\mu r \sim 350$, (34).

For the sake of simplicity, the background fluid will be called water, and the droplet will be called oil. The water density and viscosity were set to 1000 kg/m$^3$ and 1 mPas, the oil density and viscosity was set to 500 kg/m$^3$ and 2.5 mPas, and the interfacial tension was set to 0.0236 N/m. The domain has dimensions of 600 $\mu$m x 600 $\mu$m, with 10,000 cells, and a square with dimensions of 300 $\mu$m x 300 $\mu$m was placed in the middle of the domain, to represent the oil droplet (Figure 3.2). The square side ($s$) is related to the sphere radius by the following relationship: $s^2 = \pi r^2$; therefore, the final sphere radius is 169 $\mu$m, which gives a theoretical capillary pressure of 139.6 Pa, according to the pressure jump condition, Eq. 2.18.
Figure 3.2. Static droplet of oil in water, at initial conditions, and after $t\sigma/\mu r = 2500$.

The following cases have been set up for comparison:

Case interFOAM: the original solver is used, with default numerical schemes.

Case modInterFOAM_0.3: the modified solver with smoothing was used, with the numerical schemes discussed in the “Software Structure and Setup” section. The smoothing was applied twice, with a coefficient of 0.3.

Case modInterFOAM_0.5: the modified solver with smoothing was used, with the numerical schemes discussed in the “Software Structure and Setup” section. The smoothing was applied twice, with a coefficient of 0.5.

Case modInterFOAM_1.0: the modified solver with smoothing was used, with the numerical schemes discussed in the “Software Structure and Setup” section. The smoothing was applied twice, with a coefficient of 1.
Figure 3.3. Droplet dimensionless velocity vs. dimensionless time for original solver (interFOAM) and modified solver (modInterFOAM) at three levels of coefficients: 0.3, 0.5 and 1.0.

Figure 3.3 shows the results from the numerical experiments of a static droplet. The case “interFOAM” presented high magnitude of spurious currents, and the droplet moves out of the domain. In a larger domain, the droplet would move randomly, as a result of the unphysical velocities at the interface. From this figure, it is possible to observe more clearly the benefits of the smoothing on the reduction of spurious currents. The increase of the coefficient reduces the noise on the velocity response, however, it also affects the calculation of the simulated capillary pressure (Table 3.1). Therefore, a coefficient of 0.5 was selected for all simulation cases in this thesis, as it helps on the reduction of the spurious velocities, and provides a reasonable error in the calculation of capillary pressure.

For a further investigation on the effects of spurious currents in simulations at conditions applied in the cases investigated in this thesis, additional runs were set up to investigate the effect of higher viscosity and interfacial tension, and the effect of mesh size.
In one run, the fluid properties in the optimal case modInterFOAM_0.5 were modified. The oil viscosity was increased from 2.5 mPas to 100 mPas, and the interfacial tension was increased from 0.0236 N/m to 0.05 N/m. A higher viscosity is expected to dampen the effect of spurious currents, however, a higher interfacial tension results in an increase in the surface tension forces, which is expected to increase the magnitude of the un-physical velocities.

In another run, the mesh refinement of the case modInterFOAM_0.5 was increased, keeping the fluid properties unchanged. The number of cells went from 100 x 100 (10,000 cells) to 200 x 200 (40,000 cells). More mesh refinement is expected to increase the magnitude of spurious currents.

In Figure 3.4, a comparison between the modified cases mentioned above with the original modInterFOAM_0.5 is provided. It can be observed that the effect of increase in viscosity is more significant than the effect of increase in interfacial tension, and therefore, the magnitude of the velocity of the droplet decreases over time. This is an important conclusion, because the higher viscosity ratios applied in the cases of secondary imbibition are actually beneficial for numerical stability and reduction of numerical artifacts resulted from spurious currents.

For the case of mesh refinement, as expected, the magnitude of spurious currents increase, which results in an overall droplet velocity higher than the original case with 100 x 100 cells. However, as observed in Table 3.1, further mesh refinement provides little additional accuracy in the capillary pressure calculation, meaning that the 100 x 100 cells case is an optimum mesh refinement for this case.
Figure 3.4. Droplet dimensionless velocity vs. dimensionless time for modified solver (modInterFOAM) with coefficient of 0.5, with increased mesh refinement (40k cells) and increased oil viscosity (100 mPas).

The effect of these modifications on the computation of the capillary pressure can be observed in Table 3.1. In this table, the relative error is calculated as follows: \((P_{c,\text{Theo}} - P_{c,\text{Sim}})/P_{c,\text{Theo}}\). The term \(P_{c,\text{Theo}}\) corresponds to the theoretical capillary pressure calculated according to the pressure jump condition, Eq. 2.18, and the term \(P_{c,\text{Sim}}\) corresponds to the pressure jump obtained from the simulations.

Due to the high magnitude of the spurious currents in the default case (interFOAM), the relative error in capillary pressure is \(~14\%\). Applying the smoothing and the optimized numerical schemes not only reduces the magnitude of spurious velocities, but also improves the computation of the curvature, resulting in smaller errors in the calculation of capillary pressure. The relative error in the simulated capillary pressure versus the theoretical were between 5 to 6% when the optimized numerical setup and smoothing are applied.
<table>
<thead>
<tr>
<th>Case</th>
<th>Pc_Theo</th>
<th>Pc_Sim</th>
<th>Relative Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>interFOAM</td>
<td>139.5</td>
<td>120.2</td>
<td>0.139</td>
</tr>
<tr>
<td>modInterFOAM_0.3</td>
<td>139.5</td>
<td>132.3</td>
<td>0.052</td>
</tr>
<tr>
<td>modInterFOAM_0.5</td>
<td>139.5</td>
<td>131.8</td>
<td>0.056</td>
</tr>
<tr>
<td>modInterFOAM_1</td>
<td>139.5</td>
<td>130.8</td>
<td>0.063</td>
</tr>
<tr>
<td>modInterFOAM_0.5_100 mP</td>
<td>295.9</td>
<td>281.0</td>
<td>0.050</td>
</tr>
<tr>
<td>modInterFOAM_0.5_40k cells</td>
<td>139.5</td>
<td>132.0</td>
<td>0.054</td>
</tr>
</tbody>
</table>

Table 3.1. Theoretical capillary pressure (Pc_Theo), simulated capillary pressure (Pc_Sim) and calculated error.

3.3. Capillary Tube Numerical Experiments

The numerical experiments presented in the previous section showed the improvements in the solver and the selected numerical schemes that resulted in a reduction of spurious currents. In this section, numerical experiments are performed in 2-dimensional capillary tubes to evaluate capillary pressure when the interface is in contact with a solid boundary at the scales expected for typical pore throat sizes. Also, in the immiscible displacements simulated later in this thesis, the differences in viscosity are significant, therefore, it is important to evaluate how the numerical model takes into account variations in viscosity ratio.

Typical pore size distributions for sandstones, tight sandstones and shales were reviewed (40), and a seven orders of magnitude size spectrum range from molecular sizes to grain sizes was provided (Figure 3.5). According to Nelson (40), high-quality sandstone reservoirs generally have pore-throat sizes greater than 10 μm, lower quality reservoirs have pore throat sizes greater than 1 μm, and below 1 μm the reservoirs are classified as tight sandstones. The region classified as sandstones in Figure 3.5 was taken from a set of data in which the average porosity was 21% and
the geometric mean of the permeability was 30 mD. Therefore, for the cases evaluated in this thesis, pore-throat sizes are expected to be greater than 10 μm.

Figure 3.5. Spectrum range of sizes, from molecular sizes to grain sizes, including typical pore size distributions (40).  

Simple 2-dimensional capillary tubes with diameters ranging from 5 to 50 μm were used to evaluate the effect of changing viscosity on the computation of the curvature and calculation of surface tension forces. This range represents the lower limit of pore-throat sizes expected in conventional sandstones, with permeability in the order of 30 mD. The contact angle at the solid
boundaries was set to zero, meaning that the system is strongly water-wet. The numerical experiments were based on a fixed Reynolds number of 0.001, as defined in the equation below:

\[ Re = \frac{\rho v D}{\mu} \]  

Eq. 3.3

With \( \rho \) being the density of the fluid, \( v \) the injection velocity, \( D \) the capillary tube diameter and \( \mu \) the fluid viscosity. The fluid properties used to calculate Reynolds number correspond to that of the injecting fluid (oil). The density of oil and water were set to 1000 kg/m\(^3\), and oil viscosity, injection velocity and capillary diameter were varied according to Table 3.2. The geometry contains 25,000 hexahedral cells, and the interface between oil and water is placed in the middle of the capillary.

<table>
<thead>
<tr>
<th>Test ID</th>
<th>Velocity (m/s)</th>
<th>Diameter (( \mu m ))</th>
<th>Theoretical Cap. Pressure (Pa)</th>
<th>Oil Viscosity (mPas)</th>
<th>Reynolds Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cap_1d</td>
<td>2 \times 10^{-4}</td>
<td>5</td>
<td>20000</td>
<td>1</td>
<td>0.001</td>
</tr>
<tr>
<td>Cap_2d</td>
<td>1 \times 10^{-4}</td>
<td>10</td>
<td>10000</td>
<td>1</td>
<td>0.001</td>
</tr>
<tr>
<td>Cap_3d</td>
<td>0.4 \times 10^{-4}</td>
<td>25</td>
<td>4000</td>
<td>1</td>
<td>0.001</td>
</tr>
<tr>
<td>Cap_4d</td>
<td>0.2 \times 10^{-4}</td>
<td>50</td>
<td>2000</td>
<td>1</td>
<td>0.001</td>
</tr>
<tr>
<td>Cap_1e</td>
<td>10 \times 10^{-3}</td>
<td>5</td>
<td>20000</td>
<td>50</td>
<td>0.001</td>
</tr>
<tr>
<td>Cap_2e</td>
<td>5 \times 10^{-3}</td>
<td>10</td>
<td>10000</td>
<td>50</td>
<td>0.001</td>
</tr>
<tr>
<td>Cap_3e</td>
<td>2 \times 10^{-3}</td>
<td>25</td>
<td>4000</td>
<td>50</td>
<td>0.001</td>
</tr>
<tr>
<td>Cap_4e</td>
<td>1 \times 10^{-3}</td>
<td>50</td>
<td>2000</td>
<td>50</td>
<td>0.001</td>
</tr>
</tbody>
</table>

Table 3.2. Cases set-up for capillary tube numerical experiments, two levels of viscosity were used, and the velocities were changed to keep the same Reynolds number.
The results from the simulations above are provided in Figure 3.6, where the theoretical versus simulated capillary pressure is plotted. Two important conclusions can be drawn from these results: The increase in viscosity and/or decrease in capillary diameter results in less accuracy in the computation of the capillary pressure.

![Figure 3.6. Theoretical vs. simulated capillary pressures for the two levels of viscosity evaluated in the capillary tube experiments.](image)

These trends can be explained by the increase in numerical diffusion as the diameter decreases and the viscosity increases, which impacts the accuracy in the computation of the curvature. For the runs with viscosity ratio ($\mu_o/\mu_w$) of 1, significant numerical diffusion is only observed for capillary tube diameters of 5 $\mu$m or less (Figure 3.7). For viscosity ratios ($\mu_o/\mu_w$) of 50, numerical diffusion is more significant, and it is present in all diameters (Figure 3.8). These simple tests demonstrate that, although the default numerical setup is suitable for most applications of two-phase computational fluid dynamics in the industry, such as free surface flows, simulation at pore-scales have additional difficulties associated with the extremely small length scales.
As discussed in Chapter 2, in OpenFOAM interface sharpness is addressed by an artificial interface compression term that is active only in the interfacial region. For conventional simulations (e.g. free surface flows at the macro-scale), an interface compression factor (cAlpha) of 1 is
recommended for interface sharpness. In order to investigate further how to address interface sharpness at smaller length scales, additional simulations were setup for the case of viscosity ratio of 50 and a capillary diameter of 10 μm. In these runs, the compression factor cAlpha was increased until a proper interface representation was obtained. The plot (Figure 3.9) shows the capillary pressure error versus the cAlpha value used, and in each case the contour plot of the interface is given to demonstrate the effect of cAlpha in the representation of the interface.

![Figure 3.9](image)

**Figure 3.9.** Error in the simulated capillary pressure vs. cAlpha for the case of $\mu_0 = 50$ mPas and capillary diameter of 10 μm.

It can be observed that interface sharpness can be successfully achieved by the use of higher values of cAlpha. Numerical diffusion was eliminated by the use of a cAlpha of 4 for all diameters tested in the higher viscosity ratio cases.

The same approach was tested in the case of viscosity ratio of 1 and a capillary diameter of 5 μm, the only case at lower viscosity that presented significant numerical diffusion. For this case, interface sharpness was obtained with a cAlpha of 2, however, when cAlpha was increased to 4,
numerical artifacts started to appear close to the interface, represented by small droplets of the water into the oil phase (Figure 3.10).

As observed by Hoang et al. (34), increasing cAlpha results in an increase on the magnitude of spurious currents. However, for high viscosity cases, cAlpha does not have a negative impact in the magnitude of spurious velocities due to the dampening effect of viscosity, as observed in the static drop examples. It actually considerably increases accuracy in the computation of the curvature and numerical stability of the simulations. For the viscosity ratio ($\mu_o / \mu_w$) of 1 and 5 $\mu$m diameter case, an increase in cAlpha from 2 to 4 resulted in the random appearance of the numerical artifacts mentioned. Although the numerical artifacts did not affect the flowing behavior or the calculated capillary pressure, for lower viscosity cases it is recommended to keep the interface compression factor cAlpha below 2.

### 3.4. The Digital Porous Media Patterns

The simulations of two phase flows were performed in 2-dimensional geometries. The topology of the porous media is an important factor in two-phase flows, and it is important that the features
found in natural media are properly reproduced digitally. Previous experiments with steady-state two-phase flow in planar (2-dimensional) and non-planar (3-dimensional) micromodels indicated that “the nature of two-phase flow remains qualitatively the same and only quantitative differences are observed” (41). Thus, it is understood that successful numerical simulations in 2-dimensional patterns will provide insights on the physics of two-phase flow that are qualitatively representative of 3-dimensional geometries. Also, the physics in 2-dimensional simulations can be reproduced in a 3-dimensional geometry through the same methodology in order to pursue relevant quantitative information.

Two different patterns were used for the pore-scale simulations in this thesis:

Geometry 1: a two-dimensional pattern (Figure 3.11) characterized by large pore bodies, with dimensions of 0.579 mm x 0.289 mm. This geometry contains 112,016 cells and it will be used to evaluate pore-scale events at the level of one pore.

![Figure 3.11. Porous volume for 2-dimensional geometry with dimensions of 0.579 mm x 0.289 mm](image)
Geometry 2: a two-dimensional pattern (Figure 3.12) characterized by small pore-bodies and long pore throats, with dimensions of 0.727 mm x 0.445 mm, and 221,221 cells. Simulation in this geometry will allow to visualize the effect of pore-scale events on pressure fields and fluids distribution in the level of a few pores.

![Porous volume for 2-dimensional geometry with dimensions of 0.727 mm x 0.445 mm](image)

Figure 3.12. Porous volume for 2-dimensional geometry with dimensions of 0.727 mm x 0.445 mm

In porous media, the modeling of flow at the pore level (or microscopic level) involves solving equations that govern the fluid continuum filling the pore space, i.e. Navier-Stokes equations for Newtonian fluids, as described in the previous chapter. By averaging the fields in the fluid continuum that fills the porous space over a representative elementary volume (REV), we arrive at Darcy’s law:

\[
q = v_{\text{Darcy}} A = \frac{k}{\mu} \cdot (\nabla P + \rho g)
\]

Eq. 3.4
Where $\mathbf{v}_{\text{Darcy}}$ is the macroscopic velocity vector, $\mathbf{q}$ is the volumetric flow rate, $\mathbf{k}$ is a symmetric second rank tensor representing the permeability of the medium.

For the single-phase flow simulations, a steady-state problem is solved in order to obtain the average velocity and pressure drop across the porous medium. The OpenFOAM solver called simpleFOAM is used, where pressure and velocity fields are calculated using the solution algorithm (SIMPLE) Semi-Implicit Method for Pressure-Linked Equations, as described in the previous chapter.

The steady-state solution of the governing equations in a given geometry will result in final pressure and velocity fields. The velocity field is then averaged and converted to macro-scale (Bear, 1972):

$$
\mathbf{v}_{\text{Darcy}} = \frac{\sum \mathbf{v} PV}{\sum PV} \phi 
$$

Eq. 3.5

In this equation, $PV$ refers to “pore volume”, and $\phi$ is the porosity. For the 2-dimensional geometries used in this thesis, the “pore volume” term will be used to express the pore volume per unit width. The overall pressure drop and the calculated Darcy velocity is then used to obtain the absolute permeability of the medium, through Eq. 3.4.

The Darcy equation is solved in mutually orthogonal directions (i.e., x, y and z), by using the averaged fields generated from pore-scale simulations. The determination of the diagonal components of the permeability tensor represent the dependence of flow rate in one direction on pressure differences in the same direction. In the case when at least two elements of the diagonalized permeability tensor are not equal then this leads to permeability anisotropy.
Permeability anisotropy has crucial implications on the selection of oil recovery mechanisms, being one of the primary inputs in reservoir simulators.

The single-phase flow simulations were performed with a fixed flow rate at the inlet, generating a Darcy velocity of the order of $10^{-4}$ m/s, and an average pore velocity according to Table 3.3. The injected fluid has density of 1000 kg/m$^3$ and viscosity of 0.001 Pa.s. The volume of each mesh element is integrated over the entire Geometry 1 resulting in a pore volume (per unit width) of the sample of $9.98 \times 10^{-8}$ m$^2$, which gives a porosity of 59.6%. For the case of Geometry 2, the pore volume (per unit width) of the sample of $1.04 \times 10^{-7}$ m$^2$, which gives a porosity of 32%.

The pore-scale Reynolds numbers calculated according to Eq. 2.25 are given in Table 3.3, and it can be seen that their values are much smaller than 1. As $Re \ll 1$, the flows through these digital porous media were performed in a laminar flow regime.

The shape of the grains are not spherical in the geometries used in these simulations, which gives an anisotropy of $\sim 1.6$ for Geometry 1 and $\sim 2$ for Geometry 2, meaning that the x-direction has a permeability twice higher than the y-direction.

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Direction</th>
<th>$k$ (D)</th>
<th>$v$ (m/s)</th>
<th>Re</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>x</td>
<td>5.47</td>
<td>$2 \times 10^{-4}$</td>
<td>$5 \times 10^{-4}$</td>
</tr>
<tr>
<td></td>
<td>y</td>
<td>3.50</td>
<td>$2 \times 10^{-4}$</td>
<td>$4 \times 10^{-4}$</td>
</tr>
<tr>
<td>2</td>
<td>x</td>
<td>0.82</td>
<td>$8 \times 10^{-4}$</td>
<td>$1 \times 10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>y</td>
<td>0.41</td>
<td>$5 \times 10^{-4}$</td>
<td>$6 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

Table 3.3. Absolute permeability and Reynolds number for 2-dimensional and 3-dimensional cases.
3.5. Summary and Conclusions

The numerical experiments in this chapter represent conditions in which the capillary forces are the strongest, due to the small diameters used, the high interfacial tension and a zero contact angle, which makes the medium strongly water wet. Simulations with intermediate or neutral contact angle conditions, lower interfacial tension and greater pore-throat sizes will have the surface tension effects reduced in comparison with the tested cases, and therefore, more numerical stability.

Spurious currents are a well-known problem present in all interface capturing methods, and in this section a demonstration of a combination of numerical schemes and smoothing that effectively minimizes the problem was given. In addition to that, interface capturing using Volume of Fluid method may lead to high numerical diffusion, depending on the conditions of the immiscible displacements. This problem was solved by increasing the compression factor cAlpha for interface sharpness. It was observed that the simulation time for lower viscosity cases was higher than for higher viscosity cases, supporting the argument that high viscosity ratio simulations have more numerical stability due to the reduced magnitude of spurious currents even with the high cAlpha values applied.

In this section an optimized numerical set-up was provided which successfully increases the accuracy of the computational method, and a verification with simple geometries indicates that the error in the calculation of capillary pressure at the dimensions and viscosity ratios tested are lower than ~5%.

Finally, single-phase flow simulations were performed in order to characterize the digital porous media used in this thesis. Geometry 1 presents larger pore throats, and a permeability of 5.47 Darcy
in the direction of flow, while Geometry 2 presents smaller pore throats and permeability of 820 mD. While simulations in Geometry 1 will allow detailed visualization of flow dynamics in the level of an individual pore, Geometry 2 presents a higher number of pores, and it is expected that it will provide more averaged insights on the level of an elementary volume.
CHAPTER 4. PRIMARY DRAINAGE SIMULATIONS

4.1. Primary Drainage in Geometry 1

The primary drainage process involves injecting a non-wetting phase in a medium, and reducing the wetting phase saturation from 100% to an irreducible level. This process is characterized by individual pore drainage events that result in irreversible fluid rearrangement, the so called jumps or Haines jumps.

When the oil/water interface comes out of the pore throat into a pore body its curvature is reduced. This results in an unstable configuration because the interface is unable to change curvature smoothly with variations in pressure. When an unstable configuration is present, the interface moves at a high velocity into the pore body until the next constriction, leading to an almost instantaneous filling of the pore body. This is a spontaneous, irreversible process, resulted from a release of surface free energy of the system (42). Therefore, the high interfacial velocity generated during a jump is a result of the conversion of this released surface free energy into heat and kinetic energy. Due to inertial effects, the interface oscillates around an equilibrium position while propagating inside the pore body, which generates damped oscillations (43). A Haines jump generates a cascade of events that affects fluids distribution and pressure fields.

Investigation of these interfacial instabilities in a micromodel experiment (44) provided insights on the effect of Capillary number on the interfacial velocity during a Haines jump. In these experiments, a non-wetting fluid was injected into a network of pore bodies with 60 μm and pore throats with 13 μm (Figure 4.1). The experiments were conducted with a constant flux boundary condition, and the injection rates varied between runs.
The interfacial velocity was measured for several injection flow rates (Figure 4.2), and their main conclusion in this part of the experiment was that there was no correlation between injection flow rate and interfacial velocity for the cases evaluated. The differences in interfacial velocity observed in Figure 4.2 are actually related to the fluids distribution prior to an event. If sufficient fluid is available in the vicinity of a draining pore, the interfacial velocity will be high, regardless of the injection rate. However, if the nearby region drains too soon, the interfacial velocity decreases.
To evaluate if the Volume of Fluid method was able to reproduce the effects of Haines jumps observed in physical experiments, a primary drainage simulation was set up in Geometry 1. The medium is strongly water-wet, and oil with viscosity of 10 mPas was injected at the inlet, at a Darcy velocity of $4.8 \times 10^{-4}$ m/s. At the outlet, atmospheric pressure was defined, and the upper and lower walls were defined as no-flow boundaries. The density of oil and water were kept the same, 1000 kg/m$^3$, in order to eliminate gravity effects in this analysis. Reynolds number (Eq. 2.25) was $2.4 \times 10^{-4}$ and Capillary number (Eq. 2.26) was $1.6 \times 10^{-4}$ for this simulation.

The medium was initially 100% saturated with water (blue color), and an initial interface of oil was set up at the inlet (red color). An observation pore was selected in order to observe the effect of events on the level of an individual pore, as indicated in Figure 4.3.

![Flow Direction](Image)

**Figure 4.3.** Initial configuration for primary drainage simulation in Geometry 1.
During oil injection, abrupt jumps of the interface were identified in several time steps. These jumps were reflected in the pressure response, as observed in the plot of pressure difference between inlet and outlet versus time (Figure 4.4).

The noisy pressure response is a result of individual pore drainage events. As Geometry 1 has only a few pore bodies which are quite large, the effect of these events on pressure difference is magnified.

![Graph showing pressure difference and pore drainage events](image)

**Figure 4.4.** Pressure difference in a primary drainage simulation in Geometry 1, showing the effect of individual pore drainage events on pressure response.

Complete drainage of the observation pore is achieved between time steps 0.2 to 0.216 s, as indicated in the plot (Figure 4.4). A high interfacial velocity is observed, as the meniscus comes out of the pore throat into the pore body.
Figure 4.5. Pore drainage event of a large pore body (observation pore). It can be observed withdrawal of fluids in the vicinity (white arrows).

The high interfacial velocity results in a local flow rate that is higher than the injection flow rate, leading to the local fluids redistribution observed in the sequence in Figure 4.5. In other words, the drainage of one pore body may result in imbibition of several pore throats adjacent to the draining pore. As long as enough fluid is available in the vicinity, this kind of fluid redistribution will happen, which is in accordance with qualitative observations in physical experiments mentioned previously.

In order to investigate Haines jumps in more details, six simulation cases for primary drainage in Geometry 1 were set up with varying injection velocity, oil viscosity and interfacial tension. In these runs, water viscosity was set to 1 mPas, and the medium is strongly water-wet.

The simulations were set up in order to observe an individual pore-filling event in the observation pore. The initial fluid configuration was so that some fluid was already available in the vicinity of the draining pore in the beginning of the simulation (Figure 4.6).
Figure 4.6. Initial configuration for primary drainage case in Geometry 1 where pore-scale events in the observation pore will be investigated.

The inlet velocities for oil ($v_{oil}$) were $5 \times 10^{-4}$ and $1 \times 10^{-3}$ m/s, which results in Darcy velocities of $2.4 \times 10^{-4}$ and $4.8 \times 10^{-4}$ m/s, respectively. Oil viscosity, interfacial tension, Reynolds (Eq. 2.25) and Capillary (Eq. 2.26) numbers are given in Table 4.1. The properties of fluids used for Reynolds and Capillary numbers calculations correspond to that of the invading fluid, which, for primary drainage is oil.

<table>
<thead>
<tr>
<th>Case</th>
<th>$v_{oil}$ (m/s)</th>
<th>$\mu_{oil}$ (mPas)</th>
<th>$\sigma_{ow}$ (N/m)</th>
<th>$Re$</th>
<th>$Ca$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>$5 \times 10^{-4}$</td>
<td>10</td>
<td>0.025</td>
<td>$1.2 \times 10^{-4}$</td>
<td>$1.6 \times 10^{-4}$</td>
</tr>
<tr>
<td>B</td>
<td>$1 \times 10^{-3}$</td>
<td>10</td>
<td>0.025</td>
<td>$2.4 \times 10^{-4}$</td>
<td>$3.2 \times 10^{-4}$</td>
</tr>
<tr>
<td>C</td>
<td>$5 \times 10^{-4}$</td>
<td>1</td>
<td>0.025</td>
<td>$1.2 \times 10^{-3}$</td>
<td>$1.6 \times 10^{-5}$</td>
</tr>
<tr>
<td>D</td>
<td>$1 \times 10^{-3}$</td>
<td>1</td>
<td>0.025</td>
<td>$2.4 \times 10^{-3}$</td>
<td>$3.2 \times 10^{-5}$</td>
</tr>
<tr>
<td>E</td>
<td>$5 \times 10^{-4}$</td>
<td>10</td>
<td>0.050</td>
<td>$1.2 \times 10^{-4}$</td>
<td>$8.0 \times 10^{-5}$</td>
</tr>
<tr>
<td>F</td>
<td>$1 \times 10^{-3}$</td>
<td>10</td>
<td>0.050</td>
<td>$2.4 \times 10^{-4}$</td>
<td>$1.6 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

Table 4.1. Reynolds and Capillary numbers for 2-dimensional simulations in Geometry 1.
Figure 4.7. Interfacial velocity for a pore drainage event at different injection rates for the cases with oil viscosity of 10 mPas and interfacial tension of 0.05 N/m.

Figure 4.8. Interfacial velocity for a pore drainage event at different injection rates showing the effect of interfacial tension.
The meniscus velocity was measured by tracking the oil-water interface across the pore body. As per initial fluids configuration, the meniscus will jump from a throat of \(~10 \mu m\) to a large opening of \(100 \mu m\), generating a large energy release.

In Figures Figure 4.7, Figure 4.8 and Figure 4.9, it can be observed that the meniscus acquires a high velocity, as a result of this energy release due to a decrease in curvature when it invades the pore body. Menisci velocities calculated in the simulations are different from the values observed in the experiments mentioned previously (44), because the aspect ratio in the digital porous media is larger and the properties of the fluids and materials are different.

From the simulation results presented, it can be confirmed that injection rate has little or no influence on the interfacial velocity developed during a pore drainage event. However, other parameters such as fluids distribution, aspect ratio, fluid properties (Figure 4.8) and interfacial
tension (Figure 4.9) affect the dynamics of a jump, and consequently, they affect the impact on fluids redistribution and the extent of changes on pressure field due to this pore-scale event.

If we calculate the local Reynolds number for the highest values of interfacial velocities using Eq. 3.3, with the pore body diameter as characteristic length, it is possible to deduct that the inertial forces start to play a role in two-phase flows at a sub-pore scale level whenever a jump occurs. The order of magnitude of Reynolds number at these velocities are as high as 1. If pore-scale simulations are being conducted, it is important to take into account not only capillary and viscous forces, but also inertial effects, as they may not be negligible. This is an advantage of the Volume of Fluid method over other simplified models, such as pore networks.

The rearrangement of fluids distribution and changes in pressure response due to a Haines jump discussed in this section are in agreement with the observations of micromodel experiments mentioned previously (44). These pore scale events were also observed in actual three-dimensional two phase flow experiments registered with micro-CT images (45), (46), and it confirms that the numerical model can properly reproduce this type of pore scale instability. The ability to model a Haines jump has a significant impact on macro-scale properties, as the final configuration of fluids will change.

4.2. Primary Drainage in Geometry 2

Several factors are important in the evaluation of two-phase flows, such as, rock morphology, wettability, fluid properties, and flow conditions, to name a few. In this section, the effect of fluid viscosity on two phase flows during primary drainage is investigated. The main objective of this
analysis is to identify pore scale instabilities and to observe the influence of viscous forces on pore scale events and final fluids distribution.

As geometry 2 has more pores than geometry 1, the primary drainage simulations will allow to observe the extent of the effect of a jump on the saturation and pressure fields. The simulations are performed for different oil viscosities, generating viscosity ratio (Eq. 2.27), Reynolds (Eq. 2.25) and Capillary (Eq. 2.26) numbers according to Table 4.2. The properties of fluids used for Reynolds and Capillary number calculations correspond to that of the invading fluid, which, for primary drainage is oil. Also, according to the definition of viscosity ratio discussed in Chapter 2, the lower the viscosity ratio, the more stable the displacement will be.

<table>
<thead>
<tr>
<th>Case</th>
<th>( \mu_{\text{oil}} ) (mPas)</th>
<th>( M )</th>
<th>( Re )</th>
<th>( Ca )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>( 1 \times 10^{-3} )</td>
<td>( 2 \times 10^{-5} )</td>
</tr>
<tr>
<td>2</td>
<td>10</td>
<td>0.1</td>
<td>( 1 \times 10^{-4} )</td>
<td>( 2 \times 10^{-4} )</td>
</tr>
<tr>
<td>3</td>
<td>50</td>
<td>0.02</td>
<td>( 3 \times 10^{-5} )</td>
<td>( 1 \times 10^{-3} )</td>
</tr>
<tr>
<td>4</td>
<td>100</td>
<td>0.01</td>
<td>( 1 \times 10^{-5} )</td>
<td>( 2 \times 10^{-3} )</td>
</tr>
</tbody>
</table>

Table 4.2. Mobility ratio, Reynolds and Capillary Numbers for 2-dimensional simulations.

As boundary conditions, a fixed flow of oil is defined at the inlet (left side), generating a Darcy velocity of \( 2.5 \times 10^{-4} \) m/s. At the outlet (right side), atmospheric pressure is defined, and the upper and lower walls are defined as no-flow boundaries (Figure 3.12). The density of oil and water were kept the same, 1000 kg/m\(^3\), in order to eliminate gravity effects in this analysis, interfacial tension was set to 0.04 N/m and water viscosity was set to 1 mPas. The medium is strongly water-wet, with a zero contact angle at the walls.

The simulations were evaluated up to oil breakthrough, which allows a visualization of the displacement front and its effects on the amount of trapped phase (water). After breakthrough,
pressure difference decreases as oil connects to the outlet boundary, leaving trapped water at the corners of the geometry.

Figure 4.10 and Figure 4.11 highlight the patterns at breakthrough for the two extreme cases, the lowest viscosity ratio, case 1, and the highest viscosity ratio, case 4. In these figures, the volume fraction field is presented, with red indicating oil. Oil is being injected in the left side of the geometry, following a drainage process in a 100% water saturated water-wet core, which can be confirmed by the curvature of the oil phase in the pores. In this process, water fills the thin pore throats, while oil invades through the largest pore throats and occupies the pore bodies. In both cases, poor connectivity and the presence of some dead end pores lead to by-pass, leaving water trapped in some pore bodies. The final water saturation for case 1 is 0.47, and for case 4 is 0.37.

![Flow pattern at breakthrough for case 1 (1 mPas). In this case it can be observed that large areas are by-passed, leading to a water saturation at breakthrough of 0.47.](image)
Figure 4.11. Flow pattern at breakthrough for case 4 (100 mPas). Oil phase flows into the water-wet rock in a “piston-like” fashion. Water saturation at breakthrough is 0.37 in this case.

The interplay between capillary and viscous forces in porous media leads to distinct flow regimes, depending on the values of Capillary number and viscosity ratio. According to Lenormand *et al.* (47), immiscible displacement may take three different forms depending on the viscosity ratio and Capillary number (Figure 4.12):

1) Capillary fingering: at low Capillary number and negligible viscous forces, the principal force acting in the displacement is due to capillarity;

2) Stable displacement: favorable viscosity ratios, where the principal force is due to the viscosity of the injected fluid;

3) Viscous fingering: tree-like fingers are developed in unfavorable viscosity ratios.
The simulation runs performed in this study are with increasingly favorable viscosity ratios. No viscous fingering is observed, as expected, however, as oil viscosity increases, a transition from capillary fingering to stable displacement occurs. The higher viscosity of the injecting fluid results in a “piston-like displacement”, with more uniform saturation front and smaller cluster sizes than for the lower viscosity oil.

In the capillary fingering regime, oil fingers grow in different directions forming loops that lead to larger by-passed areas, and higher final water saturation. This phenomenon happens because, due to capillarity, the oil stream will deviate from narrow constrictions finding new pathways, as demonstrated in Figure 4.13.
Figure 4.13. Visualization of an oil finger for case 1 (1 mPas), under the capillary fingering flow regime.

Figure 4.14 shows an example of pressure distribution field in a primary drainage for case 4. Due to capillary pressure and wettability of the medium, oil phase has a higher pressure than the water phase. Also, as the oil has high viscosity and the pore throats are small, the pressure drop generated to push oil into this water-wet media is high (several kPa’s). The range of pressure selected in the figures allows to observe more clearly how pressure drops along the oil phase, for a fixed time step.

In addition to that, in Figure 4.14 it is possible to observe three distinct regions: the oil saturated Darcy Zone, the water saturated Darcy Zone and the “Active Jump Zone” in between. The “Darcy Zones” present steady pressure drop corresponding to viscous dissipation in the tortuous media. In these regions, only one phase is moving: a) Darcy Zone (Oil), from 0 to ~0.3 mm, where water is trapped and immobile, and only oil is moving; b) Darcy Zone (Water), from ~0.45 to 0.727 mm, where the oil phase still did not reach and only water is moving.
Figure 4.14. Pressure field during primary drainage of the 100 mPas oil (case 4).

Figure 4.15 shows the pressure drop and saturation profiles in these regions. Due to viscous dissipation, pressure gradually decreases over the length of the sample.

Figure 4.15. Pressure and Saturation behavior for primary drainage (case 4). The saturation in the oil invaded zone varies between 0.05 and 0.25, due to the presence of trapped (immobile) water.
Another region can be identified in the vicinity of the saturation front (dashed square in Figure 4.14), characterized by pressure fluctuations and large local pressure gradients, namely, the “Active Jump Zone”, between ~0.3 and ~0.45 mm. The pressure fluctuations happen due to pore draining events; when an oil meniscus jumps, the pressure in the oil and water phase close to the draining pore falls. This leads to crossflows, interfacial re-arrangements and change in fluids configuration in this zone, and, as a result, Darcy’s law cannot properly describe fluid flow in this region (48).

In order to understand the details of dynamic effects in the “Active Jump Zone”, Figure 4.16 and Figure 4.17 present the simulation results for a drainage event of a large pore body in the lower viscosity case (case 1) and the higher viscosity case (case 4). The white circle indicates the pore body in which a jump will occur in the following time steps.

Figure 4.16. Pore drainage event for lower viscosity (case 1). This event is characterized by a rapid burst of 2 to 3 milliseconds.
Figure 4.17. Pore draining event for higher viscosity (case 4). This event takes a longer time (15 to 16 milliseconds) due to the dampening effect of high viscosity in a Haines jump.

For the lower viscosity case (case 1), the drainage of a pore body is characterized by a rapid burst, and the pore is drained in less than 3 milliseconds. The black arrows in Figure 4.16 indicate imbibition occurring in adjacent pores, as the main pore body is being drained. This is a result of the high interfacial velocity generated by a Haines jump, which results in local flow rates that surpass the total injection flow rate, as discussed in the previous section.

As the viscosity of oil increases, the time required to completely drain the same pore body increases, it takes 5 to 6 milliseconds for case 2, 11 to 12 milliseconds for case 3, and 15 to 16 milliseconds for case 4. This can be explained by the fact that, as viscosity increases, the inertial effects resulted from a Haines jump are damped, leading to a slower interface motion (49). This phenomenon was also observed in the numerical experiments in Geometry 1. Ng et al. (50) indicated that the dimensionless group $\sigma \rho r_b/\mu^2$ dictates bubble dynamics in a jump ($r_b$ corresponds to radius of the pore body), and from the exponents in this equation, it can be observed...
that interface dynamics are very sensitive to viscosity, as compared to other parameters, such as interfacial tension and pore body radius.

As discussed in the previous section, the extent of the effect of a pore drainage event over the adjacent pores is dependent not only on the amount of fluid available in the vicinity, but also the overall topology of the porous media and the transport properties of the fluids. In the lower viscosity cases, drainage of a large pore results in quick withdrawal of fluids from adjacent connections, leading to a wider and more severe pressure drop, as shown in Figure 4.16 and Figure 4.17. As the viscosity increases, a slower withdrawal of fluids from the vicinity is observed, resulting in a smaller radius of influence of the draining event. As a result, as the viscosity increases, there is more incidence of simultaneous invasion into pore bodies closer to the large pore being drained.

4.3. Summary and Conclusions

Drainage processes were simulated in two geometries, and it was possible to observe the effect of capillary and viscous forces on fluids distribution and pressure fields. The most important observation is that Haines jumps will play a significant role on the pressure behavior and final distribution of fluids.

From the results of Geometry 1 simulations, it was possible to observe that the profile of the interfacial velocity during a jump is similar to experimental observations. Through these simulations, it was possible to demonstrate that the Volume of Fluid method in OpenFOAM is able to properly reproduce pore-scale instabilities such as Haines jumps.
The pressure field may be presented in distinct regions, with the Active Jump zone corresponding to the region where steep pressure and saturation gradients are present. The adjacent regions (oil and water regions) have the expected monotonic pressure decline due to viscous dissipation. The magnitude of the change in pressure due to a draining event will depend on the availability and flowing properties of the fluids in adjacent pore throats and bodies. Additionally, the size of the geometry will also influence the effect of this pressure decline on the overall pressure field. An important observation is that increasing viscous forces have a dampening effect on jumps in pore drainage events, as a result, for higher viscosity drainage cases, more jumps will happen simultaneously.
CHAPTER 5. SECONDARY IMBITION SIMULATIONS

The secondary imbibition process involves injecting a wetting phase in a medium, and reducing the non-wetting phase saturation to a residual saturation level.

For all secondary imbibition cases, the two-dimensional pattern Geometry 2 is used (Figure 5.1). Primary drainage simulation was performed previously (51) to establish an initial (immobile) water saturation of 44%.

![Porous volume for 2-dimensional geometry. The image shows the initial condition for volume fraction, with oil as red and water as blue.](image)

Figure 5.1. Porous volume for 2-dimensional geometry. The image shows the initial condition for volume fraction, with oil as red and water as blue.

As discussed in the Chapter 2, once hot fluids are injected, a temperature gradient will be established within the reservoir. Transport properties of fluids are functions of temperature (Figure 5.2), and therefore, this will lead to different flowing conditions. In order to investigate this problem, secondary imbibition numerical experiments were set, simulating flows at three different temperature points: 140°C, 180°C and 220°C. Empirical correlations were used to obtain order of
magnitude values for oil viscosity (18) and density (52). For the water viscosity and density, NIST reference values were used (53).

Figure 5.2. Viscosity of oil and water. The vertical (light grey) dashed lines indicate the temperatures in which the physical properties were taken for the numerical experiments (18), (53).

Figure 5.3. Density of oil and water. The vertical (light grey) dashed lines indicate the temperatures in which the physical properties were taken for the numerical experiments (52), (53).
As boundary conditions, a fixed velocity of water is defined at the inlet (left side), generating Darcy velocities that range from $10^{-4}$ to $10^{-3}$ m/s (Table 5.1). This level of velocity represents the upper range of velocities expected in immiscible displacements, and it will allow observation of important pore-scale events associated dynamic ganglia displacement.

At the outlet (right side), atmospheric pressure is defined, and the upper and lower walls are defined as no-flow boundaries. The interfacial tension between oil and water was set to 0.04 N/m, and a zero contact angle was defined at the solid walls (water-wet) in all simulations. The viscosity ratio ($M$) indicates if the displacement front is more likely to be stable or unstable, and it is calculated according to Eq. 2.27. The Capillary number ($Ca$) gives an indication of the balance between viscous and capillary forces, and it is defined at the micro-scale, using the pore velocity, Eq. 2.26. Secondary imbibition simulations were performed for the cases under the conditions summarized in Table 5.1:

<table>
<thead>
<tr>
<th>Case</th>
<th>Temp. (°C)</th>
<th>Darcy Vel. (m/s)</th>
<th>Pore Vel. (m/s)</th>
<th>Viscosity Ratio</th>
<th>Ca</th>
</tr>
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<tbody>
<tr>
<td>140a</td>
<td>140</td>
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<td>196</td>
<td>$2.1 \times 10^{-6}$</td>
</tr>
<tr>
<td>140c</td>
<td>140</td>
<td>$2.5 \times 10^{-4}$</td>
<td>$8 \times 10^{-4}$</td>
<td></td>
<td>$4.1 \times 10^{-6}$</td>
</tr>
<tr>
<td>140b</td>
<td>140</td>
<td>$10 \times 10^{-4}$</td>
<td>$40 \times 10^{-4}$</td>
<td></td>
<td>$2.1 \times 10^{-5}$</td>
</tr>
<tr>
<td>180a</td>
<td>180</td>
<td>$1 \times 10^{-4}$</td>
<td>$4 \times 10^{-4}$</td>
<td>91</td>
<td>$1.6 \times 10^{-6}$</td>
</tr>
<tr>
<td>180c</td>
<td>180</td>
<td>$2.5 \times 10^{-4}$</td>
<td>$8 \times 10^{-4}$</td>
<td></td>
<td>$3.2 \times 10^{-6}$</td>
</tr>
<tr>
<td>180b</td>
<td>180</td>
<td>$10 \times 10^{-4}$</td>
<td>$40 \times 10^{-4}$</td>
<td></td>
<td>$1.6 \times 10^{-5}$</td>
</tr>
<tr>
<td>220a</td>
<td>220</td>
<td>$1 \times 10^{-4}$</td>
<td>$4 \times 10^{-4}$</td>
<td>58</td>
<td>$1.2 \times 10^{-6}$</td>
</tr>
<tr>
<td>220c</td>
<td>220</td>
<td>$2.5 \times 10^{-4}$</td>
<td>$8 \times 10^{-4}$</td>
<td></td>
<td>$2.4 \times 10^{-6}$</td>
</tr>
<tr>
<td>220b</td>
<td>220</td>
<td>$10 \times 10^{-4}$</td>
<td>$40 \times 10^{-4}$</td>
<td></td>
<td>$1.2 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

Table 5.1. Calculated Viscosity Ratio, Capillary and Reynolds numbers for the numerical experiments.
From the values of viscosity ratio in this table it is possible to conclude that the displacements are highly unstable, and a viscous fingering flow regime is present.

Due to the small scales (order of microns) and high viscosities involved in these simulations, the use of interface compression constant (cAlpha) higher than 1 was needed in order to guarantee interface sharpness. The compression constant used varied from 1 to 4, with the highest value used for the highest viscosity cases (140a, b and c). The pointCellsLeastSquares numerical scheme was used for calculation of the curvature, along with a Courant number of 0.2. This combination of numerical scheme and the use of low values of Courant number were found to provide better accuracy in the calculation of the curvature, as discussed in Chapter 3.

5.1. Secondary Imbibition Results

Table 5.2 summarizes the main results from the simulations. Approximately one pore-volume of water was injected in all runs, although no appreciable additional oil production was observed after breakthrough. Recovery is expressed as %OOIP, and the coding for post-processing is presented in Appendix A.

The most important mechanism that leads to high amounts of trapped oil is viscous fingering, caused by the highly unfavorable viscosity ratios. Also, the 2-dimensional nature of the geometry and the presence of dead end pores contribute to large regions of oil to be by-passed. The pore-volumes injected at breakthrough (PVI\textsubscript{BT}) are very small (< 1), which can be explained by water fingering. The injection of water results in an unstable water/oil displacement front, and water breakthrough occurs quickly, leaving large areas of oil un-swept.
<table>
<thead>
<tr>
<th>Case</th>
<th>At breakthrough</th>
<th>Post-breakthrough</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Time$_{BT}$ (s)</td>
<td>PVI$_{BT}$</td>
</tr>
<tr>
<td>140a</td>
<td>0.425</td>
<td>0.230</td>
</tr>
<tr>
<td>140c</td>
<td>0.151</td>
<td>0.164</td>
</tr>
<tr>
<td>140b</td>
<td>0.084</td>
<td>0.457</td>
</tr>
<tr>
<td>180a</td>
<td>0.505</td>
<td>0.274</td>
</tr>
<tr>
<td>180c</td>
<td>0.163</td>
<td>0.177</td>
</tr>
<tr>
<td>180b</td>
<td>0.043</td>
<td>0.234</td>
</tr>
<tr>
<td>220a</td>
<td>0.425</td>
<td>0.231</td>
</tr>
<tr>
<td>220c</td>
<td>0.146</td>
<td>0.160</td>
</tr>
<tr>
<td>220b</td>
<td>0.031</td>
<td>0.171</td>
</tr>
</tbody>
</table>

Table 5.2. Summary of results indicating recovery, residual saturation, pressure drop and breakthrough time.

As expected, water breakthrough is reached quicker for higher velocity cases (higher injection rates), but for longer times, the cases with lower injection rates resulted in highest ultimate recovery. An exception is observed for the case of higher velocity and highest viscosity ratio (case 140b). This observation suggests that different production mechanisms are involved in heavy oil immiscible displacements, and a detailed discussion about the mechanisms will be given in the following sections.

In terms of pressure response, after breakthrough the pressure drop will depend on the water channel pathway, which can be more tortuous (generating more pressure drop) or less tortuous. This is dependent not only on flow conditions, but also on the size of the geometry and the presence of dead end pores. As it will be discussed in the section “Considerations about the geometry”, the trend observed in pressure response and oil recovery is strongly influenced by the small size of the geometry.
The start of water injection is characterized by a high pressure drop across the sample. Figure 5.4 shows the pressure profile over the length of the sample at different time steps for the simulation at 220°C and velocity of $2.5 \times 10^{-4}$ m/s. As observed, initially the pressure over the length of the sample is high, as oil is being pushed from the inlet to the outlet. This happens because of the high viscous dissipation generated when the higher viscosity oil is displaced across the porous media. This high pressure differential favors mobilization of oil ganglia, resulting in break up and coalescence.

Figure 5.4. Example of pressure profile for simulation at 220°C at $2.5 \times 10^{-4}$ m/s. The pressure over the length of the sample reduces as more water imbibition occurs.

Due to the 2-dimensional nature of the geometry, after water breakthrough appreciable pressure decline is observed, the lower viscosity of the water phase generates less pressure drop due to viscous dissipation. Therefore, water breakthrough is identified when pressure drop reaches a low and constant value (Figure 5.5). At this moment, a high velocity water channel is formed,
connecting the inlet to the outlet, and in the timeframe evaluated in these simulations, no appreciable additional oil production is obtained after that. However, as observed in physical experiments for heavy oil waterflooding (54), (14), (55), for longer simulation times after breakthrough capillary imbibition is expected to happen, generating more oil recovery in the long term. The noisy pressure response is attributed to the presence of pore-scale events (i.e. choke-off and Haines jumps), that generates rapid drainage of individual pores while oil is being pushed by water.

![Graph](image)

Figure 5.5. Example of pressure difference and oil recovery versus time for simulation at 220°C at $2.5 \times 10^{-4}$ m/s. Water breakthrough is distinguished by the low and constant value of pressure and leveling off of oil recovery.

Figure 5.6 shows a zoom of the volume fraction field for a sequence of time steps for the case at 140°C and velocity of $2.5 \times 10^{-4}$ m/s. In these images, the red color represents the oil phase, and blue represents water. The curvature of the oil phase confirms that the medium is water-wet, and water is injected in the left hand side of the geometry.
At the microscopic level, as water invades the geometry, it can be observed that the oil phase breaks into smaller ganglia as a result of a choke-off process. This phenomenon was the main mechanism of ganglia break up observed in the simulations, being present in all levels of flow rates and viscosity ratios.

In Figure 5.6, the choke-off process is indicated by the white arrows in time steps between 120 and 122 milliseconds, and between 128 and 130 milliseconds. Once the ganglion breaks up, the daughter ganglia may remain trapped, if the capillary forces in the appendices of the ganglion are high enough. The stranding of oil ganglion increases as the size of the ganglion decreases. Therefore, large ganglia tend to be mobilized more easily than smaller ganglia. Thus, different ganglion velocities are originated depending on size, which leads to collision and coalescence, an important process in immiscible displacement.

Figure 5.6. Volume fraction field for simulation at 140°C at $2.5 \times 10^{-4}$ m/s. Several pore-scale phenomena may be observed in this sequence of images, such as choke-off (from 120 to 122 milliseconds, and from 128 to 130 milliseconds), Haines-jump (from 122 to 124 milliseconds), and oil blob mobilization (sequence from 130 to 144 milliseconds).
The mobilization of an oil ganglion will depend on the balance between capillary pressure at the ends of the ganglion, which will tend to leave oil trapped, and the flow field that generates an external pressure drop. If the viscous pressure drop generated by the external flow field is sufficient to overcome the capillary forces that keep the ganglion trapped, a critical Capillary number is achieved and the ganglion will be further mobilized, as indicated by the white arrows in Figure 5.6, from time step 130 to 144 milliseconds.

Ganglia motion is characterized by successive jumps, also called ganglion rheon (56), or, as previously discussed, Haines Jump. When a meniscus is located at a pore throat, it rapidly jumps to the next pore body, which represents a lower energy position (lower curvature). As oil jumps to the next available pore body in a drainage process (usually downstream of the ganglion), the upstream appendices are displaced by imbibition, in order to conserve the total volume of the ganglion. This phenomenon happens in a timeframe of the order of milliseconds, as indicated in Figure 5.6, in the sequence from 122 to 124 milliseconds.

When water breakthrough occurs, the external pressure gradient is drastically reduced, which results in little further mobilization of oil ganglia. A movement of fluid interfaces is observed, as the ganglia settles to a more capillary stable position, but little additional recovery is obtained in the timeframe of these simulations.

**5.2. Low Capillary Number: Viscous Fingering vs. Capillary Imbibition**

Figure 5.7 represents the volume fraction field at water breakthrough for cases at 220°C and velocities of $1 \times 10^{-4}$ m/s (220a) and $1 \times 10^{-3}$ m/s (220b), with the main pathways of water
breakthrough highlighted. The pathways in which water will travel through the porous media will be dictated by the topology of the medium and the balance between capillary and viscous forces. For higher flow rate it is observed that the lower part of the geometry is invaded first, and little oil is swept in the upper parts (Figure 5.7-A). At lower flow rate, oil is still pushed to the outlet in the direction of the flow, but some imbibition is observed in the direction perpendicular to the flow, because lower injection rates results in smaller viscous pressure drop and provides more residence time for imbibition to occur (Figure 5.7-B). This phenomenon has been identified as micro-fingering (12) due to capillary imbibition. Therefore, although viscous forces are dominant in immiscible displacements at high viscosity ratio, as the velocity decreases, a higher contribution of capillary forces is observed, which considerably affects the distribution of fluids and oil recovery, as observed in the recovery results from Table 5.2. One consequence of this phenomenon is that the pathway in which water breaks through in lower injection rate cases is completely different from the cases with higher injection rates.

Figure 5.7. High velocity pathways at water breakthrough for cases at 220°C, at velocity of $1 \times 10^{-3}$ m/s in figure A, and at velocity of $1 \times 10^{-4}$ m/s in figure B.
Conventional linear displacement theory dictates that a decrease in residual oil saturation is observed as the Capillary number increases. This can be reflected on the plot of $Ca$ vs. $S_{or}$ for several experiments in the literature (Figure 2.5, in Chapter 2). In immiscible displacements in natural porous media, a $Ca$ number below ~$10^{-6}$ results in a relatively constant residual oil saturation, meaning that for typical $Ca$ numbers applied in conventional oil waterflooding ($10^{-7} – 10^{-6}$), oil recovery is independent of injection flow rate (57). Experimental observations (14), (13), (58) and simulation results reported in this study indicate that the injection rate will have an effect in the case of heavy oil immiscible displacements at low Capillary numbers.

In etched glass micromodel experiments of heavy oil waterflooding reported by Mei et al. (58), the reported results of post-breakthrough oil recovery versus Capillary number using Abrams’s correlation (Eq. 2.28) are presented in Figure 5.8. The plot of incremental recovery versus $Ca$ was not monotonic. This result was attributed to the fact that the oil viscosity used in some of the experiments (from 1.4 to 2,830 mPas) was outside the range of that used by Abrams (25).

Figure 5.8. Incremental Recovery versus Capillary number correlation by Abrams from etched glass micromodel experiments (58).
An attempt to correlate the recovery results from the secondary imbibition simulations performed in this thesis were made (Figure 5.9). The correlation included total oil recovery, which differs from the approach previously discussed (58), in which only post-breakthrough data was used. Nevertheless, a similar trend was observed, in which the result is not monotonic, and the oil recovery is a function of flow rate at low capillary numbers. Although the trend is similar to physical experiments previously reported in the literature, more simulations are required and experimental verification is recommended in order to confirm if this trend is expected for any case of heavy oil immiscible displacements. Additionally, other porous media patterns and sizes would be needed in order to draw definite conclusions, as it will be discussed in the “Considerations about the Geometry” section.

Figure 5.9. Oil recovery (% OOIP) versus Capillary number according to Abrams correlation, results are presented for the simulations performed in this thesis
5.3. High Capillary Number: High Shear Flow

In immiscible displacements at high injection rates, viscous forces are dominant and little influence of capillary imbibition is observed. In the case 140b (which has the highest velocity, $10^{-3}$ m/s, and the highest viscosity ratio evaluated in these simulations), massive oil ganglia break-up, motion and coalescence happen in all regions of the geometry. Due to high viscous dissipation, the displacement of the oil phase generates very high differential pressure, leading to displacement of the oil phase in the form of disconnected oil ganglia. This causes re-arrangement of oil in the upper parts of the geometry. Some water accumulated close to the outlet end in the upper part of the geometry is then produced, meaning that both oil and some water are produced at this stage. This explains the separation between the curves before breakthrough in the plot of pore-volumes injected versus recovery for the high velocity cases in the highest and lowest viscosity ratios (140b and 220b), as shown in Figure 5.10.

Dynamic ganglia movement is observed, which, according to definition by Payatakes (59), results in ganglia invasion through one or more pores simultaneously. This is a result of the fact that local Capillary number exceeds its critical value for ganglia mobilization. In this type of displacement, the frequency of alignment of the ganglion with the direction of the pressure gradient reduces. If narrow constrictions are presented in the direction of flow, the ganglion grows through new patterns that by-pass the region of obstruction. This behavior enhances break-up and lateral dispersion of oil blobs in different directions.
Figure 5.10. Oil recovery versus pore-volumes injected for cases at velocity of $1 \times 10^{-3}$ m/s, and viscosity of 140°C and 220°C.

The sequence in Figure 5.11 indicates how ganglia dispersion occurs. Water is injected from the left side of the geometry. However, due to its high velocity, oil ganglia is mobilized downwards, invading several pores simultaneously. This process generates several daughter ganglia, which results in smaller cluster sizes.

Figure 5.11. Sequence of time steps for the volume fraction field in a region of the geometry for case at velocity of $1 \times 10^{-3}$ m/s and viscosity of 140°C. Oil ganglia moves in a dynamic displacement mode, enhancing ganglia breakup.
As indicated in Figure 5.7, once water breaks through, a high velocity water channel is formed, and the differential pressure drops to a constant and low value. For the case 140b, after water breakthrough, some additional oil production was obtained due to a mechanism of oil stripping as a result of viscous drag. The mechanism of oil stripping was described and investigated by Rallison (60), and it has important implications to porous media flows under high shear.

Figure 5.12 represents a series of time steps in which the process of oil stripping happens. The ganglion indicated by the white arrow at a time step of 112 milliseconds is directly exposed to the high velocity stream of water. This rapid external fluid velocity over the surface of the ganglia requires larger internal pressure gradient to push internal fluid back from the tip to the center of the ganglion. Therefore, the surface tension force has to increase near the ends of the ganglion, in order to increase internal pressure gradient. This results in a decrease of radius near its ends. To conserve volume, the length of the ganglion increases, which exposes its tip to even higher velocities. At this moment, small blobs are stripped out. This sequence is shown in Figure 5.12, from time step 112 milliseconds to 119 milliseconds.

Once smaller blobs are stripped from the mother ganglion, they will be mobilized further until they get stranded. This may result in blockage and pressure build, and consequent re-mobilization of oil ganglia upstream of the blob, as observed in Figure 5.12, from time step 120 milliseconds to 130 milliseconds.

Finally, the effect of this fluid redistribution on the pressure response can be observed in the plot of pressure versus time, in Figure 5.13. It is observed that a time interval at low pressure (between ~0.075 to 0.11 seconds) is followed by a series of pressure spikes, which happen when the small blobs generated by the stripping of oil blocks pathways and induces additional oil mobilization.
This phenomena results in additional oil recovery, but it may also result in the formation of stable emulsions that may block pathways and leave oil trapped.

Figure 5.12. Sequence of oil stripping and re-mobilization after breakthrough for the case at velocity of $1 \times 10^{-3}$ m/s and viscosity of 140°C (140b).

Figure 5.13. Pressure behavior for the case at velocity of $1 \times 10^{-3}$ m/s and viscosity of 140°C (140b).
For the case 220b, the initial stages before breakthrough resulted in significant deformation of oil blobs before it broke up into smaller ganglia. Lower viscosity fluids can withstand more deformation before it actually breaks up. Although some choke-off is observed in the upper part of the geometry, most of the displacement happens in its lower part (least resistance pathway). The overall pressure drop is smaller than for the case 140b, due to the lower viscosity of oil. Therefore, oil is basically pushed from the inlet to the outlet through the least resistance path, with little dynamic ganglia movement in the upper parts. Once water breakthrough happens, a large area is by-passed, leading to very poor sweep efficiency. The high velocity pathway is located in the lower part of the geometry, where most oil has been swept, therefore, ganglia is not directly exposed to the high velocity stream, resulting in no oil stripping.

![Case 140b](image1.png) ![Case 220b](image2.png)

Figure 5.14. Final residual oil distribution for cases at velocity of $1 \times 10^{-3}$ m/s, and viscosity of 140°C (140b) and 220°C (220b).

In Figure 5.14, the final residual oil distribution for cases 140b and 220b is shown. In case 220b, a large area of oil is by-passed in the upper part of the geometry, leading to a higher residual oil saturation. A quantification of the area of each ganglia versus its corresponding fraction of the
final residual oil is presented in Figure 5.15. Note that ganglia area is computed instead of ganglia volume due to the 2-dimensional nature of the problem. In this figure it can be observed that the area of ganglia is overall smaller for the case 140b, meaning that more ganglia breakup happened. Also, it can be observed in case 220b two large oil ganglia, which basically represents a large unswept area. This large area was by-passed as a result of viscous fingering and early breakthrough, and it is still at irreducible water saturation. This analysis indicates the strong influence of viscosity ratios on cluster size distribution in immiscible displacements.

![Figure 5.15. Fraction of the final residual oil saturation versus the area of ganglia for cases at velocity of $1 \times 10^{-3}$ m/s, and viscosity of 140°C (140b) and 220°C (220b).](image)

5.4. Considerations about the geometry

For the lower velocity cases, it can be observed that the runs at 180°C present the highest recovery (Table 5.2). This result is counter-intuitive, in the sense that it is expected for the same velocity,
that oil recovery would be inversely proportional to viscosity ratio. In an attempt to investigate further this observation, another run was performed at a velocity of $2 \times 10^{-4}$ m/s (Figure 5.16). Although oil recovery does not present the expected trend for variation of oil recovery with viscosity ratio, it can be observed that the simulation results are consistent for different velocities, meaning that the results are not random.

As discussed previously, lower injection rates will allow more capillary imbibition to take place, which results in different pathways for imbibition. In a sufficiently large geometry, capillary fingers will develop in different directions, and the effect of this phenomenon on oil phase bypassing will be more representative if more pores are available to allow a visualization of macroscopic effects. Therefore, although important pore-scale features were identified in these
simulation runs, the geometry may not have enough pores to be a representative elementary volume to allow to extract substantial quantitative macroscopic results in these flows.

Other geometric factors that are relevant on the immiscible displacement simulations are the 2-dimensional nature of the geometry and the presence of dead end regions. By using this geometry for the simulations, an attempt is made to reproduce complex features of natural porous media, which allows more realistic reproduction of pore-scale events. The 2-dimensional characteristic of the geometry, however, considerably limits the possible pathways for flow. In addition to that, the presence of regions of poor connectivity creates preferred (least resistance) pathways, and, as discussed previously, the interplay between flowing conditions and rock topology will have a significant impact on the pathways that water will imbibe in the porous media. It is important to highlight that 2-dimensional simulations are extremely useful in the sense that it allows for visualization of physics in a much clearer way than 3-dimensional simulations, and the computational demands are substantially lower in the 2-dimensional runs. This reinforces the statement that 2-dimensional runs are more adequate for qualitative evaluations.

Although the initial water saturation used was constant in all simulation cases, different levels of initial water saturation will also play a role on the pathways for water imbibition, because as water imbibes in the medium, the isolated water clusters become connected.

In regards to the wetting behavior of the fluid, although the meshing used was not sufficiently small to resolve the wetting film on the solid walls, the definition of the contact angle allowed that oil ganglia motion behaved as if a lubricating film were present. On the other hand, snap-off of oil phase by water films was partially suppressed due to the poor resolution of the wetting layer at the solid boundaries.
For the case of 2-dimensional micromodels, this issue can be solved by simulating it as a 3-dimensional domain, with angular edges that would allow water to flow continuously through the corners. Another possibility is to properly represent the wetting layer by applying local grid refinement at the solid walls (34). This approach may result in a prohibitively large number of cells, especially in more complicated geometries and presence of surface roughness, and therefore it should be applied preferably when the wettability is very good and the role of wetting films becomes significant.

5.5. Summary and Conclusions

Secondary imbibition processes were simulated in 2-dimensional geometry with varying viscosity ratios and injection rates, and it was possible to observe the interplay between viscous and capillary forces, and the influence of rock topology in heavy oil immiscible displacements. The simulations were able to reproduce important features from heavy oil hot waterflooding observed in natural porous media, such as: 1. early breakthrough due to water fingering; 2. capillary imbibition in displacements at low $Ca$ number; 3. Water channeling and oil stripping.

Based on the results from the simulations, the following conclusions can be observed:

- Although viscous forces are dominant at high viscosity ratios, water imbibition will play a significant role on heavy oil/water two phase flows at low Capillary numbers. In the case of steam-assisted oil recovery (steamflooding, cyclic steam injection, etc.), the imbibition mechanism in the heated two phase zone may contribute to oil production.

- The influence of injection rates in heavy oil two-phase flow is important at a wider range of Capillary numbers, and the mechanisms of oil recovery in heavy oil immiscible displacements are
different from conventional oil, especially in regards to unstable displacement fronts leading to early breakthrough.

- High viscosity combined with high injection rates will promote massive ganglia mobilization and breakup, due to the increased pressure drop generated by viscous dissipation.

- When an oil ganglia is exposed to a high velocity stream of water, oil stripping may occur, which can block throats downstream the mother ganglia and generate additional oil mobilization. Further study is needed to evaluate the effect that viscous blobs in shear flows will have on in-situ formation of emulsions.

- At the micro-scale, it was possible to observe the mechanisms of ganglia motion, break-up and coalescence. The main mechanism of ganglia break-up was choke-off, although a better representation of the wetting film is needed in order to evaluate the effect of snap-off in these flows.

- The complex topology of the digital porous media allowed to identify important pore-scale events in the simulations. However, the geometry may not be a representative elementary volume, which explains the trends observed in the macroscopic parameters calculated.
CHAPTER 6. CONCLUSIONS AND FUTURE WORK

6.1. Final Conclusions

In this thesis, two-phase flow simulations at pore-scale were performed for primary drainage and secondary imbibition processes. This research demonstrated that the Volume of Fluid method is a powerful tool for properly reproducing fluid flow at the pore-scale.

The findings in this thesis collaborate towards the ultimate goal of the workflow of digital rock physics, which is to obtain macro-scale properties, such as relative permeability curves, from a reliable representation of a porous rock. The methodology used in this thesis for computation of two-phase flows at pore-scale has a great potential, especially if associated with additional physics. The results from the simulations provided important insights on the physics of two-phase flows and the main recovery mechanisms observed in thermal recovery processes using steam or hot water. The following conclusions can be drawn from the results presented:

1. The optimized numerical setup implemented in the interFOAM solver in OpenFOAM successfully minimized spurious currents and numerical diffusion problems, improving the accuracy of the computation of curvature and calculation of capillary pressure. The main approach for improvement of numerical stability and accuracy is the use of smoothing of the volume fraction field and a compression factor cAlpha for better interface sharpness. The optimum level of these parameters were determined by verifying the simulation results against analytical solutions, and the capillary pressure computed presented an error of $< -5\%$, which is considered acceptable.
2. Porous media patterns can be meshed and imported to OpenFOAM, which allows simulations of single and two-phase flow in more realistic geometries. Steady-state single-phase flow simulations were performed using SimpleFOAM solver in OpenFOAM, and preliminary results such as absolute permeability and anisotropy were obtained.

3. Primary drainage simulations in Geometry 1 allowed to observe how pore-scale instabilities affect interfacial velocity. The behavior of oil-water interface during a Haines jump in the simulations were similar to experimental observations, which confirms that the model can properly reproduce this kind of pore-scale phenomena. In Geometry 2, it was possible to observe how the overall pressure response is influenced by individual pore-scale events, and how viscosity ratio may have a dampening effect on a Haines jump. In addition to that, it was observed that an increase in oil viscosity (decrease in viscosity ratio, as it was defined in this thesis) results in a transition from capillary fingering to stable displacements in porous media, which affects fluids configuration and initial water saturation in primary drainage simulations.

4. As demonstrated in the “Definition of the Problem” section, at a pore-scale, the gradient of temperature and viscosity for the length scales evaluated in this thesis are negligible. Therefore, isothermal two-phase flow simulations mimicking conditions of thermal processes in a geometry with dimensions in the order of micrometers allowed to observe how different flowing conditions affect the occurrence of pore-scale events, such as Haines jumps, oil ganglia mobilization, oil stripping and capillary imbibition. The main mechanisms of heavy oil recovery observed in physical experiments were reproduced in the simulations, such as, unstable displacement leading to early breakthrough, water
fingering, spontaneous imbibition in flows at low Capillary number, additional oil recovery due to oil stripping.

6.2. Recommendations for Future Work

The main objectives of the thesis were achieved. However, additional studies are needed in order to improve the existing model and extend it to different applications. The following recommendations are made for future research:

1. Different porous media patterns and sizes need to be investigated, in order to determine the elementary volume that would be representative of a natural porous media under two-phase flow conditions. As observed in the simulations, the topology of the porous media is a critical parameter that determines the pathways in which oil and water will travel during immiscible displacements. Additionally, the concept of representative elementary volume will also depend on the topology. Different porous media patterns may need different sizes in order to properly provide averaged quantitative results relevant to macro-scale. Although the model was able to properly reproduce two-phase flow features observed in physical experiments, a larger number of pores is recommended for a proper quantitative evaluation of macro-scale properties.

2. This work is being extended to 3-dimensional porous media, therefore, calculation of macroscopic properties from pore-scale simulations and a verification of the results with physical experiment is highly recommended. For relative permeability curves calculation, it is recommended to run both transient and steady state two-phase flow numerical experiments, which can be used to match with experimental results. Different methods may
be used to calculate relative permeability from pore-scale simulations, the Johnson-Bossler-Naumann (JBN) method (61), the calculation from upscaling of sub-pore-scale forces (62), etc. An evaluation of which method will provide a better workflow for obtaining macro-scale properties needs to be performed.

3. Different models need to be tested in order to improve numerical stability. A hybrid method that combines Volume of Fluid and Level-Set methods would be an interesting field of research, because it has the advantage of mass conservation from Volume of Fluid method, added to a better interface sharpness from Level-set method. In addition to that, other models or smoothing techniques should be tested in order to reduce more the magnitude of spurious currents.

4. As 2-dimensional patterns enable a better visualization of pore scale physics, it is recommended that other solvers with additional physics combined with two-phase flows are used with this geometry. An example is compressibleInterFOAM, which adds compressibility and the energy governing equation to be able to compute temperature fields. In this case, simulations in which a transient of the temperature field is present can be performed, or simulations involving compressible fluids. The multiphaseInterFOAM solver allows to use more than two phases, which is useful for forced-gravity-drainage flows, for example. Finally, the interMixingFOAM, which adds the mass transfer governing equation, is useful in the evaluation of diffusion associated with two-phase flows (solvent diffusion in heavy oil, or surfactant flooding, for example).
REFERENCES


APPENDIX A. POST-PROCESSING SECONDARY IMIBITION DATA

First, a brief explanation of the equations used for post-processing the secondary imbibition is given. The microscopic velocity relates to the macroscopic velocity \( \mathbf{v}_{\text{Darcy}} \) by the following relationship: 
\[
\mathbf{v}_{\text{Darcy}} = \mathbf{v} \phi.
\]
The microscopic velocity \( \mathbf{v} \) is the average velocity over all cells of the domain. Therefore, we have that:
\[
\mathbf{v}_{\text{Darcy}} = \frac{\sum \mathbf{v} PV}{\sum PV} \frac{\sum PV}{BV} \tag{Eq. A-1}
\]
Where the term \( BV \) corresponds to the Bulk Volume of the sample, \( BV = dx dy dz \). The macroscopic velocity then will be:
\[
\mathbf{v}_{\text{Darcy}} = \frac{\sum \mathbf{v} PV}{dx dy dz} \tag{Eq. A-2}
\]
As \( q = \mathbf{v}_{\text{Darcy}} \cdot A \), and \( A \) corresponds to the cross-sectional area, which is \( A = dy dz \), the flow rate can be calculated from the average velocity:
\[
q = \mathbf{v}_{\text{Darcy}} \cdot A = \frac{\sum \mathbf{v} PV}{dx dy dz} \cdot dy dz = \frac{\sum \mathbf{v} PV}{dx} \tag{Eq. A-3}
\]
This equation was written in the code to calculate flow rate, which, when multiplied by the volume fraction, can give the flow rate of each phase. The complete code for post-processing secondary imbibition data is given below. It is a coded function-object, and it is saved in the controlDict file. To execute, use the command `execFlowFunctionObjects -noFlow > log`, the data will be saved in a log file which can be exported using foamLog.
flow_calc
{
    functionObjectLibs ("libutilityFunctionObjects.so");
    type coded;
    redirectType flow_calc; // Name of on-the-fly generated functionObject
    outputControl outputTime;
    code
    #{
        // Reading fields
        Info<< "Looking up fields\n" << endl;
        const volVectorField& U = mesh().lookupObject<volVectorField>("U");
        const volScalarField& alpha1 = mesh().lookupObject<volScalarField>("alpha.water");
        dimensionedScalar rho1("rho1", dimensionSet(1, -3, 0, 0, 0, 0, 0), 926); // enter density of water
        dimensionedScalar rho2("rho2", dimensionSet(1, -3, 0, 0, 0, 0, 0), 914); // enter density of oil
        volScalarField Ux1 ("Ux1", alpha1*U.component(0));
        volScalarField Ux2 ("Ux2", (scalar(1)-alpha1)*U.component(0));
        volScalarField Ux ("Ux", U.component(0));

        // fractional flow of water
        dimensionedScalar f_1("f_1", dimensionSet(0, 0, 0, 0, 0, 0, 0), pTraits<scalar>::zero);
        f_1 = fvc::domainIntegrate(Ux*alpha1)/fvc::domainIntegrate(Ux);
        Info << "f_1 = " << f_1.value() << "m" << endl;

        // total volume over all cells
        dimensionedScalar vol("vol", dimVol, pTraits<scalar>::zero);
        dimensionedScalar one("one", dimVol, 1);
        vol = gSum(mesh().V())*one;
        Info << "vol = " << vol.value() << "m3" << endl;

        // average pore velocity of water
        dimensionedScalar Uavg1("Uavg1", dimensionSet(0, 1, -1, 0, 0, 0, 0), pTraits<scalar>::zero);
        Uavg1 = fvc::domainIntegrate(Ux1)/vol;
        Info << "Uavg1 = " << Uavg1.value() << "m/s" << endl;

        // average pore velocity of oil
        dimensionedScalar Uavg2("Uavg2", dimensionSet(0, 1, -1, 0, 0, 0, 0), pTraits<scalar>::zero);
        Uavg2 = fvc::domainIntegrate(Ux2)/vol;
        Info << "Uavg2 = " << Uavg2.value() << "m/s" << endl;

        // average pore velocity
        dimensionedScalar Uavg("Uavg", dimensionSet(0, 1, -1, 0, 0, 0, 0), pTraits<scalar>::zero);
        Uavg = fvc::domainIntegrate(Ux)/vol;
        Info << "Uavg = " << Uavg.value() << "m/s" << endl;

        dimensionedScalar dx("dx", dimLength, 0.000727); // enter distance in direction of flow

        // water flow rate
        dimensionedScalar q_1("q_1", dimensionSet(0, 3, -1, 0, 0, 0, 0), pTraits<scalar>::zero);
    }
}
q_1 = (Uavg1*vol/dx);
Info << "q_1 = " << q_1.value() << " m3/s" << endl;

// oil flow rate
dimensionedScalar q_2("q_2", dimensionSet(0, 3, -1, 0, 0, 0), pTraits<scalar>::zero);
q_2 = (Uavg2*vol/dx);
Info << "q_2 = " << q_2.value() << " m3/s" << endl;

// volume occupied by oil phase
dimensionedScalar alpha_2("alpha_2", dimensionSet(0, 3, 0, 0, 0, 0, 0), pTraits<scalar>::zero);
alpha_2 = fvc::domainIntegrate((scalar(1) - alpha1));
Info << "alpha_2 = " << alpha_2.value() << " Pa" << endl;

// volume occupied by water phase
dimensionedScalar alpha_1("alpha_1", dimensionSet(0, 3, 0, 0, 0, 0, 0), pTraits<scalar>::zero);
alpha_1 = fvc::domainIntegrate(alpha1);
Info << "alpha_1 = " << alpha_1.value() << " Pa" << endl;

// saturation of water phase
dimensionedScalar sw_1("sw_1", dimensionSet(0, 0, 0, 0, 0, 0, 0), pTraits<scalar>::zero);
sw_1 = alpha_1/vol;
Info << "sw_1 = " << sw_1.value() << " " << endl;

// mass flow rate of water
dimensionedScalar qm_1("qm_1", dimensionSet(1, 0, -1, 0, 0, 0, 0), pTraits<scalar>::zero);
qm_1 = q_1*rho1;
Info << "qm_1 = " << qm_1.value() << " " << endl;

// mass flow rate of oil
dimensionedScalar qm_2("qm_2", dimensionSet(1, 0, -1, 0, 0, 0, 0), pTraits<scalar>::zero);
qm_2 = q_2*rho2;
Info << "qm_2 = " << qm_2.value() << " " << endl;

// total mass flow rate
dimensionedScalar qm_t("qm_t", dimensionSet(1, 0, -1, 0, 0, 0, 0), pTraits<scalar>::zero);
qm_t = qm_1+qm_2;
Info << "qm_t = " << qm_t.value() << " " << endl;

// total inlet volumetric flow rate
dimensionedScalar qv_1("qv_1", dimensionSet(0, 3, -1, 0, 0, 0, 0), pTraits<scalar>::zero);
qv_1 = qm_t/rho1;
Info << "qv_1 = " << qv_1.value() << " " << endl;

#};