Modelling single and two-phase flow on micro-CT images of rock samples

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Declaration

This thesis has been entirely composed by the author and has not been accepted in any previous application for a degree. The work has been undertaken by the author and all sources of information have been specifically acknowledged.

Michele Starnoni
Abstract

In this Thesis, numerical simulations of single and two-phase pore-scale flow on three-dimensional images obtained from micro-CT scanning of different reservoir rocks are presented.

For single-phase flow, the petrophysical properties of rocks, namely Representative Elementary Volume (REV), mean pore and grain size, and absolute permeability, are calculated using an integrated approach comprising image processing, statistical correlation and numerical simulations. Two rock formations, one carbonate and one sandstone, are used throughout this Thesis. It is shown that REV and mean pore and grain size are effectively estimated using the two-point spatial correlation function. A comparison of different absolute permeability estimates is also presented, showing a good agreement between the numerical value and the experimentally determined one for the carbonate sample, but a huge discrepancy for the sandstone.

For two-phase flow, the Volume-of-fluid method is used to track the interfaces. The surface tension forces are modelled using a filtered sharp formulation, and the Stokes equations are solved using the PISO algorithm. A study on the snap-off mechanism, investigating the role of several parameters including contact angle and viscosity ratio, is presented. Results show that the threshold contact angle for snap-off increases from a value of 28° for a circular cross-section to 30-34° for a square cross-section and up to 40° for a triangular one. For a throat of square cross-section, increasing the viscosity of the injected phase results in a drop in the threshold contact angle from a value of 30° when \( \mu = 1 \) to 26° when \( \mu = 10 \) and down to 24° when \( \mu = 20 \), where \( \mu \) is the viscosity ratio.

Finally, a rigorous spatial averaging procedure is presented, leading to a novel definition of the macroscopic capillary pressure. Simulations results of drainage on the scanned images of the rock samples are used to compare different estimates of the macroscopic capillary pressure. The comparison reveals that, contrary to what is commonly done following the traditional approach, use of surface average for the pressures is more appropriate than that of volume average, when averaging the microscopic balance equations relevant for pore-scale two-phase flows in porous media.
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List of Symbols

Abbreviations

CB  Cayton Bay
CFD  Computational Fluid Dynamics
CLSVOF  Coupled Level-Set Volume-of-Fluid
$CO_2$  Carbon Dioxide
CSF  Continuous Surface Force
FD  Finite Difference
FE  Finite Element
FSF  Filtered Surface Force
FV  Finite Volume
KC  Kozeny-Carman
LBM  Lattice Boltzmann Method
LS  Level-Set
$\mu$-CT  micro-Computed Tomography
MD  Molecular Dynamics
NCI  Normalized Continuity Imbalance
NS  Navier-Stokes
SIMPLE  Semi-Implicit Method for Pressure-Linked Equations
PISO  Pressure-Implicit with Splitting of Operators
PLIC  Piecewise Linear Interface Calculation
REA  Representative Elementary Area
REBMB Relative Error in the Bulk Momentum Balance
REV  Representative Elementary Volume
SEM  Scanning Electron Microscope
SIMPLEC  SIMPLE Consistent
SIMPLER  SIMPLE Revised
SPH  Smoothed Particle Hydrodynamics
VOF  Volume-of-Fluid

**Greek symbols**

\( \alpha \)  VOF indicator function
\( \hat{\alpha} \)  Sharpened VOF indicator function
\( \tilde{\alpha} \)  Smoothed VOF indicator function
\( \beta \)  Interface intercept in the PLIC algorithm
\( \beta' \)  Interface intercept in the PLIC algorithm after transformation to the standard configuration
\( \gamma_\alpha \)  Distribution function for phase \( \alpha \)
\( \delta_s \)  Dirac delta function associated with the general surface \( s \)
\( \Delta t \)  Time step
\( \Delta t_{bkz} \)  Critical time step for interfacial flow problems
\( \Delta V_f \)  Truncated volume moving through face \( f \)
\( \Delta x \)  Size of the elementary element in a structured grid
\( \epsilon \)  Some given small number, usually in the order of \( 10^{-8} \)
\( \epsilon_k \)  Error in the curvature in the two-phase benchmark tests
\( \epsilon_m \)  Error in the bulk momentum balance
<table>
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<th>Definition</th>
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<tr>
<td>$\bar{\epsilon}$</td>
<td>Average error in the interface tracking algorithm test</td>
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<td>$\epsilon_{mc}$</td>
<td>Error in mass conservation in the two-phase benchmark tests</td>
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<td>$\epsilon_v$</td>
<td>Error in the average interface velocity in the dynamic pipe test</td>
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<tr>
<td>$\eta$</td>
<td>Non-negative material coefficient accounting for dynamic effects in eq. (3.83)</td>
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<tr>
<td>$\theta$</td>
<td>Static contact angle measured between the wall and the wetting phase</td>
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<tr>
<td>$\lambda_s$</td>
<td>Vector accounting for all the tensions on the surface other than the adjacent fluids pressures in the generalized Young-Laplace equation, eq. (3.62)</td>
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<tr>
<td>$\Lambda_s$</td>
<td>Vector accounting for all the macroscopic effects other than the interface average mean curvature in the macroscopic capillary pressure definition, eq. (3.89)</td>
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<tr>
<td>$\mu$</td>
<td>Viscosity</td>
</tr>
<tr>
<td>$\overline{\mu}$</td>
<td>Viscosity ratio</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Anisotropy ratio</td>
</tr>
<tr>
<td>$\xi$</td>
<td>Binary indicator function</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density</td>
</tr>
<tr>
<td>$\rho_s$</td>
<td>Surface density</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Interfacial tension</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Viscous stress tensor</td>
</tr>
<tr>
<td>$\tau_s$</td>
<td>Surface viscous stress tensor</td>
</tr>
<tr>
<td>$\phi$</td>
<td>Porosity</td>
</tr>
<tr>
<td>$\phi_\alpha$</td>
<td>Volume fraction of phase $\alpha$</td>
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<td>$\Phi_s$</td>
<td>Capillary field</td>
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<tr>
<td>$\Phi_{s,filt}$</td>
<td>Filtered capillary field</td>
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<tr>
<td>$\Phi_{s,f}$</td>
<td>Capillary field at a cell-face</td>
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<tr>
<td>$\Phi_{s,filt}$</td>
<td>Filtered capillary field at a cell-face</td>
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</table>
\(\Phi_{s,f,\text{threshold}}\) Threshold capillary field at a cell-face

\(\chi\) Constant depending on the dimensions of the digital image

\(\psi\) General microscopic quantity

\(\psi_\alpha\) General microscopic quantity associated with phase \(\alpha\)

\(\tilde{\psi}_\alpha\) Spatial deviation of \(\psi_\alpha\)

\(\langle \psi_\alpha \rangle^\alpha\) Intrinsic average of \(\psi_\alpha\)

\(\langle \psi_\alpha \rangle\) Superficial average of \(\psi_\alpha\)

\(\psi_s\) General microscopic quantity defined on a surface

\(\psi_{\alpha\beta}\) General microscopic quantity associated with the surface \(\alpha\beta\)

\(\tilde{\psi}_{\alpha\beta}\) Spatial deviation of \(\psi_{\alpha\beta}\)

\(\langle \psi_{\alpha\beta} \rangle^\alpha\beta\) Intrinsic surface average of \(\psi_{\alpha\beta}\)

\(\overline{\psi}_{\alpha\beta}\) Superficial surface average of \(\psi_{\alpha\beta}\)

\(\omega_p\) Under-relaxation factor for pressure in the SIMPLE algorithm

\(\omega_u\) Under-relaxation factor for velocity in the SIMPLE algorithm

**Operators, dimensionless groups and special functions**

\(AR\) Aspect ratio

\(Ca\) Capillary number

\(CC\) Convergence criterion for the SIMPLE algorithm

\(CR\) Contraction ratio

\(\delta_{sf}\) Discretized delta function at a cell-face

\(F_\delta(\delta_{sf})\) function restricting the validity of the filtering kernels to the interface region

\(H(x)\) Heaviside step function

\([[]]_\alpha\) Jump condition across the interface

\([[]]_f\) Linear interpolation between nodes adjacent to face \(f\)
Re Reynolds number

$RSD_v$ Relative Standard Deviation of the average interface velocity in the dynamic pipe test

$T(u_i)$ Discretized viscous stress tensor

$Z_2$ Two-point correlation function

$\bar{Z}_2$ Discrete two-point correlation function

**Roman symbols**

$\ell, m, n$ Set of orthogonal unit vectors defining a surface $S$

$a_{\alpha\beta}$ Area of the surface between two phases $\alpha$ and $\beta$

$\hat{a}_{\alpha\beta}$ Specific area of the surface between two phases $\alpha$ and $\beta$

$a_C$ Central coefficient in the discretized momentum equations

$a_{nb}$ Neighbor coefficient in the discretized momentum equations

$a'_C$ Central coefficient in the pressure-correction equations

$a'_{nb}$ Neighbor coefficient in the pressure-correction equation

$A$ Helmholtz free energy per unit mass

$A_s$ Surface Helmholtz free energy per unit mass

$\overline{A}$ Total Helmholtz free energy

$\overline{A}_s$ Total Surface Helmholtz free energy

$b$ Source term in the general conservation equation for a bulk phase, eq. (3.35)

$b_s$ Source term in the general conservation equation for a surface, eq. (3.36)

$b_{i,C}$ r.h.s in the $i$-th component of the discretized momentum equations

$b'_{C}$ r.h.s in the first pressure-correction equation in the SIMPLE/PISO algorithm, also called the continuity imbalance

$C_j$ Constants used for filtering surface tension forces ($j = 1, \ldots, 5$)(values given in Tab. 5.1)
\(c_j\) Sides of the control volume \((j = x, y, z)\)

\(C_\sigma\) Constant for determining the magnitude of the spurious velocities

\(C_t\) Constant for determining the time step

\(\tilde{C}_p\) Constant depending on the cross-section of the pore

\(\tilde{C}_t\) Constant depending on the cross-section of the throat

\(d_\alpha\) Characteristic length scale of phase \(\alpha\)

\(D_p\) Form drag

\(D_v\) Viscous drag

\(E\) Internal energy per unit mass

\(e\) External supply of entropy

\(E_s\) Surface internal energy per unit mass

\(e_s\) Surface external supply of entropy

\(F\) Formation factor

\(f_s\) Surface tension force

\(f_{s,f}\) Surface tension force at a cell-face

\(f_{s,f,filt}\) Filtered surface tension force at a cell-face

\(f_{s,f,filt//}\) Time-dependent term for filtering surface tension forces

\(g\) Acceleration of gravity

\(h\) External supply of energy

\(i\) Flux term in the general conservation equation for a bulk phase, eq. (3.35)

\(i_s\) Flux term in the general conservation equation for a surface, eq. (3.36)

\(I\) Identity tensor

\(I^s\) Surficial identity tensor defined by eq. (3.4)

\(j\) Entropy flux
\(j_s\) Surface entropy flux

\(k\) Interface mean curvature

\(K\) Absolute permeability

\(\tilde{k}\) Smoothed interface mean curvature

\(k_f\) Interface mean curvature at a cell-face

\(L_t\) Length of the throat

\(m_1, m_2\) Constants in the Kozeny-Carman relationship

\(N\) Number of voxels in each direction

\(n_{\alpha\beta}\) Unit normal to the surface \(\alpha\beta\) pointing from phase \(\alpha\) to phase \(\beta\)

\(n\) Interface unit normal (in the PLIC algorithm pointing outwards from fluid 1)

\(n_f\) Interface unit normal at a cell-face used for filtering capillary forces

\(n'\) Interface unit normal in the PLIC algorithm after transformation to the standard configuration

\(n_w\) Unit normal to the wall pointing outwards the wall

\(n_s\) Number of smoothing iterations

\(n|_w\) Interface unit normal evaluated at the wall

\(p\) Pressure

\(p_c\) Capillary pressure

\(p^*\) First pressure field computed in the SIMPLE/PISO algorithm

\(p^{**}\) Second pressure field computed in the PISO algorithm

\(p_n\) Pressure of the non-wetting phase on its side of the interface

\(p'\) First pressure correction in the SIMPLE/PISO algorithm

\(p''\) Second pressure correction in the PISO algorithm

\(p_s\) Pressure due to surface tension forces
\( p_w \) Pressure of the wetting phase on its side of the interface

\( q \) Heat flux

\( Q \) Flow rate

\( q_s \) Surface heat flux

\( r_c \) Effective pore size

\( R_p \) Pore radius

\( R_t \) Throat radius

\( \tilde{R}_p \) Radius of the largest inscribed circle at the pore

\( \tilde{R}_t \) Radius of the largest inscribed circle at the throat

\( R_{zt} \) Longitudinal radius of curvature of the throat

\( R_{zp} \) Longitudinal radius of curvature of the pore

\( s \) Specific pore-grain surface area

\( s_\alpha \) Saturation of phase \( \alpha \)

\( S \) Internal entropy per unit mass

\( S_s \) Surface internal entropy per unit mass

\( S_f \) outward vector area of face \( f \)

\( s_w \) Vector lying in the wall and normal to the contact line

\( T \) Temperature

\( t \) Time

\( t \) Stress tensor

\( t_s \) Surface stress tensor

\( u = (u,v,w) \) Velocity

\( u_f \) Velocity component at the cell-face which is normal to the face

\( u' \) First velocity correction in the SIMPLE/PISO algorithm
Second velocity correction in the PISO algorithm

First velocity field computed in the SIMPLE/PISO algorithm

Second velocity field computed in the SIMPLE/PISO algorithm

Third velocity field computed in the PISO algorithm

Surface velocity

Control volume

Volume of fluid 1 contained within the control volume, also called truncated volume

Speed of displacement of the surface defined by eq. (3.12)

Magnitude of the spurious velocities

Velocity on the boundary curve C

Weight in the weighted interpolation method

Boundary area of the control volume V

External boundary pore area of the control volume V

Internal pore-grain interfacial area within the control volume V

General curve bounding the surface S

Pseudo-pressure in the PLIC-VOF solution algorithm

Macroscopic thermodynamic pressure of phase α

Macroscopic capillary pressure

General surface

Averaging volume

Portion of averaging volume occupied by phase α
Chapter 1

Introduction

1.1 Project background

Fluid flow in porous media is encountered in many practical engineering problems, including oil, water, and gas flow in petroleum reservoirs, transport of water and contaminants in unsaturated soils, heating and drying in industrial processes, and the storage of carbon dioxide ($CO_2$) in deep underground aquifers. These problems are usually solved numerically, using, as input, generalized physical laws such as Darcy’s law, as well as functional relationships between the different physical quantities involved, such as permeability-porosity, capillary pressure-saturation, and relative permeability-saturation curves. These relationships describe the physics of the fluid flow and transport processes at the core-scale, i.e. the scale of a lab sample (order of mm), and are usually obtained with laboratory experiments. Their role in determining the solution of the macro-scale problem (order of m to km) is paramount, since the macroscopic behaviour of a medium and its components, is dictated by the processes occurring at the pore-scale. Code comparison studies (Pruess et al., 2004) have shown that the largest discrepancies between different simulators can be traced to uncertainties in these parameters. Hence, it is of utmost importance to have accurate and reliable core-scale relationships in order to produce trustworthy and applicable macro-scale solutions.

However, obtaining these relationships through laboratory experiments can be very costly and time-consuming. Besides, reservoir conditions can be very difficult to reproduce. An alternative way to produce these relationships in a faster and more efficient way through numerical simulations has emerged over the last decade as part of a research field known as pore-scale modelling. This PhD project can be placed within this latter research area.
1.1.1 The CO2FLIP Project

This PhD is part of a major collaborative project between three UK’s Universities (Aberdeen, Leeds and Sheffield) and Tsinghua University in China. The wider research project aims at developing fundamental understanding and quantitative description of CO$_2$ migration in porous media at conditions relevant to saline aquifers encountered in carbon sequestration, and hence contributing to climate change mitigation.

The project brings together engineers and geologists from the UK and China to undertake a comprehensive research programme comprising combined experimental (flow and mineral-fluid interactions), computational and theoretical investigations. The complex two-phase flow phenomena in porous rocks are experimentally investigated using a purposely-built supercritical CO$_2$ test facility equipped with a Custom-built MRI at Tsinghua operating at conditions typical of deep saline aquifers. Complementary experiments on mineral-fluid interactions are conducted at Leeds studying the interactions between the fluids and rocks reactions of the rocks. The computational studies employ various numerical techniques combining mesoscale modelling using Lattice Boltzmann Method (LBM) (Sheffield) and conventional CFD (Aberdeen) to investigate the two-phase flow physics, and fluid-fluid and fluid-rock interactions at sub-pore levels.

The ultimate aim of the investigations is to use the new experimental and computational data to produce correlations/relationships for use with large scale simulations as well as developing further fundamental understanding of phenomena of CO$_2$/brine two-phase flow in porous media.

1.1.2 Pore-scale phenomena in the porous region

Carbon capture and storage (CCS) has been recognised as one of the measures needed to mitigate the climate change. Emitting is avoided by capturing CO$_2$ from stationary sources and transporting it into a suitable storage location. Geological storage in deep saline aquifers is one of the most favourable storage options due to its wide availability and large storage space. Geological formations in the subsurface are composed of transported and deposited rock grains, organic material, and minerals that form after the rocks are deposited. The pore space between grains or minerals is occupied by fluid (mostly water). Open fractures and cavities are also filled with fluid. Injection of CO$_2$ into the pore space and fractures of a permeable formation can displace the in situ fluid or the CO$_2$ may dissolve in or mix with the fluid or react with the mineral grains. Injection of fluids into deep geological formations is achieved by pumping fluids down into a well. Injection raises
Figure 1.1. Primary flow and transport mechanics associated with geological storage of CO$_2$ (Huppert and Neufeld, 2014).

the pressure near the well, allowing CO$_2$ to enter the pore spaces initially occupied by the in situ formation fluids. Once injected into the formation, the primary flow and transport processes that control the migration of CO$_2$ include:

- Fluid flow driven by the pressure gradients created by the injection process;
- Buoyancy caused by the density differences between CO$_2$ and the in situ formation fluid;
- Diffusion;
- Dissolution into the formation fluid;
- Mineralization;
- Pore space trapping.

The latter process is also called as "residual CO$_2$ trapping" or "capillary trapping" and refers to the amount of CO$_2$ retained in the pore space by capillary forces. Retention of gas bubbles in the pore-space is provoked by large local gradients in capillary forces which causes a ganglion of gas to break up in several bubbles when passing through a constriction. This mechanism is called "snap-off".
1.2 Motivations and aims

As part of this Project, the C++ in-house code *interpore3d* is fully developed. It computes either single or two-phase flow at the pore-scale using conventional Computational Fluid Dynamics (CFD) techniques. The full code contains the following components:

- A single-phase flow solver;
- An interface tracking algorithm;
- A two-phase flow solver;
- An ensemble of filtering techniques for surface tension forces;
- A choice of linear solvers.

Simulations are run on the High Performance Computing (HPC) cluster of the University of Aberdeen. It consists of 20 standard nodes (320 cores, 64 GB RAM), 16 high memory nodes (256 cores, 256 GB RAM) and 1 very high memory node (1 TB RAM). Visualization and postprocessing of results is done using the open-source Software Paraview. The following objectives are proposed for this Project:

- To increase fundamental understanding and quantitative description of the pore-scale mechanisms happening at conditions encountered in carbon sequestration. In particular the so-called snap-off mechanism, which is at the origin of capillary trapping, is studied. To achieve this goal, simulations are carried out on simplified pore-throat systems, and the role of various parameters such as contact angle, capillary number, and viscosity ratio is investigated.

- To produce improved correlations/relationships for use with large-scale simulations. To achieve this goal, single and two-phase flow simulations are carried out on three-dimensional digital images obtained from micro-Computed Tomography (µ-CT) scanning of several reservoir rocks, and the macro-scale parameters are calculated by spatially averaging the predicted relevant quantities.

- To provide more insight into the definition of the physical quantities involved in the description of the physics of the fluid flow at the core-scale, such as capillary pressure. To achieve this goal, an averaging procedure is proposed yielding a novel formulation for the macroscopic capillary pressure.
1.3 Thesis outline

This thesis is organized as follows:

- **Chapter 2** contains the relevant literature for this project, including a brief introduction on pore-scale modelling, a thorough presentation of the challenges in modelling both single and two-phase flow at the pore-scale, and a list of previous related studies.

- **Chapter 3** contains the theoretical background about the concept of capillary pressure. This chapter includes a presentation of the governing equations of flow for both a bulk phase and a surface of discontinuity at both the micro- and macro-scale, an insight into the definition of capillary pressure at the micro-scale and a survey of the most commonly employed approaches for upscaling capillary pressure to the macro-scale. The proposed averaging procedure yielding a novel formulation for the macroscopic capillary pressure is also presented and discussed here.

- **Chapter 4** contains the single-phase flow work done within this project. It consists in an integrated approach for calculating the petrophysical properties of rocks, comprising pore-space imaging, statistical correlation, and numerical simulations.

- **Chapter 5** contains the description of the numerical method for modelling two-phase flow at the pore-scale, as well as simulation results of benchmark problems for its validation.

- **Chapter 6** contains simulations results of several two-phase flow applications of the model, including imbibition in a capillary pipe, snap-off in constricted tubes of variable cross-sections, and drainage on μ-CT images of real rock samples.

- **Chapter 7** contains a summary of the main achievements of this PhD
Chapter 2

Pore-scale modelling of porous media flows

2.1 Introduction

This chapter is organized as follows. First, an introduction on what is pore-scale modelling and why it is important in current research in porous media is given in Sec. 2.2. The various numerical approaches for computing pore-space properties are also briefly reviewed. Then, the techniques and the challenges in simulating both single-phase and two-phase flow at the pore-scale using conventional grid-based methods are presented in Secs. 2.3 and 2.4 respectively. Finally, the main gaps in knowledge are summarized in Sec. 2.5

2.2 Background

Pore-scale (or micro-scale) modelling is the field within the immensely vast discipline of fluid flow through porous media, aiming at enhancing understanding of the pore-scale phenomena through numerical simulations. The importance of pore-scale simulations lays in the fact that fluid properties, geometry of the medium, and boundary conditions are much easier to systematically investigate in computer simulations than in experiments. Developments in pore-space visualization at very high image resolution (see Fig. 2.1), and constant increase in computer power also contributed to the popularity of this field of study. In particular, image acquisition techniques have advanced from statistical reconstruction of three-dimensional representations of the pore-space based on two-dimensional images, to three-dimensional images directly produced by micro-Computer Tomography. With modern \( \mu \)-CT scanners, an instrument housing its own source of x-rays, the 3D
representation of the pore-space is reconstructed from a series of 2D projections taken at
different angles, allowing for reproducing the exact microstructure of a rock sample down
to a resolution of 1 µm. This enables predictions to be made on many 3D images of small
rock samples, providing data that would be much more difficult or impossible to obtain
using traditional experiments. Moreover, results obtained from pore-scale simulations can
be used to obtain accurate estimates of the core-scale quantities using spatial averaging
techniques, thus reducing uncertainties in predicting larger scale phenomena. The combi-
nation of high resolution imaging techniques with the predictive capabilities of pore-scale
modelling is the approach commonly known as digital rock physics. A typical example
is the computation of the absolute permeability of a medium. Pore-scale simulations are
performed on 3D images of size taken as representative of the medium at a larger scale.
The predicted flow field is then used to average the relevant quantities and compute the
absolute permeability. Recent reviews on pore-scale imaging and modelling can be found
in Joekar-Niasar et al. (2012); Blunt et al. (2013); Bultreys et al. (2016).

In summary, the main objective of pore-scale modelling is to calculate the properties
of a medium over a Representative Elementary Volume (REV). The concept of REV is
essential in porous media and will be used often in this dissertation, thus more detail is
provided in the next paragraph.

2.2.1 The concept of REV

The concept of REV was introduced by Bear (1972). Following his approach, an REV
is the volume which allows the passage from a smaller to a larger scale, i.e. spatial
averaging over REV yields a representative large-scale description of relevant quantities.
For example, a fluid can be described at two different scales: molecular and microscopic.
At the molecular scale, the fluid is seen as composed of a number of particles (molecules)
which move and collide with each other. At the microscopic scale, instead, the concept of
fluid parcel is central and the fluid is regarded as a continuum, meaning that at any point \( P \)
of the fluid domain there is a mass of fluid with definite kinematic and dynamic properties.
The fluid parcel is an ensemble of molecules occupying a certain volume called the particle
volume, to which the mass density of the fluid is associated. Determination of the fluid
mass density and particle volume is done by considering progressively increasing volumes
centred at a point \( P \) in the fluid, until the fluid mass density no longer changes with
further changes of the volume (excluding larger scale heterogeneity). Fluid parcels thus
describe the average velocity and other properties of the fluid particles when averaging is
done over the particle volume.
Figure 2.1. Images of a sandstone obtained at different resolutions (Lamy-Chappuis et al., 2014).

Figure 2.2. Determination of porosity and REV (the volume $V_0$ in figure) for a digital image of a real sample of Cayton Bay sandstone (see Sec. 4.2 for description of the samples).
In the same way the particle volume allows for the passage in the description of the fluid from the molecular to the microscopic continuum scale, an REV can be determined for the porous medium which allows for its continuum representation at the macro-scale. The REV is usually defined through the volumetric porosity of the medium, namely the ratio between the pore volume and the total volume of the medium. Volumetric porosity is considered the main property of the porous medium. The procedure is illustrated in Fig. 2.2 for a cubic digital image of a real sample of Cayton Bay sandstone. Increasing cubic volumes, centred at the centroid of the sample, are considered and porosity is calculated as the ratio between the pore voxels and total number of voxels - a voxel is the 3D equivalent of a 2D pixel. When the single voxel containing the centroid is considered, the porosity is either 0 or 1 depending whether the voxel belongs to the pore or grain space. Increasing the volume size to 27, 125, etc. voxels initially produces fluctuations of the calculated porosity. The volume $V_0$ in Fig. 2.2 for which these fluctuations vanish, is the REV of the medium.

A schematic of the different scales involved in the description of a medium is shown in Fig. 2.3. The particle volume is the elementary point of the fluid domain of the REV in the same way as the REV is the elementary point of a macro-scale model. Analagously, as the fluid density and viscosity are defined for each point in the fluid domain, other physical properties describing core-scale processes, such as the absolute permeability or the relative permeability-saturation curves, are assigned to each point in the macro-scale model. The process of computing a larger-scale property by spatially averaging the relevant quantities over REV is called upscaling. Common issues involved by the upscaling process include identifying the REV, making constitutive hypotheses, and making assumptions based on length-scale considerations.

### 2.2.2 Pore-network models vs direct simulations

There are two ways to compute pore-space properties: direct simulations, where the real pore-space of the medium is the computational domain for the governing equations, and network modelling, where the complex geometry of the medium is replaced by a topologically representative system of larger void spaces called pores, connected by straight channels called throats. While naturally superior in that they honour the real geometry of the problem, direct simulations have the drawback of being very computationally demanding for most engineering applications. On the other hand, despite clearly making some approximations in the description of the pore-space, network modelling stands as an efficient way for larger-scale properties computation.
Pore-Network models

The first use of pore-network models for computing pore-space properties dates back to around 15 years ago (Bakke et al., 1997; Oren et al., 1998; Blunt et al., 2002; Valvatne et al., 2005). The main component of pore-network modelling is the extraction of the topologically representative network from the real porous microstructure. There are numerous ways to achieve this but their review is beyond the scope of this work. More detail can be found in the literature cited above. Pores and throats are then assigned geometrical properties such as volume and shape. For the most basic models, the pores are located at the nodes of a regular lattice and the throats have circular cross section. More refined networks were then developed to accommodate the impelling need of modelling the physics of the flow more realistically. These include irregular lattices, variable cross sections, shape factors, etc. Fig. 2.4 shows an example of an extracted pore-network from a reconstructed sandstone sample.

Direct simulations

Lattice Boltzmann methods (LBM) (d’Humieres et al., 1986; Frisch et al., 1986; Chen and Doolen, 1998; Zu and He, 2013) are the most popular approach for computing single and multiphase flow directly on the pore-space. LBM is kinetic in nature and consists of a number of particles moving in a regular lattice and undergoing momentum-conserving collisions. The resulting fluid properties are then obtained by statistical averaging. LBM...
can also be seen as a discretization of the Boltzmann equation for a particle velocity distribution field. An extensive overview on LBM methods for multiphase flow for porous media applications can be found in Liu et al. (2016). LBM is only one of a number of particle-based methods, where particles representing packets of fluid are tracked through the computational domain. Smoothed Particle Hydrodynamics (SPH) (Tartakovsky and Meakin, 2006) is another particle-based method that was first introduced to compute astrophysical fluid dynamics and is now applied to a wide range of fluid applications, including fluid flow through porous media (Holmes et al., 2011; Bandara et al., 2011, 2013; Sivanesapillai et al., 2016; Tartakovsky and Panchenko, 2016). Last, there are conceptually more traditional approaches that solve the Navier-Stokes (NS) equations using standard discretization methods. Conventional grid based methods such as finite difference (FD), finite element (FE) and finite volume (FV), are the most widely used for the solution of the incompressible NS equations for their superior computational efficiency and capability of handling multiphase fluid flow with large viscosity and density ratios. However, while these methods work well for single-phase flow simulations, they become much more complicated for multiphase flow, where they present three major inconveniences: 1) the tracking of the interfaces between the fluids, 2) the presence of localized forces due to surface tension between the two fluids and 3) the coupling with a contact angle model for accounting the dynamics of the solid-fluid-fluid contact lines. These issues have been largely overcome in the last decades by using a variety of methods for tracking the interfaces (Hirt and Nichols, 1981; Sussman et al., 1994; Jacqmin, 1999). In most cases, these methods were coupled with contact-angle models for the description of the behaviour of the fluid-fluid-solid contact lines. However, despite these recent advances, the extension
to porous media problems, where in general capillary forces are dominant, is still a challenge. In the following text, the literature review is restricted to traditional grid-based methods and it is split in two main sections: single-phase flow (Sec. 2.3) and multiphase flow (2.4). A more comprehensive review on pore-scale modelling of multiphase flow can be found in Meakin and Tartakovsky (2009).

2.3 Single-phase flow

In conventional CFD, the motion of a fluid is described by the well-known NS equations

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{2.1a}
\]

\[
\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) + \nabla p - \nabla \cdot \mathbf{\tau} - \rho \mathbf{g} = 0, \tag{2.1b}
\]

where \( \mathbf{u} \) is the velocity vector, \( p \) is the pressure, \( \mathbf{\tau} = \mu [\nabla \mathbf{u} + (\nabla \mathbf{u})^T] \) is the viscous stress tensor, \( \rho \) and \( \mu \) are the fluid density and viscosity respectively, and \( \mathbf{g} \) is the acceleration due to gravity vector.

In pore-scale modelling, simulation of single-phase flow is important for the estimation of the absolute permeability of a medium. Absolute permeability is a macroscopic property of a medium which measures the ability of a fluid to flow through it (Bear, 1972). In pore-scale modelling, estimation of the absolute permeability is usually done by solving the reduced form of the NS equations for the case of incompressible fluid (\( \rho = \text{const} \)) and when inertial effects can be neglected, i.e. \( Re \ll 1 \), where \( Re \) is the Reynolds number (\( Re = \frac{\rho v L}{\mu} \)). The resulting equations are called the Stokes equations and are written as

\[
\nabla \cdot \mathbf{u} = 0, \tag{2.2a}
\]

\[
\mu \nabla^2 \mathbf{u} - \nabla p + \rho \mathbf{g} = 0. \tag{2.2b}
\]

The equations are solved in the real pore-space geometry which covers at least an REV of the medium and averaging is then carried out to obtain the absolute permeability from the computed velocity field using Darcy’s law (see Sec. 3.3.3 for derivation).

2.3.1 Numerical methods for the solution of the Navier-Stokes equations

The Stokes equations (2.2a)-(2.2b) are a system of four partial differential equations in terms of four independent variables. However, a numerical solution of this system of PDEs is not straightforward, since an explicit equation for pressure is missing. There are
two different groups of methods for the solution of the incompressible Stokes equations. The first category is usually known as coupled approach, since both pressure and velocity are treated as simultaneous unknowns, and the Stokes equations are solved by means of the so-called artificial compressibility method (Chorin, 1967). In this method, an artificial time-dependent pressure term is added to the continuity equation by means of an artificial density. The coupling between pressure and density is provided with an artificial equation of state of the kind $p = \frac{\rho}{\beta}$, in which $\beta$ is an artificial compressibility. These artificial terms vanish approaching the steady state conditions, i.e. the steady state solution of the artificial problem does not depend on $\beta$ and thus satisfies the original equations. In other words, the artificial compressibility method consists of replacing the original incompressible problem by an unsteady compressible problem which is assumed to converge to the incompressible solution of interest.

The second category refers to a family of iterative procedures called "pressure-correction" methods. The philosophy of pressure-correction methods is to first compute an intermediate velocity field $\mathbf{u}^*$ by solving the momentum equation using a known pressure field $p$ (the initial pressure field is guessed). These velocities will generally not satisfy the continuity equation, unless the correct pressure field is employed. Thus, a Poisson-like equation is artificially built to compute a new pressure field in order to improve the velocity in such a way to satisfy the continuity equation. This process is repeated until convergence is reached and the continuity equation is satisfied. There are different pressure-correction methods, depending on how the pressure equation is built. All these methods have to be considered valid regardless of the approximations introduced, as long as they serve to ultimately satisfy all the discretized equations. The most famous formulation of a pressure-correction method is due to Patankar and Spalding (1972), namely SIMPLE (Semi-Implicit Method for Pressure-Linked Equations). In the SIMPLE algorithm, after solving the momentum equations for $\mathbf{u}^*$, a second velocity field $\mathbf{u}^{**}$ satisfying the continuity equation $\nabla \cdot \mathbf{u}^{**} = 0$ together with a new pressure field $p^*$ are sought. Defining pressure and velocity corrections as $p' = p^* - p$ and $\mathbf{u}' = \mathbf{u}^{**} - \mathbf{u}^*$ respectively, after some algebraic manipulations, a velocity-correction formula is obtained which, upon substitution into the continuity equation $\nabla \cdot \mathbf{u}^{**} = 0$, leads to an equation for $p'$.

However, in the original formulation of SIMPLE some approximations were introduced in deriving the velocity-correction formula, resulting in slow convergence of the overall procedure. In order to overcome this major issue, two modified version of SIMPLE were proposed: the SIMPLER algorithm (SIMPLE revised) by Patankar (1980) and the SIMPLEC (SIMPLE consistent) by Van Doormaal and Raithby (1984). In SIMPLER,
Figure 2.5. 2D staggered (a) and non-staggered (b) grid arrangements in the framework of the FV method.

A pseudovelocity is defined and the method does not make use of any approximation, whereas in SIMPLEC the approximation introduced in the original formulation is not removed but its magnitude is somehow alleviated.

An alternative to the SIMPLE family algorithms is a non-iterative method called PISO (Pressure-Implicit with Splitting of Operators) formulated by Issa (1986) for time-dependent problems. This method is a combination of a predictor step and one or more corrector steps during each time step. The novelty of PISO with respect to SIMPLE is that a third velocity field \( \mathbf{u}^{**} \) satisfying the continuity equation \( \nabla \cdot \mathbf{u}^{**} = 0 \) together with its corresponding new pressure field \( p^{**} \) are sought, and a second pressure-correction equation is built for \( p'' = p^{**} - p^* \). A comparison between the PISO algorithm and the steady-state version of SIMPLE has been made by Issa et al. (1986) for an axisymmetric laminar flow test, revealing that the computational effort to reach the steady-state solution for PISO is smaller. A performance assessment of all the four methods introduced here (SIMPLE, SIMPLER, SIMPLEC and PISO) can be found in Acharya et al. (2007).

Another issue when solving the NS equations in the framework of the FV method regards the grid arrangement, i.e. the choice of the points in the domain where the unknown variables are stored. Two basic grid arrangements, known as staggered and non-staggered (or collocated), are shown in Fig. 2.5. The staggered grid (Fig. 2.5a) consists of three different sets of control volumes in 2D (four for 3D). Velocities are defined at the cell faces whereas pressure is defined at the cell centre. The major advantage of this arrangement is that it avoids the use of any interpolation for the evaluation of the cell face velocities.
required by the discretization of the divergence operator in the NS equations. On the contrary, in a non-staggered arrangement (Fig. 2.5b), velocities and pressure are all defined at the cell centre, thus only one control volume is used during the computation, resulting in a significant programming simplification. This arrangement has to be preferred when complex geometries are encountered or when using a curvilinear coordinate system. However, this arrangement has been out of favour for many years because it was observed to produce non-physical oscillations in pressure (Patankar, 1980), when computing the cell-face velocities by linear interpolation between neighbouring nodes. A cure for this problem was first proposed by Rhie and Chow (1983). They suggested calculating the cell-face velocities as a linear interpolation of the discretized momentum equations of the neighbour cell-centre velocities. This approach was then refined by other authors with higher-order approximation schemes for the cell-face velocities (Papageorgakopoulos et al., 2000; Yu et al., 2002). An alternative solution was proposed by Date (1993), in which the cell face velocities are evaluated by linear interpolation and the pressure gradient in the momentum equation is interpolated in terms of the pressure gradients at its neighbours. A detailed comparison of these two grid arrangements has been made by Perić et al. (1988) for three test cases (lid-driven cavity flow, backward facing step flow and flow through a pipe with a sudden contraction). Their computations demonstrated that the performances of both arrangements are very similar.

The SIMPLE and PISO algorithms for non-staggered grid arrangements will be described in more detail in Secs 4.4.1 and 5.3.4 respectively.

2.3.2 Applications to real porous microstructures

Pioneering investigations in this field are due to Adler et al. (1990). They computed permeability values on a fictitious porous medium, sharing the same statistical properties of real Fontainebleau sandstones, and then compared the numerical values with experimental data. They found the predicted permeabilities five times greater than the measured ones, although the general shape of the experimental curve was well-reproduced. Martys et al. (1994) and Coelho et al. (1997) simulated fluid flow and dispersion through random packings of spheres and packings of grains of arbitrary shape respectively, in order to obtain universal curves for fluid permeability. Their data were found to agree well with experimentally obtained permeability values of several sandstones. The first use of 2D digital images of real porous microstructures, captured using an optical microscope, is due to Tashman et al. (2003). They first validated the numerical scheme by comparing the predicted permeability values of a medium of packed columns to a closed form solu-
tion, and then evaluated the permeability tensor of three natural granular microstructures (Glass beads of 1 mm diameter and two sands with an average particle diameter between 0.40 and 0.60 mm). Al-Omari and Masad (2004) computed fluid flow in 3D microstructures of field cores of asphalt mixes, captured using X-rays CT, with average particle diameter between 3 and 10 mm, and compared the predicted permeability values with closed form solutions. Zaretskiy et al. (2010) applied the FE method to study a digitized Fontainebleau sandstone sample, comparing their numerical performance to LBM simulations. Mostaghimi et al. (2013) simulated Stokes flow on 3D images obtained from μ-scanning of a range of porous microstructures, including sandstones (mean pore radius 15-20 μm) and carbonates (mean pore radius 10-15 μm) (Dong, 2008). They studied the existence and size of the REV showing that the REV for permeability is larger than for other properties such as porosity. Finally Guibert et al. (2015) investigated the role of mesh sensitivity in computing permeability on a Dausse sandstone, showing that mesh refinement of the original tomographic image has a non-negligible impact on the evaluation of the permeability tensor.

### 2.4 Modelling two-phase flow at the pore-scale using grid-based methods

While pore-scale simulations of single-phase flow do not present any major inconveniences other than identifying the REV, modelling two-phase flow at the pore-scale is a very difficult task. First of all, the interfaces between the two phases have to be represented and their evolution in time needs to be tracked. This poses problems not only in terms of accuracy of the interface representation but also in terms of mass-conservation. Moreover, if one aims at simulating two-phase flow taking place in real porous microstructures, the dynamics of the contact line where the interface and a solid wall meet must also be taken into account. However, what mostly makes modelling two-phase flow at the pore-scale a big challenge is the presence of localized forces of molecular nature at the interface. In most pore-scale simulations at real reservoir conditions these forces are the dominant ones, and their treatment in the NS equations must be carried out carefully, as they are prone to inducing numerical instabilities or producing non-physical results. The remainder of this section seeks to address these issues.
2.4.1 Interface representation

Interface-tracking methods can be divided into two main categories: volume-tracking and front-tracking methods. In volume-tracking methods, the fluids are marked and tracked, whereas in front-tracking methods the interface itself is marked and tracked. Front-tracking methods (Unverdi and Tryggvason, 1992) are more computationally demanding, as the interface is explicitly represented in a separate grid that moves through the stationary grid, thus grid reconstruction is necessary during the computation. On the other hand, in volume-tracking methods, the fluids are marked and tracked either by mass particles (Harlow et al., 1965) or a function. The latter can be a volume fraction (Hirt and Nichols, 1981), a level-set function (Sussman et al., 1994) or a phase-field variable (Jacqmin, 1999). Among these methods, the level-set (LS) and the Volume-of-fluid (VOF) are the most widely used for their simplicity and computational efficiency.

The VOF method

In the VOF method, a volume-fraction \( \alpha \) which lies between 0 and 1 is defined in each computational cell as the ratio of the volume of fluid 1 filling the cell and the volume of the cell as follows:

\[
\alpha = \begin{cases} 
1, & \text{if the cell is filled by fluid 1,} \\
0, & \text{if the cell is filled by fluid 2,} \\
0 < \alpha < 1, & \text{if there is an interface within the cell.}
\end{cases}
\]  

(2.3)

When \( \alpha = 1 \) the cell is completely filled by fluid 1, when \( \alpha = 0 \) the cell is filled by fluid 2 and when \( 0 < \alpha < 1 \) the cell contains both the phases, thus an interface is present within the cell.

The main feature of VOF methods is their capability to conserve mass exactly during advection of the interfaces. This is achieved by using one of a number of available algorithms designed for modelling the motion of the interfaces. The idea of these algorithms is that an interface can be represented by a line (in 2D) or a planar surface (in 3D). This line, or plane, divides the cell in two parts, each containing one fluid. The interface is then propagated by the flow and a systematic geometric calculation of moving volume fluxes is carried out to solve an advection equation. Advection is usually one-dimensional with multi-dimensionality obtained through operator splitting. The updated volume fraction field therefore results from a normalization of moving fluid volumes with respect to the cell volume.
Numerous methods have been proposed for tracking the interfaces in the framework of a VOF algorithm, such as the SLIC (Simple Line Interface Calculation) due to Noh and Woodward (1976), the piecewise constant, stair stepped method by Hirt and Nichols (1981) and the piecewise linear interface calculation (PLIC) method by Youngs (1982). In the SLIC method, the interface is represented by a straight line parallel to one of the coordinate directions. It is a direction-split algorithm so only the neighbour cells in the sweep direction are employed for the interface reconstruction. The method due to Hirt and Nichols is piecewise constant like SLIC but all the neighbour cells are used to reconstruct the interface. Finally, the PLIC method is based on the idea that the interface is represented by a straight line, or a planar surface in 3D, having unit normal $\mathbf{n}$ computed from a given distribution of the volume fraction through the computational domain, i.e. from the gradient of the volume fraction

$$
\mathbf{n} = \frac{\nabla \alpha}{|\nabla \alpha|}. 
$$

These methods are extensively reviewed in the papers of Rudman (1997) and Rider and Kothe (1998) and the different interface reconstruction techniques are illustrated in Fig. 2.6. Rudman (1997) compared the performances of the above-mentioned methods and found that the PLIC algorithm is the most accurate in terms of interface shape.

There is then another group of VOF interface capturing schemes which attempts to directly capture the interface by solving the relevant advection equation without explicit interface reconstruction. This includes the Compressive Interface Capturing Scheme for Arbitrary Meshes (CICSAM) (Ubbink, 1997), the High Resolution Interface Capturing...
(HRIC) scheme (Muzaferija et al., 1998), the Modified High Resolution Interface Capturing (MHRIC) scheme (Park et al., 2009), and the Flux Blending Interface Capturing Scheme (FBICS) (Tsui et al., 2009). These methods work well for unstructured grids, especially in the 3D case, where geometric interface reconstruction becomes more complicated.

Estimation of the interface normal, and consequently of the interface curvature, is the weak point of the VOF methods. As it will be described in the next paragraph, inaccurate discretization of the gradient operator in eq. (2.4) can lead to serious issues when modelling fluid motion driven by surface tension forces.

The LS method
In the LS method, the interface is represented as the level-set of a given function, namely the signed distance function $\Phi$, defined for each point $x$ in the domain as

$$\Phi(x, t) = \begin{cases} > 0, & \text{if } x \text{ belongs to fluid 1}, \\ 0, & \text{if } x \text{ lays in the interface}, \\ < 0, & \text{if } x \text{ belongs to fluid 2}. \end{cases}$$

(2.5)

Level-sets methods are widely employed as they allow for exact computation of the unit normal to the interface, to the limit of the approximations introduced with discretization. The unit normal to the interface is the gradient of a function normal to the level sets by definition, so it can be directly computed as

$$n = \frac{\nabla \Phi}{|\nabla \Phi|}.$$  

(2.6)

However, loss of mass is the main drawback of this method. To improve the accuracy of the solution in terms of mass conservation, Sussman et al. (1998) developed a constraint that significantly reduced the average mass error from 3% without the constraint to 1% with the constraint, for a drop collision problem.

Coupled LS-VOF methods
Bearing in mind the main advantages of the LS (direct calculation of the normal to the interface) and VOF (existence of a number of mass-conserving algorithms for the evolution of the interfaces) methods, it should be reasonable to try to develop a more robust and efficient algorithm combining the best features from these two methods. The pioneering Coupled Level Set and Volume-of-Fluid (CLSVOF) method was developed by Sussman and Puckett (2000) to have a new more accurate algorithm for tracking the interfaces.
than either LS or VOF alone. In this method both the level set and the volume fraction are advected, and the interface is represented by the best fit planar surface with normal vector computed from the LS function. Further details on the coupling between the LS and VOF functions can be found in Son and Hur (2002); Son (2003); Wang et al. (2009). Despite its superior computational efficiency, the CLSVOF method is rather complicated to implement for computing incompressible two-phase flow due to the need of solving the advection equation for both the LS and VOF functions, as well as providing the scheme for their coupling. A new approach was recently proposed by Sun and Tao (2010) based on an innovative iterative geometric procedure for the calculation of the signed distance function which avoids the solution of an advection equation for the LS function. In this method, only the advection equation of the volume fraction is solved.

### 2.4.2 Surface tension forces

Considering a system where two homogenous phases 1 and 2 are present, the surface of discontinuity between the two phases can be seen as a thin non-homogenous film called transition region, where the properties of the two phases gradually change (see Fig. 2.7). Let $A_s$ be the Helmholtz free energy per unit mass of the surface defined as

$$A_s = E_s - TS_s,$$

where $E_s$ is the internal energy per unit mass of the surface, $T$ is the temperature and $S_s$ is the internal entropy per unit mass of the surface. The surface tension $\sigma$, with units of force per unit length, can be defined as the change in Helmholtz free energy of the surface $\overline{A}_s$, per unit change of area of the surface $a_s$, at constant temperature, volume and mass.
of the components substances, as follows (Gibbs, 1878)

$$\sigma = \left( \frac{\partial A_s}{\partial a_s} \right)_{T,V,m}$$  \hspace{1cm} (2.8)

The surface tension is due to the imbalance of molecular forces in the transition region between the two phases and can be seen as the property which makes the surface of discontinuity acquire the least surface area possible. This results in the surface of discontinuity tending to assume a curved configuration except in the presence of a third phase. The relationship between surface tension and curvature is given by the Young-Laplace equation. More insight into this important relationship will be given in Sec. 3.4.

The classical method for modelling surface tension effects in fluid motion, namely the continuum surface force (CSF) model, is due to Brackbill et al. (1992). According to this model, surface tension is interpreted as a continuous, three-dimensional effect across the interface, rather than as a boundary value condition at the interface. In other words, instead of calculating the pressure for each bulk phase separately, and applying a boundary condition for surface tension at the interface, surface tension is treated as a body force concentrated at the interface, and only one pressure field is calculated, using a color function similar to the VOF indicator function for identifying the two phases. Following this approach, the surface tension force per unit interfacial area $f_s$ at the point $x_s$ on a surface $S$, can be written as

$$f_s(x_s) = \sigma k(x_s)n(x_s),$$  \hspace{1cm} (2.9)

where $\sigma$ is the surface tension, $n$ is the unit normal to the interface at $x_s$ pointing into phase 2 and $k$ is the curvature of the interface given by

$$k = -\nabla \cdot n.$$  \hspace{1cm} (2.10)

The Dirac function $\delta_s$ is then employed to convert the surface integral over the interface $S$ of $f_s(x_s)$ to an integral over a volume $V$ containing $S$, as follows

$$\int_S f_s(x_s)dA = \int_S \sigma k(x_s)n(x_s)dA = \int_V f_s(x)\delta_s dV.$$  \hspace{1cm} (2.11)

Mathematically, the Dirac’s delta $\delta(x)$ is defined as an infinitely concentrated unit-area impulse as follows (Bracewell, 1965)

$$\delta(x) = 0, \quad x \neq 0$$

$$\int_{-\infty}^{\infty} \delta(x)dx = 1.$$  \hspace{1cm} (2.12)
The Dirac’s delta can also be interpreted as the first derivative of the Heaviside step function, and has the following important property:

\[
\int_{-\infty}^{\infty} \delta(x)f(x)dx = f(0),
\]

where \( f(x) \) is any continuous function. This property is known as the sifting property of the Dirac’s delta. Generalizing \( \delta \) to the 3D case, a Dirac’s delta function for the surface \( S \) contained within \( V \), \( \delta_s(x) \), is defined for any position \( x \) within \( V \), such as

\[
\delta_s(x) = 0, \quad x \notin S
\]

\[
\int_V \delta_s(x)dV = 1,
\]

In this manner, the surface tension force can be treated as a body force concentrated at the interface and embodied in the NS equations, which thus become

\[
\frac{\partial}{\partial t}(\rho u) + \nabla \cdot (\rho uu) + \nabla p - \nabla \cdot \tau - \rho g - f_s = 0.
\]

A problem arising when modelling fluid motion with surface tension effects is the occurrence of the so-called spurious or parasitic currents near the interface (Lafaurie et al., 1994; Brackbill and Kothe, 1996; Scardovelli and Zaleski, 1999). Spurious currents are a non-vanishing velocity field occurring in the interfacial region at low capillary numbers \( Ca = \frac{\mu v}{\sigma} \), even in absence of external forces. According to Lafaurie et al. (1994), the magnitude of the spurious velocities is given by

\[
v_\sigma = C_\sigma \frac{\sigma}{\mu},
\]

where \( C_\sigma \) is a constant, which was found to be of the order of \( 10^{-2} \) in their work, leading to a minimum capillary number for which results are not meaningless, of \( 10^{-2} \).

Different remedies to this problem have been proposed since it was first discovered in LBM simulations. For VOF methods, Lafaurie et al. (1994) suggested smoothing the volume fraction away from the interface using a recursive average-interpolation scheme and employing this smoothed indicator function for computing the interface normal, eq. (2.4). More kernels to convolve the volume fraction and the interface curvature, including an hybrid method employing a parabolic indicator function, were studied by Williams et al. (1998). Renardy and Renardy (2002) developed a parabolic reconstruction of surface tension (PROST) scheme in which the curvature is computed from an optimal fit for a quadratic approximation to the interface. They showed that this method reduces the spurious currents by two to three order of magnitude. Cummins et al. (2005) assessed the accuracy of three different curvature estimation methods within a PLIC-VOF framework, namely a convolved VOF function, a height function and a reconstructed distance
Figure 2.8. Unit vectors at the contact line between a solid wall and an interface: $\mathbf{n}_{w}$ is the normal to the interface at the contact line, $\mathbf{n}_w$ is the unit normal to the wall pointing outwards from the wall and $\mathbf{s}_w$ is a unit vector lying in the wall and normal to the contact line. $\theta$ is the contact angle between the interface and the solid wall, measured towards the wetting phase.

function, showing that the height function is the method giving the best performances. Sussman and Ohta (2006) further developed the height function technique and managed to reduce the magnitude of the spurious currents by a factor of 5. Francois et al. (2006) developed a novel balance-force algorithm for interfacial flow and concluded that the order of magnitude of the spurious currents depends on the method for computing the interface curvature while the errors in pressure distribution depend on the surface tension model. Finally, Raeini et al. (2012) presented a new filtered sharp formulation for the surface tension force (FSF) which was shown to be capable of eliminating the spurious currents completely.

### 2.4.3 Contact angle

The last challenge which remains to be highlighted is the treatment of the interface at the wall boundaries where the triple solid-wetting fluid-non-wetting fluid lines meet. Usually, at a solid wall boundary, a boundary condition for the unit normal to the interface is applied, having the following form (Brackbill et al., 1992):

$$\mathbf{n}_{w} = \mathbf{n}_w \cos \theta + \mathbf{s}_w \sin \theta,$$

(2.17)
where $\mathbf{n}_w$ is the unit normal to the wall pointing outwards the wall and $\mathbf{s}_w$ is a unit vector lying in the wall and normal to the contact line and $\theta$ is the contact angle between the interface and the solid wall, measured towards the wetting phase (see Fig. 2.8).

The computation of $\mathbf{n}_w$ requires additional smoothing for avoiding the problem of the spurious currents. Huang et al. (2005) adopted a staircase-like representation of the wall normal vectors by interpolating them from the face centres to the corners. Raeini et al. (2012) further refined the model by interpolating the wall normal vectors back from the corners to the face centres. These methods can be visualized in Fig. 2.9.

The contact angle in the formulation above may be assumed as constant for a given solid-wetting fluid-non-wetting fluid system in first approximation. In reality, the contact angle strongly depends on the roughness and heterogeneity of the solid wall, as well as on the fluid properties, and it is in general not constant. In particular, it depends on whether the interface is advancing or receding, a phenomenon called hysteresis (Huh and Scriven, 1971; Blake, 2006). In order to account for these dynamic aspects, Huang et al. (2005) considered a three-angles model in their computations, where the receding angle $\theta_r$, the advancing angle $\theta_a$ and the equilibrium angle $\theta_{eq}$ are automatically selected by the model, depending on the sign of the dot product of the interface velocity and the interface normal. However, a study of capillary flow in microchannels with integrated pillars done by Saha and Mitra (2009), found that the application of dynamic contact angle models has very minor effect on the resulting predicted flow and that the use of a static contact angle is adequate when using VOF methods.

### 2.4.4 Applications to real porous microstructures

There are very few studies of multiphase flow in porous media at the pore-scale employing conventional grid-based methods. The first use of a NS flow solver coupled with an
interface-tracking method for simulating multiphase flow at the pore-scale is due to Huang et al. (2005). They solved the NS equations embodying the CSF model for surface tension forces, eq. (2.15), using the VOF method to simulate two-phase flow in a fracture with variable aperture and at a "Y-shaped" fracture intersection. Although two-dimensional and limited in applicability, their simulations showed the potential of VOF methods to successfully simulate two-phase flow in complex geometries. Ferrari and Lunati (2013) used the same techniques to simulate drainage in a 2D packing of circles. They varied the viscosity ratio to demonstrate the ability of VOF methods to capture the different displacement mechanisms, from stable displacement to viscous fingering. In a later paper Ferrari et al. (2015) compared the predicted flow patterns with the actual invasion configurations recorded during drainage experiments carried out in micromodels of analogous geometry, showing an overall agreement between simulations and experiments. Jettestuen et al. (2013) used the LS method to simulate quasistatic drainage and imbibition processes in a subset of a 3D sandstone image, showing that the method can reproduce most of the pore-scale displacement mechanisms. However, in their method a solver for the flow field within the whole computational domain is missing, and a normal velocity obtained from a balance of pressure and surface tension forces (see Prodanović and Bryant (2006)) is defined at the interface only. Arrufat et al. (2014) applied the VOF method using height functions to compute the curvature, to simulate oil drainage and compute relative permeability curves for one sandstone sample and two carbonate rocks. They varied the capillary number between $10^{-2}$ and $10^{-4}$ and observed that decreasing the capillary number results in noisy permeability data due to the numerical instability of the advancing interface front. Finally, Raeini et al. (2014b) and Raeini et al. (2015) applied their FSF formulation to simulate primary oil drainage and water injection directly on µ-CT images of a sandpack and a Berea sandstone at low capillary numbers ($Ca = 1.0 \times 10^{-5}$). They produced permeability curves and studied capillary trapping by analysing the effects of the initial non-wetting-phase saturation, capillary number and flow direction on the residual saturation. They showed that their predictions agree well with experimental capillary trapping curves.

### 2.4.5 CFD softwares for VOF models

There are commerical CFD softwares, such as ANSYS Fluent and FLOW-3D, which provide multiphase flow models based on VOF methods. However, the user can not have access to the code and therefore, there are no possibilities to check equation implementation or to add functions to the code. Moreover, it is very likely that the surface tension
formulation used in these softwares is basic and no advanced remediation methods for the spurious currents, and other sources of error are implemented. Alternatively, the open source package OpenFoam, a C++ toolbox for the development of customized numerical solvers, and pre-/post-processing utilities for the solution of continuum mechanics problems, including CFD, is available. For example, the FSF by Raeini et al. (2012) is implemented in OpenFoam.

In this work, the choice has been to develop a new in-house code for VOF models. This is motivated by the complexity of the physical phenomena which are to be modelled, and thus the necessity of having thorough understanding of the full algorithm, including possible sources of numerical instabilities and calibration of the various parameters involved. This is of paramount importance especially if one wants to use the model for applications to real case studies. Furthermore, the code will form a solid base for further multiphysics modelling.

2.5 Summary

A review of the state-of-the-art techniques for modelling single and two-phase flow at the pore-scale in porous media has been presented. Pore-scale modelling has been defined as a research field aiming at enhancing understanding of the pore-scale phenomena. Pore-scale modelling is also used as a predictive tool for producing accurate relationships for use in larger scale simulations. For this purpose, the concept of REV has been defined as the volume which allows for the passage from a smaller to a larger scale, i.e. spatial averaging over REV yields a representative large-scale description of relevant quantities. Modelling approaches can be divided into two main categories: pore-network models and direct simulations. The latter includes LBM, SPH and conventional grid-based methods. This work focuses on this latter group, particularly the FV method. While for single-phase flow an integrated approach known as digital rock physics, is now widely established in the scientific community and numerous works can be found in literature, modelling two-phase flow at the pore-scale is still a very difficult task. Challenges include identification of the REV, tracking the interfaces between the phases, accounting for the contact line dynamics and discretizing the surface tension forces. In particular, the latter can lead to numerical instabilities and non-physical results if not treated carefully. Various methods for dealing with these issues have been illustrated. However, very few studies of two-phase flow on 3D images of rock samples are available. This is due to the fact that replicating reservoir conditions ($Ca < 1.0 \times 10^{-5}$) implies that capillary forces are dominant, which, combined
with the complex microstructure of the medium, can lead to numerical instabilities of
the moving interfaces. These instabilities are caused by the local pore-scale phenomena
happening during the simultaneous movement of the two fluids through the pore-space.
A clear understanding of these important pore-scale processes, such as snap-off, is missing
due to difficulties in traditional experiments in monitoring all the dynamic parameters
involved. Moreover, rigorous theoretical background for two-phase flow is incomplete.
This latter aspect will be addressed in the next chapter.
Chapter 3

Macroscopic balance equations and definition of the macroscopic capillary pressure in porous media flows

3.1 Introduction

While a universal definition of capillary pressure exists at the micro-scale, its upscaling to the macro-scale is still rather vague, and a macroscopic capillary pressure is often defined by analogy with its microscopic definition. This chapter aims at providing better understanding of the concept of capillary pressure in porous media. It is organized as follows. First, basic notation, kinematics and auxiliary relationships are introduced in Sec. 3.2 to facilitate presentation of equations in the remainder of the chapter. Then, the general balance equations for a bulk phase and for a surface are presented in Sec. 3.3. Next, in Sec. 3.4, capillary pressure is defined at the micro-scale and a generalized form of the Young-Laplace equation accounting also for dynamic factors is derived from momentum and energy balance equivalently. The upscaling process leading to the definition of the macroscopic capillary pressure is treated in Sec. 3.5. After a review of the standard approaches that define capillary pressure at the macro-scale, a novel definition of the macroscopic capillary pressure obtained through a rigorous spatial averaging procedure is presented. Finally, findings and shortcomings of the presented theories are discussed in Sec. 3.6.
3.2 Basic notation

3.2.1 Differential geometry

Considering the surface $S$ having boundary $C$ depicted in Fig. 3.1, a set of orthogonal unit vectors $\ell$, $m$ and $n$, where $n$ is the unit normal to the surface, are defined such as

\[ \ell \cdot \ell = m \cdot m = n \cdot n = 1, \]  
\[ \ell \cdot m = m \cdot n = n \cdot \ell = 0, \]  
\[ \ell \cdot \nabla \ell = m \cdot \nabla m = n \cdot \nabla n = 0, \]

where the operator $\cdot$ denotes scalar product between two vectors. Since a surface is uniquely defined by its unit normal vector, the surficial components $\Psi_s^s$ of the general vector quantity $\Psi_s$ defined on the surface, is given by

\[ \Psi_s^s = \Psi_s - nn \cdot \Psi_s, \]

where the product $nn$ is the dyadic product. For the vectors $a$, $b$, $c$ and $d$, the dyadic product has the following properties (Brand, 1947)

\[ a(b + c) = ab + ac, \]  
\[ (a + b)c = ac + bc, \]  
\[ (ab) \cdot c = a(b \cdot c), \]  
\[ (ab) \cdot (cd) = a(b \cdot c)d \]

In the same way, the surficial components $\Gamma^s$ and $\nabla^s$ of the identity tensor $I$ and operator $\nabla$ respectively, are given by

\[ \Gamma^s = I - nn \cdot I, \]  
\[ \nabla^s = \nabla - nn \cdot \nabla. \]

The other two vectors $\ell$ and $m$ are not uniquely defined for the surface but they are constrained to be orthogonal to $n$ and to each other. In particular, at the boundary $C$, $\ell$ is tangent to $C$ and $m$ is both tangent to $S$ and normal to $C$ pointing outwards $C$, so that at the boundary $m \cdot n = 0$.

For a scalar $\varphi$, if $\Pi$ is a second-order tensor, the following relationships apply (Brand, 1947)

\[ \nabla \cdot (\varphi a) = (\nabla \varphi) \cdot a + \varphi \nabla \cdot a, \]  
\[ \nabla \cdot (ab) = (\nabla \cdot a)b + a \cdot \nabla b, \]  
\[ \nabla \cdot (\Pi a) = (\nabla \cdot \Pi)a + \Pi : \nabla a, \]
Figure 3.1. General surface $S$ with boundary $C$ and the set of orthogonal unit vectors $\ell, m$ and $n$, where $n$ is the unit normal to the surface and $\ell$ and $m$ are constrained to be orthogonal to $n$ and to each other. At the boundary $C$, $\ell$ is tangent to $C$ and $m$ is both tangent to $S$ and normal to $C$ pointing outwards from $S$.

where the operator $: :$ denotes the double-dot product. For a general function $\psi_s$ defined on a surface, the following identity holds (Gray et al., 1993)

$$n \cdot \nabla^s \psi_s = 0.$$  

(3.7)

Recalling definition (3.5), the latter identity can be used together with chains (3.6a) and (3.6b) to develop the following important identity which will be employed later in this chapter

$$\nabla^s \cdot (\psi_s I^s) = \nabla^s \psi_s - \nabla^s \cdot (\psi_s n) = \nabla^s \psi_s - \nabla^s \cdot (\psi_s n) n = \nabla^s \psi_s + \psi_s k n,$$

(3.8)

where $k$ is the mean curvature of the surface given by (Aris, 1962)

$$k = - (\nabla^s \cdot n).$$

(3.9)

3.2.2 Kinematics

For a general scalar or vector quantity $\psi$ associated with a fluid parcel, the material derivative is

$$\frac{D\psi}{Dt} = \frac{\partial \psi}{\partial t} + \nabla \psi \cdot u,$$

(3.10)

where $u$ is the velocity of the fluid parcel. The surface material derivative of the general surface quantity $\psi_s$ is

$$\frac{D_s \psi_s}{Dt} = \frac{\partial \psi_s}{\partial t} + \nabla^s \psi_s \cdot (u_s - v_s),$$

(3.11)
Figure 3.2. Averaging volume $\forall$ where three phases - two fluids $\alpha$ and $\beta$ and one solid $k$ - are present, with indication of the surface unit normal vectors.

where $u_s$ is the particle surface velocity, i.e. the time rate of change of spatial position of a fluid parcel contained within the surface, and $v_s$ is the velocity of a fixed point on the surface or the time rate of change of spatial position of a surface point. Since the surface particles are confined within the surface, the component of their velocity normal to the surface is equal to the normal component of the velocity of the surface itself, so that

$$u_s \cdot n = v_s \cdot n = v^s_n,$$

(3.12)

where $v^s_n$ is called the speed of displacement of the surface. For the tangential components, the usual fluid mechanics assumption of continuity across the surface is applied. Full account of the kinematics of a dividing surface can be found in Slattery et al. (2007).

### 3.2.3 Averaging notation

Averaging is carried out over volumes which are representative of the medium. The concept of REV has been introduced in the previous chapter and its definition is recalled: a REV is the volume for which spatial averaging over it yields a physically meaningful large-scale description of relevant quantities. Considering an averaging volume (REV) $\forall$ where $N$ phases are present, a phase distribution function $\gamma_\alpha$ is defined for each phase as
\( \gamma_{\alpha}(x,t) = \begin{cases} 
1, & \text{if } x \in \mathcal{V}_\alpha, \\
0, & \text{if } x \in \mathcal{V}_\beta,
\end{cases} \quad \alpha, \beta = 1, 2, \ldots, N \quad \beta \neq \alpha \)  

(3.13)

where \( x \) denotes the position of a particle within \( \mathcal{V} \) and the volume \( \mathcal{V}_\alpha \) occupied by phase \( \alpha \) is

\[
\mathcal{V}_\alpha = \int_{\mathcal{V}} \gamma_{\alpha} dV.
\]

(3.14)

The volume fraction of phase \( \alpha \), \( \phi_\alpha \), is defined as

\[
\phi_\alpha = \frac{\mathcal{V}_\alpha}{\mathcal{V}},
\]

(3.15)

with the constraint

\[
\sum_\alpha \phi_\alpha = 1.
\]

(3.16)

In porous media such that a solid phase \( k \) is present within the averaging volume (see Fig. 3.2), the porosity of the medium \( \phi \) is defined as

\[
\phi = \frac{\mathcal{V} - \mathcal{V}_k}{\mathcal{V}},
\]

(3.17)

and a new quantity associated with the non-solid phase \( \alpha \) called saturation \( s_\alpha \) is defined as

\[
s_\alpha = \frac{\phi_\alpha}{\phi}, \quad \alpha \neq k,
\]

(3.18)

constrained by

\[
\sum_{\alpha \neq k} s_\alpha = 1.
\]

(3.19)

The following averaging measures of the general microscopic quantity \( \psi \) associated with phase \( \alpha \), \( \psi_\alpha \), are introduced (Whitaker, 1973; Gray, 1975; Hassanizadeh and Gray, 1979)

\[
\langle \psi_\alpha \rangle = \frac{1}{\mathcal{V}} \int_{\mathcal{V}} \psi \gamma_{\alpha} dV,
\]

(3.20a)

\[
\langle \psi_\alpha \rangle^\alpha = \frac{1}{\mathcal{V}_\alpha} \int_{\mathcal{V}} \psi \gamma_{\alpha} dV,
\]

(3.20b)

where \( \langle \psi_\alpha \rangle \) is called the superficial volumetric average of \( \psi_\alpha \) and \( \langle \psi_\alpha \rangle^\alpha \) is the intrinsic volume average of \( \psi_\alpha \). The superficial and intrinsic averages are related by

\[
\langle \psi_\alpha \rangle = \phi_\alpha \langle \psi_\alpha \rangle^\alpha.
\]

(3.21)
The intrinsic average can then be used to decompose \( \psi_\alpha \) as follows (Gray, 1975)\(^1\)

\[
\psi_\alpha = \langle \psi_\alpha \rangle^\alpha + \tilde{\psi}_\alpha, 
\]

(3.22)

where the quantity \( \tilde{\psi}_\alpha \) is called the spatial deviation of \( \psi_\alpha \) and the following identity must hold

\[
\langle \tilde{\psi}_\alpha \rangle = 0. 
\]

(3.23)

Another useful identity is

\[
\langle \psi_\alpha \xi_\alpha \rangle = \langle \psi_\alpha \rangle^\alpha \langle \xi_\alpha \rangle^\alpha + \langle \tilde{\psi}_\alpha \tilde{\xi}_\alpha \rangle. 
\]

(3.24)

When the mass density of phase \( \alpha, \rho_\alpha \), is microscopically constant, the density intrinsic average is the microscopic density itself

\[
\langle \rho_\alpha \rangle^\alpha = \phi_\alpha \langle \rho_\alpha \rangle = \rho_\alpha. 
\]

(3.25)

Let \( S_{\alpha\beta} \) be a surface of discontinuity between two phases \( \alpha \) and \( \beta \), its area is given by

\[
a_{\alpha\beta} = \int_{S_{\alpha\beta}} dA. 
\]

(3.26)

In the same way as for a volume, the surface intrinsic average of the general microscopic surficial quantity \( \psi_s \) associated with the surface \( S_{\alpha\beta}, \psi_{\alpha\beta} \), is defined as (Whitaker, 1969)

\[
\langle \psi_{\alpha\beta} \rangle^{\alpha\beta} = \frac{1}{a_{\alpha\beta}} \int_{S_{\alpha\beta}} \psi_{\alpha\beta} dA. 
\]

(3.27)

The surface integral over \( S_{\alpha\beta} \) can be converted into a volume integral over the averaging volume \( \forall \) containing \( S_{\alpha\beta} \), by means of the Dirac’s delta function \( \delta_{\alpha\beta} \) defined in eq. (2.14). An additional averaging measure called superificial surface average is then introduced as

\[
\overline{\psi}_{\alpha\beta} = \frac{1}{\forall} \int_{\forall} \psi_{\alpha\beta} \delta_{\alpha\beta} dV = \frac{1}{\forall} \int_{S_{\alpha\beta}} \psi_{\alpha\beta} dA. 
\]

(3.28)

\(^1\)Originally, Whitaker (1973) represented the point values using the superficial average, i.e. \( \psi_\alpha = \langle \psi_\alpha \rangle + \tilde{\psi}_\alpha \). Thereafter, Gray (1975) claimed that using this definition for velocity would lead to a non-zero dispersion term even when \( \psi_\alpha \) is uniform. He therefore replaced the superficial average with the intrinsic average as in eq. (3.22). Whitaker himself recognized the flaw and utilized Gray’s decomposition in following papers (Whitaker, 1977, 1986a). A third approach can be found in the work of Hassanizadeh and Gray (1979). They employed the following decomposition:

\[
\psi_\alpha = \tilde{\psi}_\alpha + \tilde{\psi}_\alpha, 
\]

where \( \tilde{\psi}_\alpha \) is an alternative averaging measure, called mass average, defined as

\[
\tilde{\psi}_\alpha = \frac{1}{\langle \rho_\alpha \rangle} \int_{\forall} \rho \psi_\alpha dV. 
\]
Surface spatial decomposition is defined as

$$\psi_{\alpha\beta} = \langle \psi_{\alpha\beta} \rangle_{\alpha\beta} + \tilde{\psi}_{\alpha\beta}. \quad (3.29)$$

Finally, the specific surface area \( \hat{a}_{\alpha\beta} \) is given by

$$\hat{a}_{\alpha\beta} = \frac{a_{\alpha\beta}}{V}, \quad (3.30)$$

and the relationship between the intrinsic surface average and the superficial surface average is

$$\bar{\psi}_{\alpha\beta} = \hat{a}_{\alpha\beta} \langle \psi_{\alpha\beta} \rangle_{\alpha\beta}. \quad (3.31)$$

### Theorems

The following spatial averaging theorems are formulated for a general function \( \psi_\alpha \) (Whitaker, 1967, 1973)

\[
\langle \frac{\partial \psi_\alpha}{\partial t} \rangle = \frac{\partial}{\partial t} \langle \psi_\alpha \rangle - \frac{1}{V} \sum_{\beta \neq \alpha} \int_{S_{\alpha\beta}} u_{\alpha\beta} \cdot n_{\alpha\beta} \psi_\alpha dA, \quad (3.32a)
\]

\[
\langle \nabla \psi_\alpha \rangle = \nabla \langle \psi_\alpha \rangle - \frac{1}{V} \sum_{\beta \neq \alpha} \int_{S_{\alpha\beta}} n_{\alpha\beta} \psi_\alpha dA, \quad (3.32b)
\]

\[
\langle \nabla \cdot \psi_\alpha \rangle = \nabla \cdot \langle \psi_\alpha \rangle - \frac{1}{V} \sum_{\beta \neq \alpha} \int_{S_{\alpha\beta}} \psi_\alpha n_{\alpha\beta} dA. \quad (3.32c)
\]

where \( u_{\alpha\beta} \) is the surface velocity and \( n_{\alpha\beta} \) is the unit normal to the surface pointing from the \( \alpha \) to the \( \beta \) phase. A useful identity which immediately follows by applying theorem (3.32b) to the constant scalar quantity \( \psi_\alpha = 1 \) is (Whitaker, 1986a)

\[
\nabla \langle 1_{(\alpha)} \rangle = \nabla \phi_\alpha = -\frac{1}{V} \sum_{\beta \neq \alpha} \int_{S_{\alpha\beta}} n_{\alpha\beta} dA. \quad (3.33)
\]

For the general function \( \psi_s \) defined on a surface contained within \( \forall \), the following integration theorems hold (Gray and Hassanizadeh, 1989; Gray et al., 1993)

\[
\frac{\partial \psi_s}{\partial t} = \frac{\partial}{\partial t} \bar{\psi}_s + \nabla \cdot \left( \frac{m_{n_s}}{v_s} \bar{\psi}_s \right) + k_{n_s} \psi_s - \frac{1}{V} \int_C m \cdot w \psi_s dC, \quad (3.34a)
\]

\[
\nabla s \bar{\psi}_s = \nabla \bar{\psi}_s - \nabla \cdot \left( \frac{m n_s}{v_s} \right) - k n_s \psi_s + \frac{1}{V} \int_C m \psi_s dC, \quad (3.34b)
\]

\[
\nabla s \cdot \Psi_s = \nabla \cdot \Psi_s - k n \cdot \psi_s + \frac{1}{V} \int_C m \cdot \Psi_s dC. \quad (3.34c)
\]

where \( v_n^s \) is the speed of displacement defined by eq. (3.12) and \( w \) is the velocity on \( C \).

### 3.3 General balance equations

#### 3.3.1 Microscopic balance equations

**Volume**

The general microscopic conservation equation for an extensive thermodynamic property
Table 3.1. Variables corresponding to the general microscopic quantities for a volume in eq. (3.35).

<table>
<thead>
<tr>
<th></th>
<th>ψ</th>
<th>i</th>
<th>b</th>
</tr>
</thead>
<tbody>
<tr>
<td>mass</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>momentum</td>
<td>u</td>
<td>t</td>
<td>g</td>
</tr>
<tr>
<td>energy</td>
<td>$E + \frac{1}{2}u \cdot u$</td>
<td>$tu + q$</td>
<td>$g \cdot u + h$</td>
</tr>
<tr>
<td>entropy</td>
<td>S</td>
<td>j</td>
<td>e</td>
</tr>
</tbody>
</table>

Table 3.2. Variables corresponding to the general microscopic quantities for a surface in eq. (3.36).

<table>
<thead>
<tr>
<th></th>
<th>$\psi_s$</th>
<th>$i_s$</th>
<th>$b_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>mass</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>momentum</td>
<td>$u_s$</td>
<td>$t_s$</td>
<td>$g$</td>
</tr>
<tr>
<td>energy</td>
<td>$E_s + \frac{1}{2}u_s \cdot u_s$</td>
<td>$t_su_s + q_s$</td>
<td>$g \cdot u_s + h$</td>
</tr>
<tr>
<td>entropy</td>
<td>$S_s$</td>
<td>$j_s$</td>
<td>$e_s$</td>
</tr>
</tbody>
</table>

$\psi$ can be written as (Whitaker, 1973; Gray, 1975)

$$\frac{\partial (\rho \psi)}{\partial t} + \nabla \cdot (\rho u \psi) - \nabla \cdot i - \rho b = 0,$$

(3.35)

where $\rho$ is the density, $u$ is the velocity field, $b$ is a source term and $i$ is a transport term-tensor of one order greater than $\psi$ and $f$. The mass, momentum, energy and entropy conservation equations can be obtained by substituting the corresponding quantities given in Tab. 3.1, into eq. (3.35). $E$ is the internal energy per unit mass, $S$ is the internal entropy per unit mass, $T$ is temperature, $t$ is the stress tensor, $q$ is the heat flux, $g$ is the acceleration due to gravity, $h$ is the external supply of energy, $j$ is the entropy flux and $e$ is the external supply of entropy.

**Surface**

When a body consists of two bulk phases $\alpha$ and $\beta$ separated by a surface with unit normal $n$, the general microscopic conservation equation for a thermodynamic property $\psi_s$ on the surface takes the following form (Deemer and Slattery, 1978)

$$\frac{\partial (\rho_s \psi_s)}{\partial t} + \nabla^s \cdot (\rho_s u_s \psi_s) - \nabla^s \cdot i_s - \rho_s b_s + \| \rho \psi (u - u_s) n - in \|_s^\beta = 0,$$

(3.36)

where $\rho_s$ is the surface density with units of mass per unit area, $u_s$ is the surface velocity, $\psi_s$, $i_s$ and $b_s$ are the surface counterparts for the general quantities for the bulk phase $\psi$, $n$ is the unit normal vector, $\nabla^s$ is the surface divergence operator.
\( i \) and \( b \) (see Tab. 3.2) and the operator \([Bn]_\beta^\alpha\) is the jump condition across the interface

\[ [Bn]_\beta^\alpha = B_\alpha n_\alpha + B_\beta n_\beta. \]

### 3.3.2 Macroscopic balance equations

#### Volume

The macroscopic conservation equation for phase \( \alpha \) is obtained by taking the superficial average of the general microscopic conservation equation (3.35) as follows

\[ \langle \frac{\partial (\rho_\alpha \psi_\alpha)}{\partial t} \rangle + \langle \nabla \cdot (\rho_\alpha u_\alpha \psi_\alpha) \rangle - \langle \nabla \cdot i_\alpha \rangle - \langle \rho_\alpha b_\alpha \rangle = 0. \] (3.37)

Application of theorems (3.32a) through (3.32c) yields

\[ \frac{\partial}{\partial t} (\rho_\alpha \psi_\alpha) + \nabla \cdot (\rho_\alpha (u_\alpha \psi_\alpha)) - \nabla \cdot (i_\alpha) - \rho_\alpha (b_\alpha) + \frac{1}{\forall} \sum_{\beta \neq \alpha} \int_{S_{\alpha\beta}} [\rho_\alpha \psi_\alpha (u_\alpha - u_{\alpha\beta}) n_{\alpha\beta} - i_\alpha n_{\alpha\beta}] dA = 0. \] (3.38)

For the case of constant microscopic density within the phase, the general macroscopic conservation equation simplifies as follows

\[ \frac{\partial}{\partial t} (\rho_\alpha \langle \psi_\alpha \rangle) + \nabla \cdot (\rho_\alpha \langle u_\alpha \langle \psi_\alpha \rangle \rangle) - \nabla \cdot (\langle i_\alpha \rangle) - \rho_\alpha \langle b_\alpha \rangle + \frac{1}{\forall} \sum_{\beta \neq \alpha} \int_{S_{\alpha\beta}} [\rho_\alpha \psi_\alpha (u_\alpha - u_{\alpha\beta}) n_{\alpha\beta} - i_\alpha n_{\alpha\beta}] dA = 0. \] (3.39)

Applying id. (3.24) to the second term and using id. (3.21), the latter takes the alternative form

\[ \frac{\partial}{\partial t} (\phi_\alpha \rho_\alpha \langle \psi_\alpha^\alpha \rangle) + \nabla \cdot (\phi_\alpha \rho_\alpha \langle u_\alpha \langle \psi_\alpha \rangle \rangle) - \nabla \cdot (\langle i_\alpha \rangle) - \phi_\alpha \rho_\alpha \langle b_\alpha \rangle + \frac{1}{\forall} \sum_{\beta \neq \alpha} \int_{S_{\alpha\beta}} [\rho_\alpha \psi_\alpha (u_\alpha - u_{\alpha\beta}) n_{\alpha\beta} - i_\alpha n_{\alpha\beta}] dA = 0. \] (3.40)

#### Surface

Similarly, a macroscopic conservation equation for a surface \( S_{\alpha\beta} \) with unit normal \( n \) can be obtained by taking the superficial surface average of its microscopic counterpart, eq. (3.36), over the union of interfacial areas between the two phases of interest within the averaging volume \( \forall \), as follows

\[ \frac{\partial}{\partial t} (\rho_{\alpha\beta} \psi_{\alpha\beta}) + \nabla^s \cdot (\rho_{\alpha\beta} u_{\alpha\beta} \psi_{\alpha\beta}) - \nabla^s \cdot i_{\alpha\beta} - \rho_{\alpha\beta} b_{\alpha\beta} + \frac{1}{\forall} \sum_{\beta \neq \alpha} \int_{S_{\alpha\beta}} [\rho_\psi (u_\alpha - \text{w}) \cdot m dC] = 0. \] (3.41)

Application of theorems (3.34a) and (3.34c) to the first two terms yield

\[ \frac{\partial}{\partial t} (\rho_{\alpha\beta} \psi_{\alpha\beta}) + \nabla^s \cdot (\rho_{\alpha\beta} u_{\alpha\beta} \psi_{\alpha\beta}) = \frac{\partial}{\partial t} (\rho_{\alpha\beta} \psi_{\alpha\beta}) + \nabla \cdot (\rho_{\alpha\beta} u_{\alpha\beta} \psi_{\alpha\beta}) + \frac{1}{\forall} \int_{C} \rho_{\alpha\beta} \psi_{\alpha\beta} (u_{\alpha\beta} - \text{w}) \cdot m dC. \] (3.42)
Substituting eq. (3.42) into eq. (3.41) and applying theorem (3.34c) further to the third term in (3.41) give
\[
\frac{\partial}{\partial t}(\rho_{\alpha\beta}\psi_{\alpha\beta}) + \nabla \cdot (\rho_{\alpha\beta}u_{\alpha\beta}\psi_{\alpha\beta}) - \nabla \cdot \hat{\mathbf{i}}_{\alpha\beta} + \kappa n_{\alpha\beta} - \rho_{\alpha\beta}b_{\alpha\beta} + [\rho\psi(u - u_{\alpha\beta})n - \mathbf{in}]^\beta_{\alpha} \\
+ \frac{1}{V} \int_C [\rho_{\alpha\beta}\psi_{\alpha\beta}(u_{\alpha\beta} - \mathbf{w}) - i_{\alpha\beta}] \cdot \mathbf{mdC} = 0.
\]
(3.43)

For the special case of a vector quantity \(\mathbf{i}_{\alpha\beta}\) tangent to the surface, i.e. \(\mathbf{i}_{\alpha\beta}\mathbf{n} = 0\), the fourth term in eq. (3.43) drops out and for the case of constant microscopic surface density, eq. (3.43) simplifies to
\[
\frac{\partial}{\partial t}(\hat{\mathbf{a}}_{\alpha\beta}\rho_{\alpha\beta}\langle\psi_{\alpha\beta}\rangle) + \nabla \cdot (\hat{\mathbf{a}}_{\alpha\beta}\rho_{\alpha\beta}\langle u_{\alpha\beta}\rangle\langle\psi_{\alpha\beta}\rangle) - \nabla \cdot (\hat{\mathbf{a}}_{\alpha\beta}\rho_{\alpha\beta}\langle \tilde{u}_{\alpha\beta}\tilde{\psi}_{\alpha\beta}\rangle) \\
- \nabla \cdot (\hat{\mathbf{a}}_{\alpha\beta}(\mathbf{i}_{\alpha\beta}^s)_{\alpha\beta}) - \hat{\mathbf{a}}_{\alpha\beta}\rho_{\alpha\beta}(b_{\alpha\beta})_{\alpha\beta} + \hat{\mathbf{a}}_{\alpha\beta}([\rho\psi(u - u_{\alpha\beta})n - \mathbf{in}]_{\alpha\beta}^{\beta}) \\
+ \frac{1}{V} \int_C [\rho_{\alpha\beta}\psi_{\alpha\beta}(u_{\alpha\beta} - \mathbf{w}) - i_{\alpha\beta}] \cdot \mathbf{mdC} = 0,
\]
(3.44)

where use of (3.24) and (3.31) has been made.

### 3.3.3 Momentum equation for a homogenous single-phase system: Darcy’s law

An important application of the method of volume averaging is the derivation of Darcy’s law (Whitaker, 1986a, 1998). Since this law will be applied later in this work, the derivation is proposed here again. Considering an averaging volume \(\forall\) where only two phases are present, one fluid \(\alpha\) having constant density and viscosity \(\rho_\alpha\) and \(\mu_\alpha\), and a solid phase \(k\), substituting the relevant quantities for momentum listed in Table 3.1 into the general macroscopic balance equation, eq. (3.40), yields
\[
\frac{\partial}{\partial t}(\phi_\alpha\rho_\alpha\langle u_\alpha\rangle) + \nabla \cdot (\phi_\alpha\rho_\alpha\langle u_\alpha\rangle\langle u_\alpha\rangle) - \nabla \cdot (\phi_\alpha\langle t_\alpha - \rho_\alpha\hat{u}_\alpha\hat{u}_\alpha\rangle) - \phi_\alpha\rho_\alpha g \\
+ \frac{1}{\forall} \int_{S_{\alpha k}} [\rho_\alpha u_\alpha(u_\alpha - u_{\alpha k})n_\alpha - t_\alpha n_{\alpha k}]dA = 0,
\]
(3.45)

which, introducing the stress tensor \(t_\alpha = -p_\alpha\mathbf{I} + \mu_\alpha [\nabla u_\alpha + (\nabla u_\alpha)^T]\), and assuming Stokes flow of the incompressible fluid \(\alpha\), simplifies to
\[
\nabla(\phi_\alpha\langle p_\alpha\rangle) - \mu_\alpha \nabla \cdot \langle \nabla u_\alpha\rangle - \phi_\alpha\rho_\alpha g + \frac{1}{\forall} \int_{S_{\alpha k}} (p_\alpha\mathbf{I} - \mu_\alpha \nabla u_\alpha)n_{\alpha k}dA = 0.
\]
(3.46)

The same result could have been obtained by applying theorems (3.32a) through (3.32c) to the superficial average of the microscopic Stokes momentum equation, eq. (2.2b). A second application of theorem (3.32b) to the second term of eq. (3.46) gives
\[
\nabla \cdot \langle \nabla u_\alpha\rangle = \nabla^2 \langle u_\alpha\rangle + \nabla \cdot \left[ \frac{1}{\forall} \int_{S_{\alpha k}} n_{\alpha k} u_\alpha dA \right] = \nabla^2 \langle u_\alpha\rangle,
\]
(3.47)
where use of the no-slip condition, $u_\alpha = 0$ at $S_{\alpha k}$, has been made. Incorporating this result into eq. (3.46), gives
\[
\nabla (\phi_\alpha \langle p_\alpha \rangle^\alpha) - \mu_\alpha \nabla^2 \langle u_\alpha \rangle - \phi_\alpha \rho_\alpha g + \frac{1}{V} \int_{S_{\alpha k}} p_\alpha n_{\alpha k} dA - \frac{\mu_\alpha}{V} \int_{S_{\alpha k}} (\nabla u_\alpha) n_{\alpha k} dA = 0, \tag{3.48}
\]
where the second term is known as Brinkman correction, while the last two terms are the pressure (or form) and viscous (or friction) drag forces per unit averaging volume, respectively.

Eq. (3.48) can be further rearranged by applying chain rule to the first term and using spatial decomposition (3.22) for pressure and velocity in the following way
\[
\phi_\alpha \nabla \langle p_\alpha \rangle^\alpha + \langle p_\alpha \rangle^\alpha \nabla \phi_\alpha - \mu_\alpha \nabla \langle u_\alpha \rangle^\alpha + \frac{1}{V} \int_{S_{\alpha k}} (\langle p_\alpha \rangle^\alpha I - \mu_\alpha \nabla \langle u_\alpha \rangle^\alpha) n_{\alpha k} dA + \frac{1}{V} \int_{S_{\alpha k}} (\tilde{p}_\alpha I - \mu_\alpha \nabla \tilde{u}_\alpha) n_{\alpha k} dA = 0.
\tag{3.49}
\]

Taking the intrinsic averages out of the integrals and applying id. (3.33), the macroscopic momentum balance becomes:
\[
\nabla \langle p_\alpha \rangle^\alpha - \phi_\alpha^{-1} \mu_\alpha \nabla^2 \langle u_\alpha \rangle - \rho_\alpha g + \phi_\alpha^{-1} \mu_\alpha \nabla \phi_\alpha \nabla \langle u_\alpha \rangle^\alpha + \frac{1}{V} \int_{S_{\alpha k}} (\tilde{p}_\alpha I - \mu_\alpha \nabla \tilde{u}_\alpha) n_{\alpha k} dA = 0,
\tag{3.50}
\]
which, for the case with constant porosity, simplifies to
\[
\nabla \langle p_\alpha \rangle^\alpha - \mu_\alpha \nabla^2 \langle u_\alpha \rangle^\alpha - \rho_\alpha g + \frac{1}{V} \int_{S_{\alpha k}} (\tilde{p}_\alpha I - \mu_\alpha \nabla \tilde{u}_\alpha) n_{\alpha k} dA = 0. \tag{3.51}
\]
The last term can be removed by introducing the permeability tensor $K$ defined in such a way that the following identity holds (Whitaker, 1986a)
\[
\frac{1}{V} \int_{S_{\alpha k}} (\tilde{p}_\alpha I - \mu_\alpha \nabla \tilde{u}_\alpha) n_{\alpha k} dA = -\mu_\alpha K^{-1} \langle u_\alpha \rangle,
\tag{3.52}
\]
so that, neglecting the Brinkman correction term, the Darcy’s law is finally recovered
\[
\langle u_\alpha \rangle = \frac{K}{\mu_\alpha} (\nabla \langle p_\alpha \rangle^\alpha - \rho_\alpha g) \tag{3.53}
\]

### 3.4 Microscopic capillary pressure

In classic theory of two-phase flow of immiscible fluids in porous media, capillary pressure $p_c$ is defined as (Scheidegger, 1963; Bear, 1972)
\[
p_c = p_n - p_w, \tag{3.54}
\]
where $p_n$ and $p_w$ are the pressures of the non-wetting and wetting phases on their respective side of the interface. This jump in pressure is due to the interfacial tension existing...
between the two fluids. The relationship between capillary pressure and interfacial tension is given by the well-known Young-Laplace equation

\[ p_c = \sigma k, \]  

(3.55)

where \( \sigma \) is the interfacial tension and \( k \) is the mean curvature of the interface. It was derived considering the force balance for an infinitesimal element of a curved interface, with constant interfacial tension, in the direction normal to the interface, where the only active forces are due to the pressures exerted by the adjacent phases on either side of the interface, and the component of the interfacial tension acting in the surface normal direction. In the following, a broader relationship between capillary pressure and other relevant quantities is provided resulting from either microscopic momentum balance or the principle of minimum energy.

### 3.4.1 Generalized Young-Laplace equation

Substituting the quantities listed in Table 3.2 for mass and momentum into eq. (3.36), yields the microscopic mass and momentum conservation equations for a surface

\[ \frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}_s) + [\rho(\mathbf{u} - \mathbf{u}_s) \cdot \mathbf{n}]_\alpha^\beta = 0, \]  

(3.56)

\[ \frac{\partial}{\partial t} (\rho_s \mathbf{u}_s) + \nabla \cdot (\rho_s \mathbf{u}_s \mathbf{u}_s) - \nabla \cdot \mathbf{t}_s - \rho_s g + [\rho \mathbf{u}(\mathbf{u} - \mathbf{u}_s) \mathbf{n} - \mathbf{t} \mathbf{n}]_\alpha^\beta = 0. \]  

(3.57)

Applying chain rule to the first two terms of eq. (3.57) and combining with the mass balance, the momentum equation is rearranged as

\[ \rho_s \frac{D_s \mathbf{u}_s}{Dt} - \nabla \cdot \mathbf{t}_s - \rho_s g + [\rho(\mathbf{u} - \mathbf{u}_s)(\mathbf{u} - \mathbf{u}_s) \mathbf{n} - \mathbf{t} \mathbf{n}]_\alpha^\beta = 0. \]  

(3.58)

This form of the microscopic momentum equation was first obtained by Scriven (1960) and Aris (1962) for the case of no exchange of fluid between the surface and the adjacent phases, i.e. \( \mathbf{u}_\alpha \approx \mathbf{u}_\beta \approx \mathbf{u}_s \), and then extended by Slattery (1964) to the general case. They derived the equation governing the motion of a surface in a three-dimensional Euclidean space from Newton’s second law and then split the external force into two components, one from any external source such as gravity and one from the traction exerted by the surroundings on either side of the surface. An alternative derivation of (3.58) was provided by Gray et al. (1993). Starting from the general microscopic momentum equation for a bulk phase, they applied integration over a straight line to a thin layer of fluid in the transition region between the two phases, and then took the limit of integration over a short line segment, obtaining as a result the balance equation for the surface.
Introducing constitutive relationships, the stress tensors for the bulk phase \( \mathbf{t} \) and for the interface \( \mathbf{t}_s \) take the form

\[
\mathbf{t} = -p \mathbf{I} + \mathbf{\tau} \quad \text{with units } F \, L^{-2}, \tag{3.59a}
\]
\[
\mathbf{t}_s = \sigma \mathbf{I}^s + \mathbf{\tau}_s \quad \text{with units } F \, L^{-1}, \tag{3.59b}
\]

where \( p \) is the pressure, \( \mathbf{\tau} \) and \( \mathbf{\tau}_s \) are the viscous stress tensors for the bulk phase and the interface respectively, \( \sigma \) is the interfacial tension, \( \mathbf{I} \) is the identity tensor and \( \mathbf{I}^s \) is the surficial identity tensor defined by eq. (3.4).

Substituting eqs. (3.59a) and (3.59b) into eq. (3.58) and expanding \( \nabla^s \cdot (\sigma \mathbf{I}^s) \) through identity (3.8), the momentum balance for the surface \( nw \) dividing the wetting and non-wetting phases becomes

\[
\rho_{nw} \frac{D \mathbf{u}_{nw}}{Dt} - \nabla^s \sigma - \sigma k \mathbf{n}_{nw} - \nabla^s \cdot \mathbf{\tau}_{nw} - \rho_s \mathbf{g} + (p_n - p_w) \mathbf{n}_{nw} - (\mathbf{\tau}_n - \mathbf{\tau}_w) \mathbf{n}_{nw} + \mathbf{n}_{nw} \cdot \left[ \rho_n (\mathbf{u}_n - \mathbf{u}_{nw})(\mathbf{u}_n - \mathbf{u}_{nw}) - \rho_w (\mathbf{u}_w - \mathbf{u}_{nw})(\mathbf{u}_w - \mathbf{u}_{nw}) \right] \mathbf{n}_{nw} = 0. \tag{3.60}
\]

The tangential and normal components of the momentum balance finally read

\[
\nabla^s \sigma = \mathbf{I}^s \rho_{nw} \frac{D \mathbf{u}_{nw}}{Dt} - \mathbf{I}^s (\nabla^s \cdot \mathbf{\tau}_{nw}) - \mathbf{I}^s \rho_{nw} \mathbf{g} - \mathbf{I}^s (\mathbf{\tau}_n - \mathbf{\tau}_w) \mathbf{n}_{nw} + \mathbf{n}_{nw} \cdot \left[ \rho_n (\mathbf{u}_n - \mathbf{u}_{nw})(\mathbf{u}_n - \mathbf{u}_{nw}) - \rho_w (\mathbf{u}_w - \mathbf{u}_{nw})(\mathbf{u}_w - \mathbf{u}_{nw}) \right] \mathbf{n}_{nw}, \tag{3.61a}
\]

\[
p_n - p_w = -\rho_{nw} \frac{D \mathbf{u}_{nw}}{Dt} \cdot \mathbf{n}_{nw} + \sigma k + (\nabla^s \cdot \mathbf{\tau}_{nw}) \cdot \mathbf{n}_{nw} + \rho_{nw} \mathbf{g} \cdot \mathbf{n}_{nw} + \mathbf{n}_{nw} \cdot (\mathbf{\tau}_n - \mathbf{\tau}_w) \mathbf{n}_{nw} - \mathbf{n}_{nw} \cdot \left[ \rho_n (\mathbf{u}_n - \mathbf{u}_{nw})(\mathbf{u}_n - \mathbf{u}_{nw}) - \rho_w (\mathbf{u}_w - \mathbf{u}_{nw})(\mathbf{u}_w - \mathbf{u}_{nw}) \right] \mathbf{n}_{nw}. \tag{3.61b}
\]

It is important to note that no assumptions on the nature of the flow nor on the properties of the fluids have been made so far, thus equations (3.61a) and (3.61b) have to be considered always valid. In particular, eq. (3.61b) written as

\[
p_n - p_w = \sigma k + \mathbf{\lambda}_s \cdot \mathbf{n}_{nw}, \tag{3.62}
\]

where the vector \( \mathbf{\lambda}_s \) accounts for all the momentum balance terms other than the adjacent fluids pressures, can be interpreted as an extension of the Young-Laplace equation to the dynamic case. For the most general case, \( \mathbf{\lambda}_s \) is given by the following combination of terms

\[
\mathbf{\lambda}_s = \lambda_p + \lambda_{\tau_s} + \lambda_g + \lambda_{\tau} + \lambda_{\mathbf{u}_{nw}}. \tag{3.63}
\]
where

\[ \lambda_\rho = -\rho_s \frac{D_s u_s}{Dt}, \quad (3.64a) \]

\[ \lambda_{\tau_s} = (\nabla^s \cdot \tau_s), \quad (3.64b) \]

\[ \lambda_g = \rho_s g, \quad (3.64c) \]

\[ \lambda_r = (\tau_n - \tau_w) n_n w, \quad (3.64d) \]

\[ \lambda_{u_s} = -[\rho_n (u_n - u_s)(u_n - u_s) - \rho_w (u_w - u_s)(u_w - u_s)] n_n w. \quad (3.64e) \]

Considering the surface massless \((\lambda_\rho = \lambda_g = 0)\), neglecting the viscous part of the interface stress tensor \((\lambda_{\tau_s} = 0)\) and assuming no fluid exchange between the interface and the surroundings \((\lambda_{u_s} = 0)\), the normal component of the momentum balance simplifies to

\[ p_n - p_w = \sigma k + \lambda_r \cdot n_n w. \quad (3.65) \]

The Young-Laplace equation \((3.55)\) is only recovered with further neglection of the net viscous stress between the adjacent bulk phases \((\lambda_r = 0)\) while, under all these assumptions, eq. \((3.61a)\) eventually leads to \(\nabla^s \sigma = 0\).

### 3.4.2 Definition of capillary pressure at thermodynamic equilibrium

Substituting the quantities listed in Table 3.2 for energy and combining with the mass balance \((3.56)\), the microscopic energy equation for a surface is written as

\[ \rho_s \frac{D_s}{Dt} \left( E_s + \frac{u_s \cdot u_s}{2} \right) - \nabla^s \cdot q_s - \nabla^s \cdot (t_s u_s) - \rho_s g \cdot u_s - \rho_s h - \left[ q \cdot n \right]^w_n - \left[ u \cdot n \right]^w_n + \left[ \rho(u - u_s) \left( E + \frac{u \cdot u}{2} - E_s - \frac{u_s \cdot u_s}{2} \right) \cdot n \right]^w_n = 0, \quad (3.66) \]

where \(E_s\) and \(q_s\) are the internal energy per unit mass and the heat flux of the surface respectively.

The first term in eq. \((3.66)\) represents the rate of change of energy of the surface, the second term is the heat conduction, the third is the mechanical work of the interface stress per unit time, the fourth is the mechanical work of the body forces and the last three terms account for the energy exchange between the interface and the adjacent bulk phases.

Neglecting heat fluxes and external energy supplies, expanding the surface operators, assuming no mass exchange between the interface and the surroundings and using the notation defined in equations \((3.64a)\) through \((3.64e)\), the energy balance becomes

\[ \rho_s \frac{D_s}{Dt} \left( E_s + \frac{u_s \cdot u_s}{2} \right) = (\nabla^s \sigma + \sigma k n_n w + \lambda_{\tau_s} + \lambda_g + \lambda_r) \cdot u_s + \tau_s : \nabla^s u_s - (p_n - p_w) v_n^s. \quad (3.67) \]
where $v_s^n$ is the surface speed of displacement defined by eq. (3.12). This form of the energy balance clearly indicates that the capillary pressure is related to the change of energy of the surface. In order to relate this change of energy to some properties of the surface, it is convenient to introduce the surface Helmholtz free energy per unit mass $A_s$ defined by eq. (2.7), so that, in isothermal conditions, the energy balance becomes

$$
\rho_s D_s \left( A_s + \frac{u_s \cdot u_s}{2} \right) + \rho_s T \frac{D_s S_s}{D t} = \left( \nabla^s \sigma + \sigma k n_{nw} + \lambda r_s + \lambda g + \lambda s \right) \cdot u_s + \tau_s : \nabla^s u_s - (p_n - p_w) v_s^n,
$$

which can be interpreted as a re-statement of the first principle of thermodynamics, that is: for an isothermal process with no entropy production, the work done on the surface is equal to the increase in the surface Helmholtz free energy.

A general criterion of equilibrium with respect to every possible change is that the free energy remains unchanged in any infinitesimal process occurring at constant temperature and pressure (Lewis et al., 1923). Furthermore, at equilibrium the rate of strain also vanishes so that the energy balance reduces to

$$
(p_n - p_w) v_s^n = \left( \nabla^s \sigma + \sigma k n_{nw} + \lambda g \right) \cdot u_s - \frac{\rho_s D_s}{2} \frac{D t}{D t} (u_s \cdot u_s),
$$

which is the Young-Laplace equation (3.55) in the form derived by Gibbs (1906) for the special case of uniform displacement of the interface in the direction normal to itself.

### 3.5 Macroscopic capillary pressure

#### 3.5.1 Standard approaches

At the macro-scale, capillary pressure is usually defined in analogy with its microscopic definition as (Whitaker, 1977; Bear and Verruijt, 1987)

$$
P_c = \langle p_n \rangle^n - \langle p_w \rangle^w.
$$

Although almost universally used in macro-scale applications of two-phase flow in porous media, eq. (3.70) has two major inconsistencies. The first one is related to the scale of the averaging measures. In fact, it does not seem possible to obtain eq. (3.70) from a rigorous averaging of the relevant microscopic balance equations. Moreover, eq. (3.60) is only valid at the interface and therefore its averaging would yield surface averages rather than intrinsic averages over the REV such as the ones appearing in eq. (3.70). An attempt to derive a macroscopic definition of capillary pressure through surface averaging
was made by Whitaker (1986b). He took the surface average of the normal component of the microscopic momentum equation for a surface, eq. (3.65), and employed the spatial decomposition (3.22) to obtain

\[
\langle p_n \rangle^n - \langle p_w \rangle^w = \sigma \langle k \rangle^{nw} + O \left( \frac{\mu_i \langle u_i \rangle^i}{d_i} \right),
\]  
(3.71)

where the subscript \( i \) refers to the largest contribution from the two fluid phases and \( d_i \) is the characteristic length scale of phase \( i \). This formulation for the macroscopic capillary pressure clearly highlights this averaging incongruity: at the left hand side intrinsic volume averages are present, while at the right hand side a surface average appears. Eq. (3.71) was derived by taking the surface average of a balance equation for a surface, thus averaged quantities are defined on that surface only. Volume averaging measures for the bulk pressures were then introduced through spatial decomposition. The trick was to use volume averages to decompose a quantity defined on a surface. This might not be very rigorous for real porous materials since it is generally false that the average of a quantity over the sum of the interfacial areas contained within an averaging volume is equal to the average of the same quantity over the whole averaging volume. More recently, Jackson et al. (2009), using the same averaging procedure of Whitaker, expressed the macroscopic capillary pressure in terms of the intrinsic surface averages as

\[
\langle p_n \rangle^{nw} - \langle p_w \rangle^{nw} = \sigma \langle k \rangle^{nw} + \langle \rho_{nw} g \cdot n_{nw} \rangle^{nw}.
\]  
(3.72)

Another weak point of these relationships is the fact that the spatial distribution of different orientated interfaces which may be present in a real porous material are not taken into account, instead they simply give the magnitude of the resultant force per total interfacial area. For these reasons, as already pointed out by Scheidegger (1963), formulations of such a kind seems to be suitable only for a single capillary or at best for a porous geometry formed by an assemblage of regular tubes. At present, such an averaging procedure for upscaling capillary pressure to the macroscale is still lacking and the macroscopic capillary pressure is usually given using functional relationships of the kind

\[
P_c = \mathcal{F}(s_w),
\]  
(3.73)

where \( s_w \) is the saturation of the wetting phase.

The second inconsistency of eq. (3.70) comes from dynamic considerations. It has been already pointed out that even at the microscopic level, dynamics effects neglected by the Young-Laplace equation can play a role under certain circumstances, and that the Young-Laplace equation must be seen merely as a condition of thermodynamic equilibrium. At
the macroscopic level this is exacerbated. The movement of one or more interfaces within a porous medium involves changes in phase saturations, interfacial areas and interfacial curvatures, as well as local mechanisms such as contact-angle hysteresis, snap-off and Haines jumps, which may provoke abrupt jumps in the interface configuration. Reducing all these features to the difference in the intrinsic average bulk pressures only, appears to be a rather implausible simplification.

3.5.2 Thermodynamic approach

Alternative definitions of the macroscopic capillary pressure can be obtained using thermodynamic principles. Morrow (1970) applied the first principle of thermodynamics to an idealized system for reversible immiscible displacement and obtained

\[ P_c = -\sum_{\alpha\beta} \sigma_{\alpha\beta} \frac{da_{\alpha\beta}}{d\phi} = -\sum_{\alpha\beta} \sigma_{\alpha\beta} \frac{d\hat{a}_{\alpha\beta}}{ds_w}, \quad \alpha\beta = nw, nk, wk \tag{3.74} \]

This expression for the macroscopic capillary pressure has two main problems: the first one was recognized by Morrow himself, who pointed out that this relationship cannot be applied to a real porous medium as changes in volume and interfacial area do not take place reversibly. The second one is that eq. (3.74) does not consider any change in free energy of the bulk phases. Moreover, the meaning of an interfacial tension for a fluid-solid surface is at best obscure.

A step forward was made by Allen (1986) who applied the second law of thermodynamics to the system formed by the bulk phases to obtain

\[ P_c = -s_w \rho_w \frac{\partial A_w}{\partial s_w} + s_n \rho_n \frac{\partial A_n}{\partial s_n}. \tag{3.75} \]

However, this definition is incomplete since it does not include any contribution from the interfaces.

A broader definition was given by Hassanizadeh and Gray (1990) and Gray and Hassanizadeh (1991) in the framework of a thermodynamic theory of two-phase flow in porous media. They started from the macroscopic mass, momentum, energy and entropy conservation equations for a bulk phase and for an interface. They then formulated constitutive hypotheses on the dependence of the Helmholtz free energies of the bulk phases and the interfaces on certain state variables such as density, phase saturation, temperature, interfacial area and porosity. Next, combining the second law of thermodynamics with the mass, energy and entropy balance equations, they recovered a combination of terms contributing to the entropy inequality for the whole system, which for isothermal conditions...
and in absence of any other thermodynamic forces satisfies
\[ \dot{s}_w \left[ P_w - P_n - s_w \rho_w \frac{\partial A_w}{\partial s_w} + s_n \rho_n \frac{\partial A_n}{\partial s_n} - \sum_{\alpha \beta} \hat{a}_{\alpha \beta} \rho_{\alpha \beta} \frac{\partial A_{\alpha \beta}}{\partial s_w} \right] \geq 0, \quad \alpha \beta = nw, nk, wk \]

(3.76)

where \( \dot{s}_w \) is the material time derivative of the saturation of the wetting phase, \( A_\alpha \) is the Helmholtz free energy per unit mass of phase \( \alpha \), \( A_{\alpha \beta} \) is the Helmholtz free energy per unit mass of interface \( \alpha \beta \) and the macroscopic pressure \( P_\alpha \) is given by the following thermodynamic definition \(^2\)

\[ P_\alpha = (\rho_\alpha)^2 \frac{\partial A_\alpha}{\partial \rho_\alpha}, \quad \alpha = n, w \]  

(3.77)

They then rearranged eq. (3.76) as

\[ -\dot{s}_w [(P_n - P_w) - P_c] \geq 0, \]

(3.78)

where they proposed the following definition for the macroscopic capillary pressure \( P_c \)

\[ P_c = -s_w \rho_w \frac{\partial A_w}{\partial s_w} + s_n \rho_n \frac{\partial A_n}{\partial s_n} - \sum_{\alpha \beta} \hat{a}_{\alpha \beta} \rho_{\alpha \beta} \frac{\partial A_{\alpha \beta}}{\partial s_w}. \]  

(3.79)

According to this definition, the macroscopic capillary pressure is thus related to the changes in free energy of both the bulk phases and the interfaces present within the system. If one takes the macroscopic interfacial tension \( \sigma_{\alpha \beta} \) as (Hassanizadeh and Gray, 1990)

\[ \sigma_{\alpha \beta} = -\hat{a}_{\alpha \beta} \rho_{\alpha \beta} \frac{\partial A_{\alpha \beta}}{\partial \hat{a}_{\alpha \beta}}, \]

(3.80)

and having postulated the dependence of \( A_{\alpha \beta} \) on \( \hat{a}_{\alpha \beta} \), application of the cyclic chain rule to the last term in eq. (3.79) yields

\[ \sum_{\alpha \beta} \hat{a}_{\alpha \beta} \rho_{\alpha \beta} \frac{\partial A_{\alpha \beta}}{\partial \hat{a}_{\alpha \beta}} = -\sum_{\alpha \beta} \hat{a}_{\alpha \beta} \rho_{\alpha \beta} \frac{\partial A_{\alpha \beta}}{\partial \hat{a}_{\alpha \beta}} \frac{\partial \hat{a}_{\alpha \beta}}{\partial s_w} = \sum_{\alpha \beta} \sigma_{\alpha \beta} \frac{\partial \hat{a}_{\alpha \beta}}{\partial s_w}, \]

(3.81)

so that eq. (3.79) becomes

\[ P_c = -s_w \rho_w \frac{\partial A_w}{\partial s_w} + s_n \rho_n \frac{\partial A_n}{\partial s_n} - \sum_{\alpha \beta} \sigma_{\alpha \beta} \frac{\partial \hat{a}_{\alpha \beta}}{\partial s_w}, \]

(3.82)

which resembles the definition obtained by Morrow, eq. (3.74), except that Morrow did not consider the changes in free energy of the bulk phases and thus only the last term of eq. (3.82) arises in his formulation. On the other hand, if this "Morrow’s term" is

\[^2\text{A physical interpretation of this different pressure coming from change in energy with respect to volume and the physically measurable pressure related to the trace of the stress tensor can be found in Bennethum and Weinstein (2004).}\]
neglected in eq. (3.82), one recovers Allen’s definition, eq. (3.75). In fact, eq. (3.82) can be interpreted as a combination of these two works, or, the other way, eqs. (3.74) and (3.75) are special cases of eq. (3.82).

Eq. (3.78) can be used to illustrate the different displacement mechanisms which may occur under different dynamic conditions. When \((P_n - P_w) > P_c\), \(\dot{s}_w\) must be negative and therefore drainage takes place. When instead \((P_n - P_w) < P_c\), the entropy inequality demands \(\dot{s}_w\) be positive, corresponding to imbibition taking place. Only at equilibrium conditions, when \(\dot{s}_w = 0\), the condition \((P_n - P_w) = P_c\) holds.

In a companion paper, Gray and Hassanizadeh (1993) concluded suggesting a first-order constitutive equation for \(\dot{s}_w\) in the form

\[
\dot{s}_w = -\eta^{-1}[(P_n - P_w) - P_c],
\]

where \(\eta\) is a non-negative material coefficient accounting for dynamic effects. Thereafter, Hassanizadeh et al. (2002) recast eq. (3.83) into a slightly different form introducing the following notation

\[
P_{c^{dyn}} - P_{c^{stat}} = -\eta \dot{s}_w,
\]

where \(P_{c^{dyn}}\) is the difference between the pressures of the bulk phases and the macroscopic capillary pressure is denoted now as equilibrium or static capillary pressure \(P_{c^{stat}}\). Dahle et al. (2005) and Mirzaei and Das (2007) defined \(P_{c^{dyn}}\) as the difference between the intrinsic volume averages of the pressures in the non-wetting and wetting phases while Jackson et al. (2009) used for the equilibrium capillary pressure \(P_{c^{stat}}\) the intrinsic surface average of the interface mean curvature, so that one can write

\[
P_c = \langle \sigma k \rangle^{nw} = \mathcal{F}(s_w, \text{other parameters}) = \langle p_n \rangle^n - \langle p_w \rangle^w + \eta \dot{s}_w.
\]

While still maintaining the averaging scale inconsistency, eq. (3.85) resolves the second shortcoming of eq. (3.70) in the sense that now dynamic effects are embodied in the macroscopic capillary pressure definition through the coefficient \(\eta\). There are numerous studies available in literature attempting to evaluate this coefficient both experimentally and numerically (Hassanizadeh et al., 2005; O’Carroll et al., 2005; Sakaki et al., 2010; Camps-Roach et al., 2010; Bottero et al., 2011), but this is beyond the scope of this chapter.
3.5.3 Proposed averaging approach

The microscopic momentum conservation equation for the surface $nw$ is recalled

\[
\frac{\partial}{\partial t}(\rho_{nw}\mathbf{u}_{nw}) + \nabla \cdot (\rho_{nw}\mathbf{u}_{nw}\mathbf{u}_{nw}) - \nabla \sigma + \mathbf{g} + (p_n - p_w)\mathbf{n}_{nw} - (\mathbf{\tau}_n - \mathbf{\tau}_w)\mathbf{n}_{nw} + [\rho_n\mathbf{u}_n(\mathbf{u}_n - \mathbf{u}_{nw}) - \rho_w\mathbf{u}_w(\mathbf{u}_w - \mathbf{u}_{nw})] = 0.
\]

(3.87)

The superficial average of eq. (3.86) is taken as

\[
\frac{1}{V} \int_{S_{nw}} \frac{\partial}{\partial t}(\rho_{nw}\mathbf{u}_{nw})dA + \frac{1}{V} \int_{S_{nw}} \nabla \cdot (\rho_{nw}\mathbf{u}_{nw}\mathbf{u}_{nw})dA - \frac{1}{V} \int_{S_{nw}} \nabla \sigma dA
- \frac{1}{V} \int_{S_{nw}} \rho_{nw}\mathbf{g}dA + \frac{1}{V} \int_{S_{nw}} (p_n - p_w)\mathbf{n}_{nw}dA
- \frac{1}{V} \int_{S_{nw}} (\mathbf{\tau}_n - \mathbf{\tau}_w)\mathbf{n}_{nw}dA + \frac{1}{V} \int_{S_{nw}} [\rho_n\mathbf{u}_n(\mathbf{u}_n - \mathbf{u}_{nw}) - \rho_w\mathbf{u}_w(\mathbf{u}_w - \mathbf{u}_{nw})]\mathbf{n}_{nw}dA = 0.
\]

(3.87)

Applying averaging theorems (3.34a) through (3.34c) to eq. (3.87) and using id. (3.24) yield

\[
\frac{\partial}{\partial t}(\bar{a}_{nw}\rho_{nw}\langle \mathbf{u}_{nw} \rangle^{nw}) + \nabla \cdot (\bar{a}_{nw}\rho_{nw}\langle \mathbf{u}_{nw} \rangle^{nw}\langle \mathbf{u}_{nw} \rangle^{nw}) + \nabla \cdot (\bar{a}_{nw}\rho_{nw}\langle \mathbf{n}_{nw} \mathbf{u}_{nw} \rangle^{nw})
- \nabla \langle \bar{a}_{nw}\langle \sigma \rangle^{nw} \rangle + \nabla \cdot (\bar{a}_{nw}\langle \mathbf{n}_{nw} \mathbf{n}_{nw} \mathbf{\sigma} \rangle^{nw}) - \nabla \cdot (\bar{a}_{nw}\langle \mathbf{\tau}_{nw} \rangle^{nw}) - \bar{a}_{nw}\rho_{nw}\mathbf{g}
+ \bar{a}_{nw}\langle (p_n - p_w)\mathbf{n}_{nw} \rangle^{nw} - \bar{a}_{nw}\langle (\mathbf{\tau}_n - \mathbf{\tau}_w)\mathbf{n}_{nw} \rangle^{nw} + \bar{a}_{nw}\langle \rho_n\mathbf{u}_n(\mathbf{u}_n - \mathbf{u}_{nw}) \rangle^{nw}
- \rho_w\mathbf{u}_w(\mathbf{u}_w - \mathbf{u}_{nw})\rangle^{nw} + \frac{1}{V} \int_{S} [\rho_{nw}\mathbf{u}_{nw}(\mathbf{u}_{nw} - \mathbf{w}) \cdot \mathbf{m} - \mathbf{\sigma}\mathbf{m} + \mathbf{\tau}_{nw}\mathbf{m}] d\mathbf{C} = 0.
\]

(3.88)

The same result could have been easily obtained by substituting the correspondent quantities for momentum from Tab. 3.2 into the general macroscopic conservation equation (3.44) derived in Sec. 3.3.2. Applying surface spatial decomposition (3.29) to the pressures in eq. (3.88), the macroscopic momentum balance is rearranged as follows

\[
\bar{a}_{nw}\langle (p_n)_{nw} \rangle^{nw} - \langle p_w \rangle_{nw}^{nw} = \nabla \langle \bar{a}_{nw}\langle \sigma \rangle^{nw} \rangle - \nabla \cdot (\bar{a}_{nw}\langle \mathbf{n}_{nw} \mathbf{n}_{nw} \mathbf{\sigma} \rangle^{nw}) + \Lambda_s,
\]

(3.89)

where the l.h.s. is the macroscopic capillary pressure $P_c$ and $\Lambda_s$ is defined in analogy with the microscopic quantity $\lambda_s$ used for the microscopic capillary pressure in Sec. 3.4, as

\[
\Lambda_s = \Lambda_p + \Lambda_{\tau_n} + \Lambda_g + \Lambda_{\tilde{p}} + \Lambda_{\tau} + \Lambda_{\tilde{u}_n} + \Lambda_c.
\]

(3.90)
with
\[ \Lambda_{\rho} = -\frac{\partial}{\partial t}(\hat{a}_{nw}\rho_{nw}\langle u_{nw}\rangle_{nw}) - \nabla \cdot (\hat{a}_{nw}\rho_{nw}\langle u_{nw}\rangle_{nw}^{nw} \langle u_{nw}\rangle^{nw}) \] (3.91a)
\[ - \nabla \cdot (\hat{a}_{nw}\rho_{nw}\langle u_{nw}\rangle_{nw}^{nw}) \]
\[ \Lambda_{\tau_{x}} = \nabla \cdot (\hat{a}_{nw}\langle \tau_{nw}\rangle_{nw}^{nw}), \] (3.91b)
\[ \Lambda_{g} = \hat{a}_{nw}\rho_{nw}g, \] (3.91c)
\[ \Lambda_{\tilde{p}} = -\hat{a}_{nw}\langle (\tilde{p}_{n} - \tilde{p}_{w})n_{nw}\rangle_{nw}^{nw}, \] (3.91d)
\[ \Lambda_{\tau} = \hat{a}_{nw}\langle (\tau_{n} - \tau_{w})n_{nw}\rangle_{nw}^{nw}, \] (3.91e)
\[ \Lambda_{u_{s}} = -\hat{a}_{nw}\langle [\rho_{n}u_{n}(u_{n} - u_{nw}) - \rho_{w}u_{w}(u_{w} - u_{nw})]n_{nw}\rangle_{nw}^{nw}, \] (3.91f)
\[ \Lambda_{c} = -\frac{1}{\forall} \int_{C} [\rho_{nw}u_{nw}(u_{nw} - w) \cdot m - \sigma m + \tau_{nw}m] dC. \] (3.91g)

From eq. (3.89), the macroscopic capillary pressure is now expressed as a vector in the direction of the average unit normal to the interface, and is defined as the macroscopic force due to capillary pressure acting on all the \( nw \) interfaces per unit averaging volume
\[ \mathcal{P}_{c} = \hat{a}_{nw}(\langle p_{n}\rangle_{nw}^{nw} - \langle p_{w}\rangle_{nw}^{nw})\langle n_{nw}\rangle_{nw}^{nw}. \] (3.92)

This new definition of the macroscopic capillary pressure has three major merits. Firstly, its derivation is rigorous - it is based solely on application of integration theorems to general microscopic balance equations. Moreover, use of the Dirac function in eq. (3.28) allows for conveniently converting surface integrals into volume integrals and therefore carrying out averaging over the whole averaging volume. The latter aspect is particularly relevant if one wants to remove the scale inconsistency of traditional definitions of macroscopic capillary pressure. Secondly, no assumptions on the flow regime nor on the properties of the different phases have been made. Hence, eq. (3.89) has to be considered valid for all possible flow conditions, static or dynamic, laminar or turbulent, as well as regardless of the fluids compressibility. Finally, the definition of macroscopic capillary pressure in vector form as a resultant force due to interfacial effects acting within the averaging volume permits to consider the actual spatial configuration of the various interfaces which may be present in real complex porous microstructures.

If now one introduces the following set of common simplifications for two-phase flow in porous media:

- No material interchange between the interface and the surrounding, i.e. \( \Lambda_{u_{s}} = 0 \),
- Inertial forces are negligible, i.e. \( \Lambda_{\rho} = 0 \),
- Gravity effects on the interface are neglected \( \Lambda_{g} = 0 \),
• The viscous part of the interface stress tensor is neglected, i.e. $\Lambda_{\tau_s} = 0$,

• Constant interfacial tension,

the macroscopic momentum balance becomes

$$\hat{a}_{nw}(\langle p_n \rangle^{nw} - \langle p_w \rangle^{nw})\langle n_{nw} \rangle^{nw} = \sigma \left[ \nabla \hat{a}_{nw} - \nabla \cdot (\hat{a}_{nw}\langle n_{nw}n_{nw} \rangle^{nw}) + \frac{1}{\nu} \int_C m dC \right] + \Lambda_{\tilde{p}} + \Lambda_{\tau}. \tag{3.93}$$

The term in square brackets multiplying $\sigma$ can be simplified by noting that applying theorem (3.34b) to the constant scalar quantity $\psi_s = 1$ defined on a surface $S$, yields

$$\int_C m dC = -\nabla a_s + \nabla \cdot (a_s\langle n_{ns}\rangle^s) + a_s\langle k_{ns} \rangle^s. \tag{3.94}$$

By incorporating the latter result into eq. (3.93), the macroscopic capillary pressure is written as

$$\hat{a}_{nw}(\langle p_n \rangle^{nw} - \langle p_w \rangle^{nw})\langle n_{nw} \rangle^{nw} = \hat{a}_{nw}\sigma\langle k_{nw} \rangle^{nw} + \Lambda_{\tilde{p}} + \Lambda_{\tau}. \tag{3.95}$$

The same result would have been obtained if the term $\nabla^s\sigma$ had been neglected in first instance in eq. (3.86). The last two terms in eq. (3.95) can be estimated as (Whitaker, 1986a,b, 1998)

$$\Lambda_{\tilde{p}} + \Lambda_{\tau} = \hat{a}_{nw}(\langle \tilde{p}_n - \tilde{p}_w \rangle n_{nw})^{nw} + \hat{a}_{nw}(\langle \tau_n - \tau_w \rangle n_{nw})^{nw} = O\left(\frac{\mu_i\langle u_i \rangle^i}{d_i^2}\right), \tag{3.96}$$

where the same length-scale considerations which led to eq. (3.71) have been used. By incorporating this result into eq. (3.95), the macroscopic capillary pressure takes its final form

$$\hat{a}_{nw}(\langle p_n \rangle^{nw} - \langle p_w \rangle^{nw})\langle n_{nw} \rangle^{nw} = \hat{a}_{nw}\sigma\langle k_{nw} \rangle^{nw} + O\left(\frac{\mu_i\langle u_i \rangle^i}{d_i^2}\right). \tag{3.97}$$

This form of the macroscopic capillary pressure resembles the one obtained by Whitaker (1986b), eq. (3.71), with two major distinctions. The first and most striking one lays in the fact that eq. (3.71) is in scalar form while eq. (3.97) is in vector form. This difference comes from the more rigorous approach chosen for averaging the relevant microscopic balance equations. Whitaker took the average of the normal component of the surface microscopic momentum balance, eq. (3.62), only, while here averaging of the microscopic momentum balance for the surface, eq. (3.60), is carried out over the whole averaging volume through use of the Dirac function. The second distinction is the use of the intrinsic surface average to define the macroscopic capillary pressure in eq. (3.92). As already pointed out, Whitaker instead employed intrinsic volume averages. This difference in averaging measures arises from the different choice in applying spatial decomposition to
the pressure terms. Although it is acknowledged that spatial decomposition is a fictitious treatment of the microscopic quantities made by the authors, nevertheless it does seem more rigorous to be consistent with the averaging domain over which averaging is being carried out. Since averaging in eq. (3.88) is taken over interfacial areas, intrinsic surface averages are used. The two approaches coincide only if the wetting and the non-wetting phase have constant pressure within the averaging volume.

### 3.6 Summary

A detailed and thorough exposition of the theory of capillary pressure in porous media has been presented. At the microscopic level, capillary pressure is taken by definition as the difference between the pressures of the surrounding fluids on their respective side of the interface. Its relationship with the properties of the fluids and the geometrical characteristics of the interface is given by the well-known Young-Laplace equation, eq. (3.55). The Young-Laplace equation relates the capillary pressure solely to the properties of the fluids, through the interfacial tension, and to the shape of the interface, i.e. the interface mean curvature. For this reason, the capillary pressure can be regarded as an intrinsic property of the medium for a given pair of fluids. In reality, it has been shown as the Young-Laplace equation holds only at thermodynamic equilibrium and a generalized Young-Laplace formulation has been derived from the full momentum balance for a surface, eq. (3.62). This broader formulation is to be considered valid for all possible flow conditions and properties of the fluids mixture. However, for most real cases, the flow of two immiscible fluids through porous media occurs at very low velocities and thus the balance of forces given by the Young-Laplace equation is approximately correct at the scale of a single pore.

At the macroscopic level, there is no clear definition of capillary pressure. Generally, the macroscopic capillary pressure is given in analogy with its microscopic definition as the difference between the intrinsic averages of the bulk pressures taken over the REV, eq. (3.70). However, aside from the fact that it does not come from any averaging procedure, this definition clearly embodies a number of approximations which seem to be rather implausible when modelling complex phenomena taking place during fluid flow and transport in real porous materials. Other authors have sought a thermodynamic basis of capillary pressure at the macro-scale, i.e. eqs. (3.74), (3.75) and (3.79)-(3.82). On one hand, thermodynamic definitions of the macroscopic capillary pressure have the quality of being undoubtedly more theoretically sound than simple hysteretic functions.
of saturation, but on the other hand, they result from constitutive hypotheses which are axiomatically introduced by the authors. Furthermore, these thermodynamic definitions do not provide a clear relationship between thermodinamically defined pressure and pressures related to the stress tensor, and no proper thermodynamic characterization of the solid-fluid-fluid contact lines is provided.

Finally, there are more traditional approaches which attempt at taking the surface average of the microscopic governing equations over the union of all the interfaces present within the REV, i.e. eqs. (3.71) and (3.72). A new averaging procedure which interprets the macroscopic capillary pressure as a macroscopic force per unit averaging volume has been presented here. This novel definition of the macroscopic pressure, eq. (3.92), resolves most of the shortcomings of the previous studies, such as the averaging-scale inconsistency, the lack of dynamic terms in momentum balance and the accounting for the different orientation of interfaces within the averaging volume. However, for as much one gains in rigour and theoretical soundness with this novel definition, as much is lost in applicability, since evaluation of a mean interface normal and curvature can potentially be an enormous task for real macro-scale applications. Nevertheless, this approach could be very useful for interpreting the results of the pore-scale simulation models such as the one developed within this project, and also for interpreting $\mu$-CT results. Prediction of the flow variables from pore-scale simulations of drainage/imbibition on digital images of reservoir rocks will provide capillary pressure and water saturation time series at a scale smaller than that of a lab sample, and thus more insight into the $P_c - S_w$ relationship. Moreover, as oppose to traditional coreflooding experiments, where $P_c$ is simply calculated from the pressures at both ends of the core, numerical simulations has the advantage that different measures of $P_c$ can be obtained. This results in more rigorous $P_c - S_w$ relationships.

Eventually, it should be noted that none of the presented theories embrace a thorough physical and/or thermodynamic description of the solid-fluid-fluid contact lines. This could potentially be subject of a future more comprehensive study.
Chapter 4

Simulation of single-phase flow

4.1 Introduction

In this chapter, an integrated approach for calculating the petrophysical properties of rocks, comprising rock imaging, statistical spatial correlation and numerical simulations, is presented. Statistical correlation is a quick and efficient way for preliminary estimation of the pore-space properties such as specific pore-grain surface area and mean pore and grain size, while the results of the single-phase flow simulations carried out on the \( \mu \)-CT images, are used to calculate the permeability tensor. The analysis is carried out on 3D digital images of two rock formations: one sandstone and one carbonate. The chapter is organized as follows. First, the morphological properties of the rocks are described in Sec. 4.2. Statistical correlation tools are illustrated in Sec. 4.3. In Sec. 4.4, the numerical method for simulating single-phase flow at the pore-scale is presented, and simulation results are shown together with a comparison of various permeability estimates obtained from different approaches. Finally, a novel convergence criterion for the SIMPLE algorithm, and more generally for the family of pressure-correction methods, based on bulk momentum balance, is presented in Sec. 4.5.

4.2 Rocks description

Core plugs of two rock formations are used in this work: one sandstone (Fig. 4.1a) and one carbonate (Fig. 4.1b). These rock formations have never been studied before, and were specifically selected as typical reservoir rocks. Cylindrical cores of the former one (5 cm long and 3.75 cm in diameter) were drilled from a single sample block of Jurassic Lower Calcareous Gritstone Formation from Cayton Bay (CB), Scaraborough (UK). The cores consist mainly of quartz (76%), muscovite (7.5%) and mitrocline (6.5%) with a range of
Calcite comprising about 4-5% of the rock mass. Measured porosity and permeability were ranging between 30.5% and 35% (average 33%) and from 8 to 12 mDa respectively. Mean pore diameter observed from Scanning Electron Microscope (SEM) images is 100 μm. Further details on the morphology of this rock can be found in Lamy-Chappuis et al. (2014).

The second rock formation studied is a carbonate of late Cambrian age. This was cut from an outcrop sample of the Al Bashair Formation, Huqf High, Oman. It is an oolitic grainstone (grains range in size from 200-480 μm, median 330 μm) with scattered lime mudstone clasts up to 3 cm in length (< 1 cm thickness). The sample is composed entirely of calcite and, despite its age, contains significant intergranular porosity which has been solution enhanced forming small vugs in places. The intergranular/vuggy pore spaces observed in SEM images range from 90 μm to 700 μm diameter, together with microporosity (< 20 μm) within grains (Haines et al., 2015). As with many carbonate samples, the pore system is heterogeneous. Porosity of 15.98% and permeability of approximately 1500 mDa were measured on a 4.48 cm in length and 2.53 in diameter core plug. A specimen was then manually detached from the core plug and scanned.

CT imaging of the sandstone sample was carried out using a μ-CT scanner housed in the Department of Mechanical Engineering, University of Leeds, at 5 and 10 μm pixel resolution (Lamy-Chappuis, 2015). The carbonate sample was scanned using Zeiss XRadia Versa 410 microscope with a 140kV/10W X-rays source housed in the School of Engineering, University of Aberdeen, at pixel resolution of 8.3 μm and the field of view covering 16.6 x 16.6 x 16.6 mm (see Fig. 4.2). Acquisition of 2D and the reconstruction of 3D images was performed using the software supplied by the respective manufacturers. The
Figure 4.2. CT imaging of the carbonate sample: 2D sections corresponding to the three orthogonal planes (a, b and c) and the reconstructed 3D microstructure (d).

latter step involved applying an optimum pixel shift in order to compensate for a slight miss-alignment of the centre of rotation for the sample bottom and top, and an optimum beam hardening constant in order to minimise the effect of beam hardening. Manual thresholding of the reconstructed 3D images, done in such a way to match the experimentally measured porosity, produced 3D binary models consisting of void and solid voxels. Different sub-samples were then extracted from these initial binary images and used as FV meshes. For the sandstone, sub-samples from three different locations were taken (CBsandstone1, 2 and 3) while for the carbonate, sub-samples were extracted by keeping a fixed origin point and considering cubic volumes of increasing size centered at this point.

A list of all the sub-samples considered in this study is given in Table 4.1 while Fig. 4.3 shows an example of the reconstructed microstructures for both the rocks.
Table 4.1. List of samples used in this study.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Size $[mm^3]$</th>
<th>Resolution $[\mu m]$</th>
<th>Voxels $[\phi]$</th>
<th>$\phi[%]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CBSandstone1a</td>
<td>1</td>
<td>10</td>
<td>100$^3$</td>
<td>31.9</td>
</tr>
<tr>
<td>CBSandstone1b</td>
<td>1</td>
<td>5</td>
<td>200$^3$</td>
<td>32.1</td>
</tr>
<tr>
<td>CBSandstone2</td>
<td>1</td>
<td>5</td>
<td>200$^3$</td>
<td>30.9</td>
</tr>
<tr>
<td>CBSandstone3</td>
<td>8</td>
<td>5</td>
<td>400$^3$</td>
<td>29.6</td>
</tr>
<tr>
<td>Carb200</td>
<td>4.6</td>
<td>8.3</td>
<td>200$^3$</td>
<td>16.5</td>
</tr>
<tr>
<td>Carb300</td>
<td>15.6</td>
<td>8.3</td>
<td>300$^3$</td>
<td>15.8</td>
</tr>
<tr>
<td>Carb400</td>
<td>36.6</td>
<td>8.3</td>
<td>400$^3$</td>
<td>15.9</td>
</tr>
<tr>
<td>Carb500</td>
<td>71.5</td>
<td>8.3</td>
<td>500$^3$</td>
<td>15.8</td>
</tr>
</tbody>
</table>

Figure 4.3. Reconstructed 3D digital images of the samples CBSandstone1a (a) and Carb300 (b).
4.3 Two-point spatial correlation function

A binary indicator function $\xi$ is defined for any position $\mathbf{x}$ in the medium as follows

$$
\xi(\mathbf{x}) = \begin{cases} 
1, & \text{if } \mathbf{x} \text{ is in the pore space}, \\
0, & \text{if } \mathbf{x} \text{ is in a grain}.
\end{cases} \tag{4.1}
$$

The two-point correlation function $Z_2$ is defined as the probability that two points separated by a distance $r$ will both lie in the pore space. It is mathematically given by (Berryman, 1985; Berryman and Blair, 1986)

$$
Z_2(r) = \langle \xi(\mathbf{x})\xi(\mathbf{x} + \mathbf{r}) \rangle, \tag{4.2}
$$

where angle brackets denote superficial volume averaging over all positions $\mathbf{x}$ and $Z_2(0) = \phi$. The two-point correlation function for a 2D square digital image is computed using the method by Berryman (1985). The discrete form of eq. (4.2) for progressive one-pixel increments $k$ is given by

$$
Z_2(k) = \frac{1}{2k + 1} \sum_{l=0}^{2k} Z_2(k\cos\varphi, k\sin\varphi), \quad \varphi = \frac{\pi l}{4k}, \quad 0 \leq k \leq N/2, \tag{4.3}
$$

where $N$ is the number of pixels along each side of the image and the discrete function $Z_2(m, n)$ has the form

$$
Z_2(m, n) = \frac{1}{N_{\max}} \sum_{1 \leq i \leq i_{\max}} \sum_{1 \leq j \leq j_{\max}} \xi_{ij} \xi_{i+m,j+n}, \tag{4.4}
$$

where $i_{\max} = N - m$, $j_{\max} = N - n$ and $N_{\max} = i_{\max} j_{\max}$. The procedure is schematically illustrated in Fig. 4.4. When $\varphi$ takes values other than 0 and $\pi/2$, i.e. the discrete point does not coincide with a lattice node, $Z_2(m, n)$ for a diagonal segment is computed using bilinear interpolation from the 4 closest nodes. The extension to the 3D case is straightforward, with eqs. (4.3) and (4.4) modified as follows

$$
Z_2(k) = \frac{1}{(2k + 1)^2} \sum_{l_1, l_2=0}^{2k} Z_2(k\sin\theta \cos\varphi, k\sin\theta \sin\varphi, k\cos\theta), \quad \theta = \frac{\pi l_1}{4k}, \quad \varphi = \frac{\pi l_2}{4k}, \quad 0 \leq k \leq N/2, \tag{4.5}
$$

$$
Z_2(m, n, o) = \frac{1}{N_{\max}} \sum_{1 \leq i \leq i_{\max}} \sum_{1 \leq j \leq j_{\max}} \sum_{1 \leq k \leq k_{\max}} \xi_{ijk} \xi_{i+m,j+n,k+o}, \tag{4.6}
$$

where $k_{\max} = N - o$, $N_{\max} = i_{\max} j_{\max} k_{\max}$ and $Z_2(m, n, o)$ is computed using trilinear interpolation from the 8 closest nodes.
Figure 4.4. Schematic of the method employed for computing the two-point correlation function $Z_2(k)$ on a 2D digital image (Berryman, 1985). The discrete two-point correlation function $Z_2$ is computed at triangular points located along the perimeters of circles centered at the reference point. The circles radii are 1 pixel ($k=1$), 2 pixels ($k=2$), etc.
This correlation function has the important feature that many physical properties of the porous material, such as porosity $\phi$, pore-grain specific surface area $s$ and effective pore size $r_c$, can be obtained from it. Berryman and Blair (1986) showed that

$$\lim_{r \to \infty} Z_2(r) = \phi^2,$$

$$Z'_2(0) = -\frac{s}{\chi},$$

$$r_c = \frac{\phi(1 - \phi)}{Z'_2(0)},$$

where $\chi$ is 4 for 2D and 6 for 3D images (Yeong and Torquato, 1998) and the initial slope $Z'_2(0)$ is computed using ordinary least squares to the first four or five points of the curve. Specific surface area can then be used to estimate the absolute permeability $K$ following the Kozeny-Carman (KC) approach. KC empirical formulations relate permeability to porosity and hydraulic radius, the latter defined as the ratio of the pore volume and the wetted area. The KC relation developed by Walsh and Brace (1984) is used here:

$$K = \frac{\phi^2}{m_1 Fs^2},$$

where $m_1$ is a constant depending on the pore shape (2 for circular tubes and 3 for cracks) and $F$ is the electrical formation factor which can be estimated using Archie’s formula (Archie et al., 1942)

$$F = \phi^{-m_2},$$

where $m_2$ is a constant ranging between 1.8 and 2 for sandstones.

Figure 4.5 shows the computed two-point correlation function for the CB sandstone images. For each sample, four curves are displayed, corresponding to the whole 3D image and three 2D cross-sections chosen with the same areal porosity as the volumetric one. The 3D curve is computed using eqs. (4.5) and (4.6), while the 2D curves are computed using (4.3) and (4.4). The 3D curve smoothly approaches the asymptotic value of $\phi^2$ with the same trend for all the samples, suggesting that for this rock 1 $mm^3$ can be assumed as REV for the pore geometry. However, for the smaller samples (CBsandstone1a, 1b and 2, having all volume of 1 $mm^3$), the 2D curves behave differently from the 3D one. They all show a distinct minimum corresponding to the mean grain size and then tend to their respective asymptotic value with an oscillatory behaviour. This discrepancy vanishes for the bigger sample (CBsandstone3 having volume of 8 $mm^3$), suggesting that 4 $mm^2$ can be assumed as representative area (REA).

The same analysis has been conducted on the carbonate images. The computed two-point correlation functions are shown in Figure 4.6. As for the CB samples, the 2D curves
Figure 4.5. Computed two-point correlation function for the CB sandstone samples. For each sample, four curves are displayed, corresponding to the whole 3D image (continuous line) and three 2D cross-sections chosen with the same areal porosity as the volumetric one.
Figure 4.6. Computed two-point correlation function for the carbonate samples. For each sample, four curves are displayed, corresponding to the whole 3D image (continuous line) and three 2D cross-sections chosen with the same areal porosity as the volumetric one.
show an oscillatory behaviour which is progressively damped with increasing the size of the sample. However, existence of an REV and REA for this rock remains undetermined, due to the significant variability of the carbonate pore system. This heterogeneity is made clearer by plotting the predicted mean pore radius, computed using eq. 4.9, as a function of the image characteristic size, for all the processed images (Fig. 4.7). For each sample, 10 values are reported: one for the whole 3D image, and three for each of the three orthogonal planes, i.e. three 2D cross-sections for each plane. For the CB sandstone a homogenous value in the range of 35-45 $\mu$m is obtained, corresponding to a mean pore diameter of 70-90 $\mu$m, in agreement and in fact a more accurate estimate than the one based on image observations only given by Lamy-Chappuis et al. (2014). On the other hand, a larger dispersion is observed for the carbonate. In particular, a drop on the predicted mean pore size is observed for the biggest 3D image. This is due to the heterogenous nature of this rock reflected by the presence of large lithological clusts (see Figure 4.1b) which were not picked up by the smaller size images. The range of predicted pore radius 60 —130 $\mu$m corresponds to mean pore diameters of 120 —260 $\mu$m which falls into the broader interval of 90 $\mu$m to 700 $\mu$m observed in SEM images. Furthermore, the mean grain size predicted by the two-point spatial correlation function, i.e. the minimum value of $Z_2$ in its initial descending branch, ranging between 240 and 380 $\mu$m, is also in good agreement with the morphological data (200-480 $\mu$m). This confirms the effectiveness of the method in fully characterizing the pore-system.

In order to assess anisotropy, the two-point correlation function is sampled only following the orthogonal directions, as in Yeong and Torquato (1998) and Øren and Bakke (2002). These components are then averaged to obtain a function for the whole medium, and compared with the one-dimensional isotropic function computed using the extended Berryman’s method for 3D images, eq. (4.5). Results are shown in Figs. 4.8 and 4.9 for the sandstone and carbonate samples respectively. One striking aspect is that sample Carb500 is strongly anisotropic. Fig. 4.9 clearly shows how the 3 directional functions have all different slope in their initial descending branch. This is the only sample displaying this feature. Another aspect which is worth highlighting is that the average directional $Z_2$ is very close to the Berryman’s one-dimensional isotropic function. The latter has obviously a smoother profile, as sampling is done along multiple directions. However, sampling along multiple directions has a very high computational cost, which makes Torquato’s method preferable.
Figure 4.7. Summary of the estimated mean pore size for all the samples considered in this study. For each sample, 10 values are reported: one for the whole 3D image, and three for each of the three orthogonal planes, corresponding to the three selected 2D cross-sections for each plane.
Figure 4.8. Directional two-point correlation functions (left column) and comparison between the average directional and the 3D isotropic Berryman's function (right column) for the sandstone samples.
Figure 4.9. Directional two-point correlation functions (left column) and comparison between the average directional and the 3D isotropic Berryman's function (right column) for the carbonate samples.
4.4 Computation of fluid flow and permeability prediction

4.4.1 Numerical method

The Stokes equations of creeping flow for incompressible fluids are recalled

\[ \nabla \cdot \mathbf{u} = 0, \quad (4.12) \]

\[ \mu \nabla^2 \mathbf{u} - \nabla p + \rho g = 0, \quad (4.13) \]

where \( \mathbf{u} \) is the velocity vector, \( p \) is the pressure, \( \rho \) and \( \mu \) are the fluid density and viscosity respectively, and \( \mathbf{g} \) is the acceleration due to gravity vector. The Stokes equations are solved using the FV-SIMPLE algorithm by Patankar (1980). The discretized Stokes equations along the \( i-th \) coordinate within a non-staggered structured grid arrangement (see Fig. 2.5b) can be written as:

\[ \sum_{nb,NB} a_{nb} u_{i,NB} - a_{C} u_{i,C} - \Delta_i p \Delta x + b_{i,C} = 0, \quad i = x, y, z \quad (4.14) \]

where the sum is over the six direct neighbor cells (the small index denotes a cell-face, the capital index a cell-centre), \( \Delta x \) is the grid size and the coefficients \( a_{nb}, a_{C} \) and \( b_{i,C} \) have the following form:

\[ a_{nb} = \mu, \]

\[ a_{C} = \sum_{nb} a_{nb}, \quad (4.15) \]

\[ b_{i,C} = \rho g_i \Delta x^2. \]

The SIMPLE algorithm works as follows: first an intermediate velocity field \( \mathbf{u}^\star \) is computed by solving the momentum equations using a known pressure field \( p \) (the initial pressure field is guessed). These velocities will generally not satisfy the continuity equation, unless the correct pressure field is employed, therefore a second velocity field \( \mathbf{u}^{**} \) satisfying the continuity equation \( \nabla \cdot \mathbf{u}^{**} = 0 \), together with a new pressure field \( p^* \) are sought. Defining pressure and velocity corrections as \( p' = p^* - p \) and \( \mathbf{u}' = \mathbf{u}^{**} - \mathbf{u}^\star \) respectively, after some algebraic manipulations, the following Poisson equation for \( p' \) is recovered

\[ \sum_{nb,NB} a'_{nb} p'_{i,NB} - a'_{C} p'_{C} = b'_{C}, \quad (4.16) \]
where the coefficients $a'_{nb}$, $a'_C$ and the continuity imbalance $b'_C$ have the following form

\begin{align}
a'_{nb} &= \lfloor \frac{1}{a_C} \rfloor_{nb}, \quad (4.17a) \\
a'_C &= \sum_{nb} a'_{nb}, \quad (4.17b) \\
b'_C &= \int_V \nabla \cdot \mathbf{u}^* dV, \quad (4.17c)
\end{align}

the operator $\lfloor \rfloor_{nb}$ denotes a linear interpolation scheme and the coefficients $a_C$ are the central coefficients resulting from the discretized momentum equations (4.15). Evaluation of the cell-face velocities required by the discretization of the divergence operator in eq. (4.17c) is done using the momentum interpolation method by Rhie and Chow (1983) as follows

\begin{align}
\mathbf{u}^*_f &= \lfloor \mathbf{u}^*_i \rfloor_f + \left[ \lfloor \frac{\mathbf{p}^*}{a_C} \rfloor_f - \lfloor \frac{1}{a_C} \rfloor_f \Delta f \mathbf{p} \right] \Delta x, \quad (4.18)
\end{align}

where the operator $\Delta f$ denotes the difference of nodal values across the face $f$. After the solution of the pressure correction equation, the new intermediate velocity field is computed as

\begin{align}
\mathbf{u}^{**}_i &= \mathbf{u}^*_i - \frac{\Delta p'_i}{a_C} \Delta x. \quad (4.19)
\end{align}

This process is repeated until convergence is reached and the continuity equation is satisfied. As the whole iterative scheme is prone to divergence, due to some approximations introduced when deriving the velocity-correction formula (Patankar, 1980), under-relaxation is used. A common practice is to solve the momentum equations with a relaxation factor $\omega_u$ and then update pressure with the following formula:

\begin{align}
p^* = \bar{p} + \omega_p p'. \quad (4.20)
\end{align}

Optimum under-relaxation parameters are problem-dependent. The resulting linear systems of equations are iterated until the ratio between the average absolute residual after an inner sweep and its initial value is less than 0.2. More insight into the convergence criterion for the overall procedure is given in Sec. 4.5.

### 4.4.2 Validation

The numerical model has been validated considering the Stokes flow past a sphere benchmark problem. For this test, a fluid of viscosity $\mu = 0.001 \text{ Pa}\cdot\text{s}$ flowing around a sphere of radius $R=1 \text{ mm}$ with freestream uniform velocity $v_0=0.01 \text{ m/s}$ was considered. The computational domain is a cube of size $2L^3$ centered at the sphere centre, where $L = 15R$ is the distance of the inlet boundary from the centre of the sphere. The domain was discretized using cubic voxels of resolution $R/\Delta x = 4$. Boundary conditions consist of the
Figure 4.10. Sphere test: computed pressure (a) and velocity component in the direction of the flow (b) on a cross-section parallel to the main flow direction passing through the centre of the sphere. The flow is directed upwards along the depicted line.

Freestream uniform velocity at the inlet, prescribed pressure at the outlet and symmetry at the other 4 faces. The numerically evaluated pressure and velocity component in the direction of the flow on a cross section passing through the centre of the sphere are shown in Figs. 4.10a and 4.10b respectively. Comparison between numerical and analytical values is made in terms of normalized pressure and velocity along the line depicted in Fig. 4.10. Along this line, the analytical solution is:

\[ p = -\frac{3}{2}\mu v_0 \cos \theta \frac{R}{r^2}, \quad (4.21a) \]

\[ v = v_0 \left[ 1 - \frac{3}{2} \left( \frac{R}{r} \right) + \frac{1}{2} \left( \frac{R}{r} \right)^3 \right] \cos^2 \theta, \quad (4.21b) \]

where \( \theta \) is the angle formed with the flow direction. Velocity and pressure are normalized against the freestream uniform velocity \( v_0 \) and the maximum value of pressure at the sphere \( p_{\text{max}} = 1.5\mu v_0/R \) respectively, while the x-axis representing the distance \( r \) of a point from the centre of the sphere is normalized against \( L \). As Fig. 4.11 clearly shows, numerical results are in good agreement with the analytical solution and only small errors can be ascribed to the influence of the boundary conditions and the poor discretization of the sphere.

4.4.3 Results

Results of the simulations carried out on the 3D images listed in Table 4.1 are presented here. Boundary conditions consist of an applied pressure gradient along the main direction, symmetry at the other four faces and no-slip conditions at the pore-grain interfaces.
Figure 4.11. Sphere test: comparison between analytical and computed pressure (a) and velocity component in the direction of the flow (b) along the line depicted in Fig. 4.10. Legend: continuous line is the analytical solution, asterisk marks are the predicted values.

Internal connectivity of the porous microstructure was assessed before starting the simulations and isolated dead-end pores (pores that are not connected to the boundary) were set as grains. Predicted pressure field and velocity in form of streamlines are shown in Figs. 4.12-4.13 and 4.14-4.15 for the CBsandstone1a and Carb300 samples respectively.

Permeability is then predicted from the computed fluid flow using Darcy’s law, eq. (3.53), as follows:

$$K = \mu \frac{QL}{A \Delta p},$$  \hspace{1cm} (4.22)

where $Q$ is the flow rate, $A$ is the area of the face normal to the flow, $\mu$ is fluid viscosity and $\Delta p/L$ is the applied pressure gradient. For a structured cubic grid of characteristic size $L = N \Delta x$ and area $A = N^2 \Delta x^2$, permeability is calculated as

$$K = \mu \frac{\Delta x \sum_j u_j}{N \Delta p},$$  \hspace{1cm} (4.23)

where $u_j$ is the velocity component in the direction of the flow and the sum is over all the pore cells on a plane normal to the flow direction. Constant values of $\mu=0.001 \text{ Pa} \cdot \text{s}$ and $\Delta p=1 \text{ Pa}$ were used in all the simulations.

Anisotropy was also evaluated by running three separate simulations with applied pressure gradient along each of the three orthogonal directions, and then calculating the following anisotropy ratio (Clavaud et al., 2008):

$$\nu = \frac{K_{\text{min}}}{\sqrt{K_{\text{max}} K_{\text{int}}}},$$  \hspace{1cm} (4.24)
Figure 4.12. Computed pressure field (a) and velocity in form of streamlines (b) for the sample CBsandstone1a.

Figure 4.13. Computed velocity magnitude on two cross-sections of the sample CBsandstone1a.
Figure 4.14. Computed pressure field (a) and velocity in form of streamlines (b) for the sample Carb300.

Figure 4.15. Computed velocity magnitude on two cross-sections of the sample Carb300.
Table 4.2. Predicted FV permeability for all the samples considered.

<table>
<thead>
<tr>
<th>Sample</th>
<th>$K_x$ [Da]</th>
<th>$K_y$ [Da]</th>
<th>$K_z$ [Da]</th>
<th>$\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CBsandstone1a</td>
<td>1.13</td>
<td>1.30</td>
<td>0.84</td>
<td>0.69</td>
</tr>
<tr>
<td>CBsandstone1b</td>
<td>1.13</td>
<td>1.36</td>
<td>0.84</td>
<td>0.68</td>
</tr>
<tr>
<td>CBsandstone2</td>
<td>0.87</td>
<td>1.06</td>
<td>0.85</td>
<td>0.88</td>
</tr>
<tr>
<td>CBsandstone3</td>
<td>0.86</td>
<td>1.05</td>
<td>0.91</td>
<td>0.88</td>
</tr>
<tr>
<td>Carb300</td>
<td>2.05</td>
<td>3.17</td>
<td>1.76</td>
<td>0.69</td>
</tr>
<tr>
<td>Carb400</td>
<td>2.99</td>
<td>2.70</td>
<td>2.76</td>
<td>0.94</td>
</tr>
<tr>
<td>Carb500</td>
<td>0.90</td>
<td>1.46</td>
<td>0.18</td>
<td>0.15</td>
</tr>
</tbody>
</table>

where $K_{\text{max}} > K_{\text{int}} > K_{\text{min}}$ are the three components of the permeability tensor along the three orthogonal directions $x$, $y$, $z$, sorted in descending order.

The predicted permeability values are listed in Table 4.2. For the CB sandstone, permeability remains constant in the narrow range $\langle 0.8 - 1.\rangle > \text{Da}$ with increasing the size of the volume and for different locations of the samples, confirming the homogeneity of the rock and the REV of 1 $\text{mm}^3$ observed using statistical correlation. Anisotropy also disappears for the biggest volume considered. As far as the carbonate is concerned, strong anisotropy is observed for the biggest sample (Carb500) and no clear determination of a REV can be made.

In order to predict the flow more accurately, the original digital images were refined by subdividing each image voxel into up to 64 sub-voxels. Fig. 4.16 shows the predicted permeability as a function of the number of sub-voxels for the sample CBsandstone1a. This graph shows that permeability tends to decrease with increasing mesh resolution, but it does not change significantly its order of magnitude.

### 4.4.4 Comparison of different permeability estimates

All the available permeability estimates for the two rock formations considered, are compared here. Fig. 4.17 shows the estimated values plotted against the experimentally determined value, the latter measured on the larger core plugs. The FV value has been computed as mean value of the 3 components listed in Table 4.2, while the KC value has been calculated using eq. (4.10). An estimated value from LBM simulations is also available from the CO2FLIP Project partners from University of Leeds for the CB sandstone only (S.He, Y. Zu, J. Xie, personal communication, 2014).

For the carbonate sample, the measured permeability ($\sim 1500 \text{ mDa}$) is roughly twice as...
Figure 4.16. Predicted permeability as a function of the number of sub-voxels for the sample CBsandstone1a.

much the average FV value of ∼850 mDa computed for the largest sample Carb500, while is roughly half the average FV value of ∼2800 mDa computed for the smaller Carb400 sample. This inconsistency is probably due to the already highlighted heterogeneity of the rock, as well as the difference in scale of the samples, resulting in significant changes in connectivity and tortuosity.

For the CB sandstone, a good agreement between permeability estimates obtained from different numerical approaches (i.e. FV and LBM) is observed. However, divergence up to almost two orders of magnitude appears between the predicted values and the experimentally determined permeability of ∼10 mDa. Again, this discrepancy can be attributed to the complex microstructure of the rock, in particular the presence of micro-imperfections, i.e. calcite shells fragments (Lamy-Chappuis, 2015), that cannot be detected by the resolution used for scanning the samples. As a result, very intricate pores filled with sub-micro fragments, which in reality have very high pore-grain surface area and very low net pore-volume, are converted into large open pores during the segmentation process, resulting in a much greater predicted permeability than the actual one.

Another source of uncertainty is the resolution of the numerical mesh. However, results showed in Fig. 4.16 indicate that increasing mesh resolution does not impact the order of magnitude of the predicted permeability significantly.

Finally, the KC equation fitted with the specific surface area value estimated using statistical correlation gives results close to the numerical ones for both rock formations, confirming the validity of statistical correlation as powerful tool for preliminary pore-space
4.5 Bulk momentum balance and a new convergence criterion for the SIMPLE algorithm

The traditional convergence criterion for the SIMPLE algorithm utilizes the continuity imbalance, i.e. the r.h.s. of eq. (4.16), as a residual. It is then demanded that its normalization to an appropriate quantity be less than a given tolerance (Patankar, 1980; Perić et al., 1988). For example, Mostaghimi et al. (2013) proposed as a convergence criterion to check the normalized continuity imbalance (NCI), defined as the ratio of the average continuity imbalance \( b'_{c} \) over the average flow rate \( Q \) as follows:

\[
NCI = \frac{b'_{c}}{Q}
\]  

(4.25)

and to terminate the computation when NCI is less than a given tolerance \( \lambda \). Alternatively, a general stopping criterion based on the reduction of the residual can be used (Ferziger and Peric, 2012). In this case, iterations are stopped when the average residuals of all equations, namely pressure-correction and x, y, z momentum, are reduced to a given fraction of its original size. However, both these criteria are based on local satisfaction of the governing equations, and no information is provided at the macroscopic level. The latter aspect is of particular interest for pore-scale modelling of reservoir rocks, especially when one wants to use the pore-scale results for upscaling over REVs, as in case of...
permeability estimation. Darcy’s law, which is used here, is indeed none other than expression of the macroscopic momentum balance (see Sec. 3.3.3).

Let us write the momentum equation (4.13) integrated over a control volume $V$ having boundary area $A$ as follows:

$$
\mu \int_A \frac{\partial u_j}{\partial x_i} n_i dA - \int_A p n_j dA + B = 0,
$$

(4.26)

where $n$ is the unit normal pointing outwards the surface and $B$ accounts for body forces. Considering the whole bulk medium as control volume, each of the two areal integrals in eq. (4.26) can be decomposed into two sub-integrals: one over the external boundary pore area $A_p$ and one over the internal pore-grain interfacial area $A_s$. The momentum equations for the whole medium can therefore be written as

$$
\mu \int_{A_p} \frac{\partial u_j}{\partial x_i} n_i dA - \int_{A_p} p n_j dA + \mu \int_{A_s} \frac{\partial u_j}{\partial x_i} n_i dA - \int_{A_s} p n_j dA + B = 0,
$$

(4.27)

where the third and fourth terms are the viscous and pressure drag forces, $D_v$ and $D_p$ respectively, which have been introduced in Sec. 3.3.3 (see eq. (3.48)). The first term in eq. (4.27) is zero because of the applied boundary conditions (zero velocity-gradient at boundaries where pressure is prescribed and simmetry at the other four faces), while the second term is the macroscopic force due to the applied pressure difference $\Delta p$. Eq. (4.27) in its compact form $\Delta P + B = D_p + D_v$ represents a balance of forces at the macroscopic level and must be satisfied by the solution of the Stokes equations (4.12)-(4.13).

Hence, the proposed convergence criterion consists on monitoring the Relative Error in the Bulk Momentum Balance (REBMB) defined as

$$
REBMB = \left| \frac{\Delta P + B - (D_p + D_v)}{\Delta P + B} \right|.
$$

(4.28)

This new criterion has the major merit of giving a clear physical interpretation of the approximate solution, i.e. how close one is to satisfy the bulk momentum balance and therefore how confident one can be in using Darcy’s law for predicting the absolute permeability. This makes the criterion particularly useful for pore-scale modelling of reservoir rocks.

To test the new convergence criterion, a test on the sample CBsandstone1b was performed. Results are shown in Fig. 4.18. Four quantities were monitored: the normalized average residuals of the momentum component in the flow direction and pressure-correction equations, the normalized continuity imbalance, eq. (4.25), and the proposed REBMB, eq. (4.28). As the graph clearly shows, the normalized average residuals of both equations keep decreasing linearly as the solution of the respective PDE improves.
NCI displays a similar behaviour. The REBMB instead converges to an asymptotic value as the macroscopic balance of forces in the flow direction can no longer be further refined with additional iterations. The achieved REBMB is less than 0.07% which can be considered an accurate measure. The fact that an asymptotic value is reached offers a valuable stopping criterion, provided that continuity must be satisfied as well. In light of this, the best convergence criterion appears to be a combination of the new one based on bulk momentum balance and the classical ones based on residual reduction. A suggested stopping criterion, used in previous computations, is the scenario where the asymptotic value of REBMB is reached and the residuals have been reduced by 4-5 order of magnitude. Finally, it must be noted that this overall convergence criterion is only related to the quality of the final approximate solution and does not impact the optimum computing time, the latter being determined primarily by the method for the solution of the linear systems.

4.6 Summary

An integrated approach comprising computer-tomography, statistical correlation and numerical simulations, for predicting the petrophysical properties of reservoir rocks, namely
REV, mean pore size and permeability, has been presented. The study has been carried out on 3D digital images obtained from µ-CT scanning of two rock formations: one sandstone and one carbonate. By analyzing several binarized small samples (order of mm) scanned at a resolution down to 5 μm, the potential of this approach to provide thorough characterization of reservoir rocks was shown. In particular, the two-point spatial correlation function was shown to be an effective way for estimating REV and REA, as well as a powerful method for evaluating the mean pore and grain sizes. Rock homogeneity and anisotropy were also effectively evaluated using spatial correlation tools. This can be very helpful when selecting the most representative sample for use in more sophisticated numerical analyses.

The 3D Stokes equations of creeping flow have been solved using the FV SIMPLE algorithm. Permeability obtained from these simulations was compared to other estimates obtained from different approaches, including LBM simulations and KC empirical relationships, against the experimentally determined value, measured on larger core-plugs. Comparison of all the available estimates revealed good agreement between different numerical estimates, i.e. FV and LBM, but a discrepancy was observed with the experimentally measured value. The latter is probably due to the difference in scale of the samples, resulting in significant changes in connectivity and tortuosity, as well as the presence of sub-micro imperfections that cannot be detected by the resolution used to resolve the pore space. More samples from different rock formations therefore need to be studied in order to establish a relationship between permeability estimates at different scales.

Finally, a new convergence criterion for the SIMPLE algorithm, and more generally for the family of pressure-correction methods, based on the bulk momentum balance, has been presented. This criterion provides information into significant fluid mechanics quantities such as form and friction drags, and is particularly useful for pore-scale modelling of reservoir rocks, especially when the predicted flow quantities are used for upscaling, e.g. Darcy’s law. Moreover, the distribution of the error as a function of the iterations showed an asymptotic behaviour. This provides a valuable stopping criterion when the new convergence indicator is effectively used in combination with classical normalized residuals.
Chapter 5

Modelling two-phase flow at the pore-scale

5.1 Introduction

In this section, the numerical method for modelling two-phase flow at the pore-scale using the VOF method is presented. Fluids incompressibility is assumed throughout this Thesis to simplify the development of the code. The primary interest here is to build a robust and accurate algorithm, and to determine which are the parameters and the flow conditions leading to numerical instabilities. Incorporation of fluids compressibility is left for a later stage. The chapter is organized as follows. First, the interface tracking algorithm is presented in Sec. 5.2. Next, the techniques for the solution of the NS equations accounting for surface tension effects, including discretization of surface tension forces and wettability conditions, are illustrated in Sec. 5.3. The whole algorithm is then summarized in Sec. 5.4. Finally, simulation results of benchmark problems for validation of the model are presented in Sec. 5.5.

5.2 The interface tracking algorithm

5.2.1 The VOF method

The VOF method is a volume-tracking method for the representation of the interfaces in interfacial flow problems, in which the fluids are marked and tracked by means of a volume fraction, also called indicator function. In a FV framework, the indicator function \( \alpha \) is defined for each cell as the ratio between the volume of fluid 1 contained within the
cell, $V^\alpha$, and the volume of the cell $V$ as

$$\alpha = \frac{V^\alpha}{V}. \quad (5.1)$$

This means that the indicator function is bounded between 0 and 1 as follows

$$\alpha = \begin{cases} 
1, & \text{if the cell is filled by fluid 1,} \\
0, & \text{if the cell is filled by fluid 2,} \\
0 < \alpha < 1, & \text{if there is an interface within the cell.} 
\end{cases} \quad (5.2)$$

A 2D example of a volume fraction distribution for the representation of a circle is shown in Fig. 5.1. There are various ways for mathematically describing the interface from a given volume fraction distribution, some of them have been revised in Sec. 2.4.1. In this work, the PLIC method by Youngs (1982) is adopted and will be illustrated in the next section.

### 5.2.2 Mathematical description of the interface

In the PLIC method, the interface is described as a planar surface defined by equation

$$\mathbf{n} \cdot \mathbf{x} - \beta = 0, \quad (5.3)$$

where $\beta$ is a constant and $\mathbf{n}$ is the interface unit normal vector pointing outwards from fluid 1:

$$\mathbf{n} = -\frac{\nabla \alpha}{|\nabla \alpha|}. \quad (5.4)$$
The minus sign in eq. (5.4) comes from the choice of the normal pointing direction. Discretization of the gradient operator in eq. (5.4) is done using a 27 points-stencil Finite Difference scheme (Fig. 5.2). The gradient of the volume fraction is stored at the cell-centre of the reference cell C (see Fig. 5.3) and is computed as average of the gradient evaluated at the 8 corners

$$\nabla \alpha = \frac{1}{8} \sum_{kji} (\nabla \alpha)^{kji}, \quad kji = tne, tnw, bnw, bne, tse, tsw, bsw, bse$$  \hspace{1cm} (5.5)

where each corner value is computed as average of the gradient of the volume fraction evaluated across the 4 faces concurrent to that corner. For example, the three components of the gradient evaluated at the top-north-east corner (see Fig. 5.4) are given by

$$\begin{align*}
(\nabla_x \alpha)^{tne} &= -\frac{1}{4c_x} (\alpha^{TNE} - \alpha^{TN} + \alpha^{TE} - \alpha^T + \alpha^{NE} - \alpha^N + \alpha^E - \alpha^C), \\
(\nabla_y \alpha)^{tne} &= -\frac{1}{4c_y} (\alpha^{TNE} - \alpha^{TE} + \alpha^{TN} - \alpha^T + \alpha^{NE} - \alpha^N + \alpha^N - \alpha^C), \\
(\nabla_z \alpha)^{tne} &= -\frac{1}{4c_z} (\alpha^{TNE} - \alpha^{NE} + \alpha^{TN} - \alpha^N + \alpha^{TE} - \alpha^T - \alpha^C),
\end{align*}$$  \hspace{1cm} (5.6a, 5.6b, 5.6c)

where \(c_j, j = x, y, z\) are the cell lengths in \(x, y, x\) directions respectively. If there are no solid wall boundaries within the 27 cells involved in the discretization stencil, the cell-centre gradient can be directly computed as

$$\begin{align*}
(\nabla_x \alpha) &= -\frac{1}{32c_x} (\alpha^{TNE} + 2\alpha^{TE} + \alpha^{TSE} + 2\alpha^{NE} + 4\alpha^E + 2\alpha^{SE} + \alpha^{BNE} + 2\alpha^{BE} + \alpha^{BSE} \\
&\quad - \alpha^{TNW} - 2\alpha^{TW} - \alpha^{TSW} - 2\alpha^{NW} - 4\alpha^W - 2\alpha^{SW} \\
&\quad - \alpha^{BNW} - 2\alpha^{BW} - \alpha^{BSW}), \\
(\nabla_y \alpha) &= -\frac{1}{32c_y} (\alpha^{TNW} + 2\alpha^{TN} + \alpha^{TNE} + 2\alpha^{NW} + 4\alpha^N + 2\alpha^{NE} + \alpha^{BNW} + 2\alpha^{BN} + \alpha^{BNE} \\
&\quad - \alpha^{TSW} - 2\alpha^{TS} - \alpha^{TSE} - 2\alpha^{SW} - 4\alpha^S - 2\alpha^{SE} \\
&\quad - \alpha^{BSW} - 2\alpha^{BS} - \alpha^{BSE}), \\
(\nabla_z \alpha) &= -\frac{1}{32c_z} (\alpha^{TNW} + 2\alpha^{TN} + \alpha^{TNE} + 2\alpha^{TW} + 4\alpha^T + 2\alpha^{TE} + \alpha^{TSE} + 2\alpha^T + \alpha^{TSE} \\
&\quad - \alpha^{BNW} - 2\alpha^{BN} - \alpha^{BNE} - 2\alpha^{BW} - 4\alpha^B - 2\alpha^{BE} \\
&\quad - \alpha^{BSW} - 2\alpha^{BS} - \alpha^{BSE}).
\end{align*}$$  \hspace{1cm} (5.7a, 5.7b, 5.7c)

The case with at least one solid wall cell within the discretization stencil will be treated in Sec. 5.3.2.
Figure 5.2. 27 points-stencil used for the discretization of the gradient of the volume fraction evaluated at the reference cell C.

Figure 5.3. Reference cell C with indication of its 6 faces - e, w, n, s, t, b - and 8 corners - tne, tnw, bnw, bne, tse, tsw, bsw, bse.

Figure 5.4. Zoom at the top-north-east (tne) corner with indication of the 8 cells used for evaluating the gradient of the volume fraction at it.
Once the normal is computed, one has to find the intercept $\beta$ to fully characterize the interface. This is done by matching the interface truncated volume $V(n, \beta)$ to the actual fluid volume $V^\alpha$ contained in the cell. With reference to the standard configuration (Fig. 5.5), where the interface unit normal has all positive components, the portion of volume contained within the control volume $V$ and laying below the interface (the volume ABCDIJKL in Fig. 5.5) is called the "truncated volume" and is given by (Gueyffier et al., 1999):

$$V(n, \beta) = \frac{1}{6n_xn_yn_z} \left[ \beta^3 - \sum_{j=x,y,z} H(\beta - n_j c_j)(\beta - n_j c_j)^3 \right. + \left. \sum_{j=x,y,z} H(\beta - \beta_{max} + n_j c_j)(\beta - \beta_{max} + n_j c_j)^3 \right],$$

(5.8)

where $c_j$ are the sides of the control volume, $\beta_{max} = n_x c_x + n_y c_y + n_z c_z$ and $H(x)$ is the Heaviside step function defined as 0 if $x < 0$ and 1 otherwise. The truncated volume is computed using a sequence of geometrically-based operations, which all together constitute a geometric toolbox (some relations can be found in Scardovelli and Zaleski (2000)). This geometric toolbox provides automatic solution to two distinct problems, namely

- the direct problem: given an interface of unit normal $n$ and intercept $\beta$ cutting a volume $V$, find the truncated volume $V(n, \beta)$

- the inverse problem: given an interface of unit normal $n$ and the truncated volume $V^\alpha$ cutting a volume $V$, find the position of the interface $\beta$ for which $V(\beta) = V^\alpha$. 
**Figure 5.6.** 2D schematic of a linear transformation \( x' = cx - x \) for bringing a non-standard configuration of the truncated volume, i.e. \( n_x < 0 \), to the standard configuration of Fig 5.5.

**The direct problem**

This problem is direct in the sense that it does not require iterations to find a solution. The surface is fully characterized, i.e. the unit normal \( n \) and the intercept \( \beta \) are known, and thus one has only to apply eq. (5.8) to calculate the truncated volume. However, eq. (5.8) applies only to the standard configuration depicted in Fig. 5.5, where all the normal components are positive, and therefore, in order to avoid a number of if-else if possible scenarios, the following automatic procedure is carried out:

1. Bring the configuration to standard case

   In order to employ eq. (5.8) for the calculation of the truncated volume, the geometry is brought to the standard case by applying to any negative component of the normal \( n_j \) the linear transformation \( x_j' = c_j - x_j \), as shown in Fig. 5.6. The interface equation thus becomes

   \[
   n' \cdot x' - \beta' = 0, \tag{5.9}
   \]

   where

   \[
   n_j' = \begin{cases} 
   n_j, & \text{if } n_j > 0, \\
   -n_j, & \text{if } n_j < 0,
   \end{cases}
   \]

   \[
   \beta' = \beta + \sum_j F(n_j)n_jc_j, \tag{5.10}
   \]

   \[
   F(n_j) = \begin{cases} 
   0, & \text{if } n_j > 0, \\
   -1, & \text{if } n_j < 0.
   \end{cases}
   \]

2. Calculate the truncated volume
The three positive components \( n'_j \) are sorted in ascending order \( n'_1 < n'_2 < n'_3 \) and those components smaller than a given tolerance \( \epsilon \) are set to zero to avoid numerical instabilities. The truncated volume \( V(\mathbf{n}', \beta') \) is then computed as

\[
V(\mathbf{n}', \beta') = \begin{cases} 
  \text{eq. (5.8)}, & \text{if } n'_1 \neq 0, \\
  \frac{c_1}{2n'_2n'_3} [\beta'^2 - \sum_{j=1,2} H(\beta' - n'_j c_j) ], & \text{if } n'_1 = 0 & n'_2 \neq 0, \\
  \frac{c_1 c_2}{n'_3} \beta', & \text{if } n'_2 = n'_1 = 0.
\end{cases} 
\]  

(5.11)

The first of the (5.11) refers to the full 3D case where all the normal components are non-zero while the second and third cases are reduced problems to 2D (one null normal component) and 1D (two null normal components) respectively.

**The inverse problem**

This is the typical problem occurring in the computation of the intercept \( \beta \) given the surface unit normal \( \mathbf{n} \) and the actual fluid volume \( V^\alpha \) contained within the cell. This is done by solving the non-linear problem \( V(\beta) = V^\alpha \) in the following manner:

1. Bring the configuration to standard case

   This step is identical to the one illustrated for the direct problem.

2. Calculate \( \beta' \)

   \( \beta' \) is calculated by solving the non-linear problem \( V(\beta') = V^\alpha \) using Brent’s method (Press et al., 1996), where \( V(\beta') \) is computed as in the direct problem.

3. Bring back the configuration to its actual position

   After \( \beta' \) is computed, the interface is brought back to its original configuration and the actual intercept \( \beta \) is calculated by reversing the second of the (5.10) equations:

\[
\beta = \beta' - \sum F(n_j)n_j c_j.
\]  

(5.12)

**5.2.3 Interface advection**

Starting from a known initial distribution, the volume fraction is updated in time by solving the following advection equation

\[
\frac{\partial \alpha}{\partial t} + \mathbf{u} \cdot \nabla \alpha = 0,
\]  

(5.13)
where \( \mathbf{u} \) is the velocity vector. The advection equation in non-conservative form, eq. (5.13), can be recast in conservative form by adding the divergence term \( \alpha \nabla \cdot \mathbf{u} \) to both sides, resulting in
\[
\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{u}) = \alpha \nabla \cdot \mathbf{u},
\] (5.14)
where the divergence term at the right hand side is retained even for incompressible fluids to enforce mass conservation locally (Rider and Kothe, 1998). Since \( V^\alpha = \int_V \alpha dV \) is the actual volume of fluid 1 contained within the control volume \( V \), integrating eq. (5.14) over a volume and applying Gauss’ theorem gives
\[
\frac{\partial V^\alpha}{\partial t} + \int_{\partial S} \alpha \mathbf{u} dS = V^\alpha \nabla \cdot \mathbf{u}.
\] (5.15)
Discretizing eq. (5.15) in time and approximating the surface integral as a discrete sum of control volume faces \( f \), yields
\[
V^{\alpha,n+1} - V^{\alpha,n} + \sum_f \Delta V_f^n = \Delta t V^{\alpha,n+1} \nabla \cdot \mathbf{u}.
\] (5.16)
Rearranging eq. (5.16) for the indicator function \( \alpha \) gives the final form of the discretized advection equation
\[
\alpha^{n+1} = \frac{\alpha^n}{1 - \Delta t \nabla \cdot \mathbf{u}},
\] (5.17)
where the terms \( \Delta V_f \) represent truncated volumes moving either in or out the cell through the face \( f \) during the time interval \( \Delta t \). The advection equation can therefore be interpreted as a mass conservation equation in which the updated indicator function results from the difference between the total amounts of fluid entering and leaving the cell during the time interval \( \Delta t \). Advection is done through operators-splitting, i.e the interface is advanced in time with three independent sweeps along each of the three directions
\[
\hat{\alpha} = \frac{\alpha^n - \Delta V_e - \Delta V_w}{V} \frac{1}{1 - \frac{\Delta t}{c_x} (u_e - u_w)}
\]
\[
\hat{\alpha} = \frac{\Delta V_n - \Delta V_s}{V} \frac{1}{1 - \frac{\Delta t}{c_y} (v_n - v_s)}
\]
\[
\alpha^{n+1} = \hat{\alpha} - \frac{\Delta V_t - \Delta V_b}{V} \frac{1}{1 - \frac{\Delta t}{c_z} (w_t - w_b)}
\] (5.18)
where the order of the sweeps is alternated at each time step to ensure better stability, and the face truncated volumes \( \Delta V_f \) are computed using the same geometric toolbox.
Figure 5.7. 2D schematic of an advection sweep along the x-direction. The top-row shows the interface configuration for the known volume fraction distribution $\alpha^n$ at time $t^n$. The velocity field is also known. In the middle-row, the truncated volumes $\Delta V_f$ are displayed. The bottom-row shows the initial (dashed) and updated (solid) interface configurations, the latter computed from the newly computed volume fraction distribution $\alpha^{n+1}$ at time $t^{n+1}$.

described in the previous section for the direct problem. The procedure is schematically illustrated in Fig. 5.7 for a 2D sweep along the x-direction. For the reference cell C, the updated volume of fluid 1 contained within the cell, $V^{\alpha,n+1}_C$, results from the combination of three contributions: the volume of fluid 1 originally contained within the cell before the advection sweep, $V^{\alpha,n}_C$, and the volumes of fluid 1 entering and leaving the cell through the west face, $\Delta V_w$, and the east face, $\Delta V_e$, respectively. In the same way $V^{\alpha,n+1}_W = V^{\alpha,n}_W + \Delta V_{ww} - \Delta V_w$ and $V^{\alpha,n+1}_E = V^{\alpha,n}_E - \Delta V_{ee} + \Delta V_e$.

To reduce the computational cost of the whole procedure, advection is done only on potential interface cells, i.e. those cells where actual change in the indicator function is possible. To avoid numerical instabilities, cells are first set as "ZERO" ($\alpha = 0$) if $\alpha < \epsilon$, "UNIT" ($\alpha = 1$) if $\alpha > 1 - \epsilon$, and "INT" if $\epsilon < \alpha < 1 - \epsilon$, where $\epsilon$ is some given small number. Then a loop over all cells is done to flag potential interface cells. These includes "UNIT_MID" cells ("UNIT" cells with at least one "INT" or "ZERO" neighbour)
and "ZERO_MID" cells ("ZERO" cells with at least one "INT" or "UNIT" neighbour). Finally, "INT" cells surrounded by "ZERO" cells are flagged as "ISOLATED" and no action is done on them. A last remark regards the CFL condition which from geometrical considerations cannot be greater than 0.5. This constraint has the meaning of not allowing the fluid to potentially invade the cell from both sides for more than the amount of fluid that the cell can actually contain.

5.3 Discretization of the Navier-Stokes equations with surface tension forces

The Navier-Stokes equations with surface tension forces are recalled

$$\frac{\partial}{\partial t} (\rho u) + \nabla \cdot (\rho uu) + \nabla p - \nabla \cdot \tau - \rho g - f_s = 0,$$

(5.19)

where \( p \) and \( u = (u, v, w) \) are the pressure and velocity fields, \( \tau = \mu \left[ \nabla u + (\nabla u)^T \right] \) is the viscous stress tensor, \( g \) is the gravitational acceleration, \( f_s \) is the surface tension force and \( \rho \) and \( \mu \) are the fluid density and viscosity, which in the VOF method are computed as

$$\rho = \alpha \rho_1 + (1 - \alpha) \rho_2,$$

$$\mu = \alpha \mu_1 + (1 - \alpha) \mu_2.$$

(5.20)

The use of the VOF method for the representation of the interface between two immiscible fluids offers the advantage that the numerical techniques for the solution of the NS equations are the same for two-phase systems as in single-phase flow. The two-phase flow problem can thus be seen as the flow of a single fluid with spatially and temporally variable physical properties. However, the presence of localized interfaces generates additional forces of chemical nature due to the change of molecular forces in the transition region between the two fluids. These forces are embodied in the Navier-Stokes equations as body forces concentrated at the interface, i.e. the term \( f_s \) in eq. (5.19), and their discretization must be treated carefully. Following the CSF model by Brackbill et al. (1992), the surface tension force \( f_s \) is computed as a body force using the Dirac delta function \( \delta_s \) concentrated at the interface as follows:

$$f_s = \sigma k n \delta_s,$$

(5.21)

where \( \sigma \) is the interfacial tension, \( k \) is the interface curvature defined as

$$k = -\nabla \cdot n,$$

(5.22)
and \( \mathbf{n} \) is the unit normal to the interface computed using eq. (5.4).

A problem often arising in numerical simulations when accounting for surface tension effects is the occurrence of the so-called “spurious currents”, a non-vanishing velocity field which appears in the interface transition region even in absence of external forces. Several remedies have been proposed over the last two decades to overcome this problem. Some of them have been presented in Sec. 2.4.2. The technique developed by Raeini et al. (2012), which so far gives the best results in practice in terms of eliminating the spurious currents, is used here and described in the following.

Following their approach, the pressure \( p \) is split into two terms to avoid numerical singularities at the interface and a pseudo-pressure field \( \varphi \) is defined as:

\[
\varphi = p - p_s, \tag{5.23}
\]

where \( p_s \) is the pressure due to surface tension forces, computed as:

\[
\begin{align*}
\nabla \cdot \nabla p_s &= \nabla \cdot \mathbf{f}_s, \\
\frac{\partial p_s}{\partial n} &= 0, \\
p_s &= \bar{p}_s, \quad \text{at } x = x,
\end{align*}
\tag{5.24}
\]

where \( n \) is the normal to the boundaries. Rearranging terms in eq. (5.19) and neglecting the convective term in the assumption of Stokes flow, the following form of the momentum equation is obtained:

\[
\frac{\partial}{\partial t} (\rho \mathbf{u}) = \nabla \cdot \mathbf{\tau} - \nabla \varphi + \rho \mathbf{g} + \Phi_s, \tag{5.25}
\]

where \( \Phi_s \) is called the capillary field (Raeini et al., 2014a) and is calculated as:

\[
\Phi_s = f_s - \nabla p_s. \tag{5.26}
\]

Besides, in order to reduce numerical instabilities in the transition region, the indicator function \( \alpha \) is smoothed by interpolating from the cell-centre to the cell-face and then averaging back, recursively for \( n_s \) iterations:

\[
\tilde{\alpha}_{s+1} = \frac{1}{6} \sum_{f} [\tilde{\alpha}_s]_f, \tag{5.27}
\]

where the operator \([ ]_f\) denotes linear interpolation between nodes adjacent to face \( f \), and \( \tilde{\alpha}_0 = \alpha \). The smoothed indicator function \( \tilde{\alpha} \) is then used for the calculation of the curvature and the average density and viscosity.
Figure 5.8. Computation of the gradient of the volume fraction at the east-face, \((\nabla \alpha)_e\), as average of the volume fraction gradient vectors evaluated at the four corners delimiting the face. The normal vectors at the corners are calculated using eqs. (5.6a) through (5.6c).

5.3.1 Discretization of the curvature

In absence of solid walls, the curvature is computed as (Brackbill et al., 1992)

\[
k = \frac{1}{|\nabla \alpha|} \left[ \mathbf{n} \cdot \nabla(|\nabla \alpha|) - \nabla \cdot \nabla \alpha \right].
\]  

(5.28)

The first term in brackets is discretized as

\[
\mathbf{n} \cdot \nabla(|\nabla \alpha|) = n_x \left( \frac{|\nabla \alpha|_e - |\nabla \alpha|_w}{c_x} \right) + n_y \left( \frac{|\nabla \alpha|_n - |\nabla \alpha|_s}{c_y} \right) + n_z \left( \frac{|\nabla \alpha|_t - |\nabla \alpha|_b}{c_z} \right),
\]  

(5.29)

where \(\mathbf{n}\) is computed as described in Sec. 5.2.2 and the magnitude of the gradient of the volume fraction at a cell-face \(|\nabla \alpha|_f\) is computed as the average of the magnitude of the volume fraction gradient vectors evaluated at the four corners of the face. For example, with reference to Fig. 5.8, the magnitude of the gradient of the volume fraction at the east-face \(|\nabla \alpha|_e\) is computed as

\[
|\nabla \alpha|_e = \frac{1}{4} \left( |(\nabla \alpha)^{tne}| + |(\nabla \alpha)^{tse}| + |(\nabla \alpha)^{bse}| + |(\nabla \alpha)^{bne}| \right),
\]  

(5.30)

where \((\nabla \alpha)^{kji}\) at the \(kji\) corner is calculated using eqs. (5.6a) through (5.6c).

The second term in brackets, namely the divergence of the gradient of the volume fraction, is computed as

\[
\nabla \cdot \nabla \alpha = \frac{(\nabla_x \alpha)_e - (\nabla_x \alpha)_w}{c_x} + \frac{(\nabla_y \alpha)_n - (\nabla_y \alpha)_s}{c_y} + \frac{(\nabla_z \alpha)_t - (\nabla_z \alpha)_b}{c_z},
\]  

(5.31)
where the \( i-th \) component of the gradient of the volume fraction evaluated at a cell-face \((\nabla_x \alpha)_f\) is computed as the average of the \( i-th \) components of the volume fraction gradient vectors evaluated at the four corners, i.e. for the east-face
\[
(\nabla_x \alpha)_e = \frac{(\nabla_x \alpha)_{tne} + (\nabla_x \alpha)_{tse} + (\nabla_x \alpha)_{bse} + (\nabla_x \alpha)_{bne}}{4}.
\] (5.32)

The curvature is then smoothed away from the interface recursively for \( n_s \) iterations (Raeini et al., 2012):
\[
\tilde{k}_{s+1} = 2\sqrt{\alpha(1-\alpha)}k + \left(1 - 2\sqrt{\alpha(1-\alpha)}\right)\tilde{k}_{s+1}^*,
\] (5.33)
where \( \tilde{k}_{s+1}^* \) is computed as
\[
\tilde{k}_{s+1}^* = \frac{\sum_f |w\tilde{k}_s|_f}{\sum_f |w|_f}, \quad w = \sqrt{\alpha(1-\alpha)} + \epsilon,
\] (5.34)
where \( \epsilon \) is a small given number and \( \tilde{k}_0 = k \).

### 5.3.2 Contact angle boundary condition at solid walls

Since \( \theta \) is the contact angle measured between the wall and the wetting phase, the normal at solid walls takes the form (Brackbill et al., 1992)
\[
\mathbf{n}|_w = \mathbf{n}_w \cos \theta + \mathbf{s}_w \sin \theta,
\] (5.35)
where \( \mathbf{n}_w \) is the unit normal to the wall pointing outwards from the wall and \( \mathbf{s}_w \) is a vector lying in the wall and normal to the contact line given by (Qaseminejad Raeini, 2013)
\[
\mathbf{s}_w = \frac{\mathbf{n} - (\mathbf{n} \cdot \mathbf{n}_w)\mathbf{n}_w}{|\mathbf{n} - (\mathbf{n} \cdot \mathbf{n}_w)\mathbf{n}_w|}.
\] (5.36)
Eq. (5.35) replaces eq. (5.4) in the interface tracking algorithm for "INT" cells which are in direct contact with a solid wall boundary, i.e. those "INT" cells having at least one solid wall cell among the direct east-west-north-south-top-bottom neighbour cells. These cells are flagged as "INT_WALL".

The normal \( \mathbf{n}|_w \) is also used for extrapolating the indicator function at a solid wall cell in the calculation of \( \nabla \alpha \). Extrapolation of the indicator function is needed when at least one solid wall cell is present within the 27 points-stencil used for the discretization of the gradient. In this case, the gradient of the volume fraction across a face \( f \) between a normal cell \( c \) and a solid wall cell is computed as
\[
(\nabla f \alpha)|_w = n|_w |\nabla \alpha|_c,
\] (5.37)
where the subscript \( i \) refers to the direction of the normal to the face \( f \). Since \( n\big|_w \) and \( n \) are interdependent, the whole interface normal computation procedure is done recursively with \( \alpha \) reflected at the wall during the first iteration. In the case no solid wall cells are present within the 27 points-stencil, eq. (5.7) is applied. Computation of the curvature is also modified in "INT_WALL" cells. For these cells the following discretized form of eq. (5.22) is used:

\[
k = -\left( \frac{(n_x)e - (n_x)w}{c_x} + \frac{(n_y)n - (n_y)s}{c_y} + \frac{(n_z)t - (n_z)b}{c_z} \right),
\]

(5.38)

where the \( i \) - \( th \) component of the unit normal evaluated at a cell-face \( f \), \( (n_i)_{f} \), is equal to \( n_i\big|_w \) if the face \( f \) is a solid wall or to the normalized average of the four corner values otherwise.

### 5.3.3 Discretization of surface tension forces

The FSF method presented in this section was originally formulated by Raeini et al. (2012). It is here further refined following personal communication with these authors (February 16, 2015). Discretization of the divergence operator at the r.h.s of the surface tension pressure equation (5.24) requires the evaluation of the surface tension forces at the cell-face

\[
f_{s,f} = \sigma k_f \delta_{s,f},
\]

(5.39)

where \( k_f \) is calculated using a weighted interpolation method

\[
k_f = \frac{[wk]_f}{[w]_f}, \quad w = \sqrt{\alpha(1 - \alpha) + \epsilon},
\]

(5.40)

and \( \delta_{s,f} \) is computed from a sharpened indicator function \( \hat{\alpha} \) as follows:

\[
\delta_{s,f} = \nabla f(\hat{\alpha}),
\]

(5.41)

where \( \hat{\alpha} \) takes the form:

\[
\hat{\alpha} = \frac{1}{1 - C_1} \left[ \min \left( \max \left( \alpha, \frac{C_1}{2} \right), 1 - \frac{C_1}{2} \right) - \frac{C_1}{2} \right],
\]

(5.42)

and \( C_1 \) is a coefficient controlling the sharpness of the interface.

After the solution of the surface tension pressure equation (eq. 5.24), the capillary field \( \Phi_s \) is first computed at the cell-face as

\[
\Phi_{s,f} = f_{s,f} - \nabla f p_s,
\]

(5.43)

and then reconstructed at the cell centre and employed in eq. (5.25) as a body force:

\[
\Phi_s = \frac{\sum_f (\Phi_{s,f}) S_f}{\sum_f S_f},
\]

(5.44)
Table 5.1. Values of the various constants used for filtering surface tension forces.

<table>
<thead>
<tr>
<th>$C_1$</th>
<th>$C_2$</th>
<th>$C_3$</th>
<th>$C_4$</th>
<th>$C_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>1</td>
<td>0.1</td>
<td>0.001</td>
<td>0.1</td>
</tr>
</tbody>
</table>

where $S_f$ is the outward vector area of face $f$.

In order to reduce the magnitude of the so-called spurious currents, the surface tension forces are filtered in the following manner:

$$f_{s,f,\text{filt}} = f_{s,f} - F_\delta(\delta_{sf})C_2f^{\text{old}}_{s,f,\text{filt}/}/,$$  \hspace{1cm} (5.45)

where $F_\delta(\delta_{sf})$ (=1 if $\delta_{sf} \neq 0$ and 0 otherwise) is a function restricting the validity of the filter to the interface region and $f_{s,f,\text{filt}/}$ is a time-dependent term updated as

$$f^{n+1}_{s,f,\text{filt}/} = F_\delta(\delta_{sf})\left[f^n_{s,f,\text{filt}/} + C_3\left[\Phi_{s,\text{filt}}\right]_{f,\text{filt}}\right],$$  \hspace{1cm} (5.46)

with $[\Phi_{s,\text{filt}}]_{f,\text{filt}}$ computed as:

$$[\Phi_{s,\text{filt}}]_{f,\text{filt}} = [\Phi_{s,\text{filt}}]_f - ([\Phi_{s,\text{filt}}]_f \cdot n_f)n_f,$$

$$n_f = [n]_f.$$  \hspace{1cm} (5.47)

Finally, a second filter applies to the capillary field which is set to zero below a threshold value chosen as:

$$\Phi_{s,f,\text{filt}} = \Phi_{s,f} - \max\left(\min\left(\Phi_{s,f}, \Phi_{s,f,\text{threshold}}\right), -\Phi_{s,f,\text{threshold}}\right),$$

$$\Phi_{s,f,\text{threshold}} = C_4\left[|f_{s,f}| + C_5\sigma(\delta_{sf})^2\right].$$  \hspace{1cm} (5.48)

$C_2$, $C_3$, $C_4$ and $C_5$ are constants and their values used in this work are given in Tab. 5.1.

### 5.3.4 Solution of the Navier-Stokes equations

The governing equations of flow are solved in the framework of the Finite-Volume method using the PISO algorithm by Issa (Issa, 1986), which is more suitable than SIMPLE for unsteady problems. The discretized NS equations (5.25) along the $i-th$ coordinate within a non-staggered structured grid arrangement ($c_x = c_y = c_z = \Delta x$) can be written as:

$$T(u_i) - a_Cu_{i,C} - \Delta_i p \Delta x + b_{i,C} = 0, \quad i = x, y, z$$  \hspace{1cm} (5.49)

where $T(u_i)$ is the discretized viscous stress tensor and the coefficients $a_C$ and $b_{i,C}$ have the following form:

$$a_C = \sum_{nb} \mu_{nb} + \rho_C \Delta x^2 / \Delta t,$$

$$b_{i,C} = (\rho g_i + \Phi_{s,i} + \rho^{\text{old}}u_i^{\text{old}} / \Delta t)C \Delta x^2.$$  \hspace{1cm} (5.50)
Starting from the available quantities \((\mathbf{u}, \varphi, \rho)^n\), the PISO algorithm works as follows:

- **Predictor step:** starting from the known pressure field \(\varphi^n\), the discretized momentum equations:
  \[
  T(u^*_i) - a_C u^*_{i,C} - \Delta_i \varphi^n \Delta x + b_{i,C} = 0. \tag{5.51}
  \]
  are solved implicitly for a guessed velocity field \(\mathbf{u}^*\).

- **First corrector step:** a second velocity field \(\mathbf{u}^{**}\) satisfying the continuity equation \(\nabla \cdot \mathbf{u}^{**} = 0\) together with a new pressure field \(\varphi^*\) are sought. The discretized momentum equation for these two fields can be written as:
  \[
  T(u^*_i) - a_C u^{**}_{i,C} - \Delta_i \varphi^* \Delta x + b_{i,C} = 0. \tag{5.52}
  \]

This step is solved in the same way as in the SIMPLE algorithm for single-phase flow. Pressure and velocity corrections are defined as \(\varphi' = \varphi^* - \varphi^n\) and \(\mathbf{u}' = \mathbf{u}^{**} - \mathbf{u}^*\) respectively, and a Poisson-like equation for \(\varphi'\) is built of the same form of eq. (4.16). The only difference compared to the single-phase solution resides in the calculation of the continuity imbalance, i.e. the r.h.s. of the pressure-correction equation \(\nabla \cdot \mathbf{u}^*\), which now accounts also for the capillary field \(\Phi_s\). The cell-face velocity \(u^*_f\) is thus calculated using the momentum interpolation method by Rhie and Chow (1983) as:

\[
  u_f^* = \left( u_f^* \right)_{SP} - \left[ \frac{\Phi_s,i}{a_C} f - \frac{1}{a_C} f \Phi_s,f \right] \Delta x^2, \tag{5.53}
\]

where \(\left( u_f^* \right)_{SP}\) is the cell-face velocity computed for single-phase flow in absence of the capillary field:

\[
  \left( u_f^* \right)_{SP} = \left[ u_i^* \right]_f + \left[ \frac{\Delta_i \varphi^n}{a_C} f - \frac{1}{a_C} f \Delta_f \varphi^n \right] \Delta x. \tag{5.54}
\]

After the solution of the pressure-correction equation, the velocity field is updated both at the cell-centre and at the cell-face in the following way:

\[
  u_i^{**} = u_i^* - \frac{\Delta_i \varphi'}{a_C} \Delta x, \tag{5.55}
\]
\[
  u_f^{**} = u_f^* - \frac{1}{a_C} f \Delta_f \varphi' \Delta x.
\]

This cell-face velocity, which already satisfies the continuity equation \(\nabla \cdot \mathbf{u}^{**} = 0\) and therefore does not need any further correction, will be employed in the calculation of the truncated volumes for advancing the indicator function. Contrary to SIMPLE, no relaxation is needed for updating the pressure field, i.e. \(\varphi^* = \varphi^n + \varphi'\).
• Second corrector step: the novelty of PISO with respect to SIMPLE is that a third velocity field $u^{***}$ satisfying the continuity equation $\nabla \cdot u^{***} = 0$ together with its corresponding new pressure field $\varphi^{**}$ are sought. The discretized momentum equation are now given by:

$$T(u_i^{**}) - a_C u_{i,C}^{***} - \Delta_i \varphi^{**} \Delta x + b_{i,C} = 0.$$  \hspace{1cm} (5.56)

As for the first corrector step, defining a second pressure-correction $\varphi'' = \varphi^{**} - \varphi^*$, taking the difference between eq. (5.56) and eq. (5.52) and combining with the continuity equation $\nabla \cdot u^{***} = 0$, yields

$$\sum_{nb,NB} a'_{nb} \varphi''_{NB} - a'_C \varphi''_C = \nabla \cdot \left[ \frac{T(u')}{a_C} \right],$$  \hspace{1cm} (5.57)

which is solved for $\varphi''$ and where the coefficients $a'_{nb}$ and $a'_C$ are given by eqs. (4.17a)-(4.17b). Finally, velocity and pressure are updated at the cell-centre as

$$u_i^{***} = u_i^{**} + \frac{T(u_i') - \Delta_i \varphi'' \Delta x}{a_C},$$

$$\varphi^{**} = \varphi^* + \varphi''.$$  \hspace{1cm} (5.58)

All the resulting linear systems of equations are solved using the PBCG method with incomplete LU factorization as pre-conditioner (Saad, 2003).

### 5.4 Final algorithm

The whole algorithm is summarized here.

1. Store variables at time $n$: $(\alpha, \varphi, u, f_s, f_{s,filt//}, \rho)^n$.

2. Update interface for half time step (eq. 5.18),

3. Outer-corrector loop ($n_{outer} = 2$):

   a. Update interface for the second half time step (eq. 5.18),

   b. Smooth $\alpha$ (eq. 5.27),

   c. Compute averaged density and viscosity (eq. 5.20) and curvature (eq. 5.22),

   d. Smooth $k$ (eq. 5.33),

   e. Compute surface tension forces (eq. 5.39),

   f. Correct surface tension forces (eq. 5.45),

   g. Solve surface tension pressure equation (eq. 5.24),
(h) Compute capillary field (eq. 5.43).

(i) Filter capillary field:
   i. Threshold capillary filed (eq. 5.48),
   ii. Reconstruct capillary field at the cell centre (eq. 5.44),
   iii. Update $f_{s,f,fit//}$ (eq. 5.46).

(j) Solve momentum equations (eq. 5.25):
   i. Solve predictor step (eq. 5.51),
   ii. Compute cell-face velocities (eq. 5.53),
   iii. Solve first pressure-correction equation (4.16),
   iv. Correct velocity field at both cell-centre and cell-face (eq. 5.55),
   v. Solve second pressure-correction equation (5.57),
   vi. Correct velocity field at cell-centre (eq. 5.58).

4. Advance to the next time step.

There is a stability condition to respect when solving the NS equations with surface tension forces, i.e. the numerical method is stable when the time step resolves the capillary wave propagation (Brackbill et al., 1992)

$$\Delta t < \sqrt{\frac{\langle\rho\rangle \Delta x^3}{2\pi\sigma}},$$

where $\langle\rho\rangle$ is the average density of the two fluids. In order to facilitate the presentation of the numerical setup for the various tests where surface tension forces are involved, a modified time step constraint is introduced:

$$\Delta t = C_t \Delta t_{bkz},$$

where $C_t$ is a constant and $\Delta t_{bkz}$ is the r.h.s. of eq. (5.59).

5.5 Validation of the model

5.5.1 Advection test: translation and rotation of a cube

These tests aim at validating the advection scheme, in particular its mass-conservation and shape-preserving properties. In both tests, a cube of variable size $L=8^3$, $16^3$ and $32^3$ unit cells is placed in a computational domain of size $(3L)^3$ where a constant velocity field $u_0 = (u_0, u_0, u_0)$ is imposed. In the first test, the cube is placed at the bottom-south-west...
corner of the domain, translated with a uniform unit velocity field for twice as its size and then returned to its original position. The total translation distance is therefore $4\sqrt{L}$.

In the second test, the cube is placed at the centre of the domain, rotated around the $z$-axis with a constant vorticity field of angular velocity $\omega = 2/(\sqrt{2}L)$ and then returned to its original position with a counter-rotation $-\omega$. The total body rotation is therefore $2\pi\sqrt{2}L$. A CFL number of 0.45 is used in all the calculations. The initial and final volume fraction distributions for the translation and rotation tests are shown in Figs. 5.9 and 5.10 respectively, for different sizes of the cube.

The error is estimated from the initial and final volume fraction distributions, $\alpha^0$ and $\alpha^f$ respectively. Two measures of error are defined as

$$\epsilon_{mc} = \frac{|V_f^\alpha - V_0^\alpha|}{V_0^\alpha},$$  \hspace{1cm} (5.61)

$$\tau = \frac{1}{N} \sum_{i=1,N} |\alpha_i^f - \alpha_i^0|,$$  \hspace{1cm} (5.62)

where $N$ is the total number of cells and $V_\alpha = \sum \alpha_i V_i$. The first measure of error $\epsilon_{mc}$ is a normalized difference between the total fluid volumes at the beginning and at the end of the calculations, and can be considered as an indicator of the mass-conservation
Table 5.2. Advection test: measures of error for different tests and different resolutions. Tests: 'T' = translation, 'R' = rotation.

<table>
<thead>
<tr>
<th>Test</th>
<th>L</th>
<th>$\epsilon_{mc}$</th>
<th>$\tau$ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>T</td>
<td>8</td>
<td>2.1e-7</td>
<td>2.96</td>
</tr>
<tr>
<td>T</td>
<td>16</td>
<td>9.7e-9</td>
<td>1.93</td>
</tr>
<tr>
<td>T</td>
<td>32</td>
<td>1.7e-8</td>
<td>0.97</td>
</tr>
<tr>
<td>R</td>
<td>8</td>
<td>3.9e-7</td>
<td>7.04</td>
</tr>
<tr>
<td>R</td>
<td>16</td>
<td>1.9e-8</td>
<td>2.23</td>
</tr>
<tr>
<td>R</td>
<td>32</td>
<td>2.3e-8</td>
<td>0.93</td>
</tr>
</tbody>
</table>

properties of the method. The second error $\tau$ is an average of the error in each cell and is a measure of the accuracy of the reconstruction algorithm. The estimated errors for all the calculations carried out are listed in Tab. 5.2. As expected, and as Figs. 5.9 and 5.10 clearly show, the average error $\tau$ decreases with increasing the resolution of the cube. Generally the error is localized at the corners, where the gradient of the volume fraction is sharper, and as a result the cube tends to assume a spherical shape when it is poorly resolved (Fig. 5.9b). With increasing the resolution, the cube appears adequately resolved (Figs. 5.9c and 5.9d). Mass is always conserved with error $\epsilon_{mc}$ of the order of the tolerance used as threshold for the indicator function.

5.5.2 Surface tension test: static drop

In this test, both a 2D and a 3D incompressible gas bubble immersed in another incompressible fluid approaching its equilibrium state in absence of gravity are studied. The gas has viscosity $\mu_g = 10^{-5}$ Pa$\cdot$s and density $\rho_g = 1$ kg/m$^3$ while the other fluid is water with viscosity $\mu_w = 10^{-3}$ Pa$\cdot$s and density $\rho_w = 1000$ kg/m$^3$. The interfacial tension coefficient $\sigma = 0.07$ N/m. Initially the bubble has square (2D) and cubic (3D) shape of size $L=40$ µm and is placed at the centre of a computational domain of size 2.5L to allow for the drop deformation. This setup is chosen for comparison with the work of Raeini et al. (2012). Velocity is set to zero everywhere at the boundary. Simulations with $C_t = 0.5$ are carried out for different resolutions $L/\Delta x = 3, 4, 8, 16$ and 32.

The aim of this test is to demonstrate that the model is able to eliminate the so-called
Figure 5.11. Static drop test: initial (a) and final (b) volume fraction distribution for the 2D drop ($L/\Delta x=16$).

Figure 5.12. Static drop test: initial (a) and final (b) volume fraction distribution for the 3D drop ($L/\Delta x=16$).
Table 5.3. Static drop test: values of $n_s$ used in the simulations (The same values were applied to both 2D and 3D simulations).

<table>
<thead>
<tr>
<th>$L/\Delta x$</th>
<th>3</th>
<th>4</th>
<th>8</th>
<th>16</th>
<th>32</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_s$</td>
<td>2</td>
<td>2</td>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
</tbody>
</table>

spurious currents and to show the convergence of the bubble to its exact curvature:

$$k_{\text{exact}} = \begin{cases} 
1/r, & \text{with } r = \sqrt{\frac{A'_f}{\pi}}, \quad 2D \\
2/r, & \text{with } r = \sqrt{\frac{3V'_f}{4\pi}}, \quad 3D 
\end{cases}$$

(5.63)

where $A'_f$ and $V'_f$ are the bubble area and volume respectively in the final equilibrium configuration. The initial and final drop equilibrium configurations can be visualized in Figs. 5.11 and 5.12 for the 2D and 3D drop respectively. As far as eliminating the spurious currents is concerned, Fig. 5.13 clearly shows how the velocity eventually tends to zero everywhere in the domain. This was the main goal of the test. The error in the drop curvature is measured as

$$\epsilon_k = \frac{|k_{\text{num}} - k_{\text{exact}}|}{k_{\text{exact}}}$$

(5.64)

where the numerical curvature $k_{\text{num}}$ is computed using a weighted average as:

$$k_{\text{num}} = \frac{\sum k_i |\nabla \alpha'_f|_i V_i}{\sum |\nabla \alpha'_f|_i V_i}.$$ 

(5.65)

The error in the drop curvature plotted as a function of grid resolution is shown in Fig. 5.14 exhibiting convergence towards zero with increasing grid resolution. This optimum behaviour was obtained by increasing the number of smoothing iterations, i.e. varying $n_s$ in equations (5.27) and (5.33), with increasing the size of the computational domain (values given in Table 5.3). For example, for the 2D case with $L/\Delta x=32$, using the same value of $n_s = 3$ as for the case with $L/\Delta x=16$ produced an error of 0.6%, which is much greater than the error of 0.25% obtained for the coarser grid. Increasing the value of $n_s$ to 4 gave the error of 0.07% plotted in Fig. 5.14. On the other hand, attention must be paid not to exaggerate with smoothing in the opposite case of coarse grids. Simulations with $L/\Delta x=3$ and 4 were run with $n_s = 2$ as using greater values were seen to impede convergence to zero of the velocity field. However, as indicated by the following simulations, this bothersome grid size-dependent behaviour seems to be relevant to solid wall boundary-free problems only.
Figure 5.13. Static drop test: computed max velocity in the computational domain as a function of time ($L/\Delta x=16$).

Figure 5.14. Static drop test: error in the drop curvature as a function of grid resolution.
5.5.3 Contact angle test: static capillary pipe

The same pair of fluids of test 5.5.2 are used here for the simulation of a static bubble on a circular pipe of radius \( R = 12.5 \mu m \) and length \( L = 50 \mu m \). This test aims at validating the contact angle formulation described in Sec. 5.3.2, showing the convergence of the bubble to the exact curvature:

\[
 k_{\text{exact}} = \frac{2 \cos \theta}{R},
\]

(5.66)

where \( \theta \) is the static contact angle. Simulations are carried out for different contact angles \( \theta = 30^\circ, 45 \) and \( 60^\circ \) and for different resolutions \( R/\Delta x = 2, 5, 10 \). Velocity is set to zero everywhere at both the inlet and the outlet, while no-slip conditions are applied at wall boundaries. \( C_t \) values are 0.5 and 0.25 for \( R/\Delta x = 2, 5 \) and \( R/\Delta x = 10 \), respectively.

The initial and final fluids configuration can be visualized in Fig. 5.15 for \( \theta = 30^\circ \) and \( R/\Delta x = 10 \). The interface location along the centre plane is displayed in Fig. 5.16. The velocity field converged to zero for all simulations (see Fig. 5.17) while the error in the drop curvature is shown in Fig. 5.18. Contrary to the drop test, no smoothing is applied here to the volume fraction as values of \( n_s \) greater than 1 were seen to result in lower accuracy in the drop curvature.

5.6 Summary

A stable and accurate algorithm for modelling two-phase flow at the pore-scale in porous media has been presented. The model consists of three main components: an interface-tracking algorithm, a model for the surface tension forces and a solver for the NS equations. The interfaces are tracked using the PLIC-VOF method. The interfaces are then evolved
Figure 5.16. Static capillary pipe test: free surface profile along the centre plane for all contact angles considered ($R/\Delta x=10$).

Figure 5.17. Static capillary pipe test: computed max velocity in the computational domain as a function of time for different values of the contact angle $\theta$ ($R/\Delta x=10$).
in time by solving an advection equation, with advection done through operator splitting. The surface tension forces are modelled using the FSF method of Raeini et al. (2012). Wettability conditions are enclosed in the model by means of a boundary condition at the wall, which gives the normal to the interface at a solid wall as a function of the static contact angle, the normal to the wall and the gradient of the VOF indicator function. The NS equations are solved using the PISO algorithm.

Simulation results of benchmark problems for validation of the model have also been presented. These includes a test for the interface tracking algorithm, and two static tests for the surface tension model at low capillary numbers, in absence and presence of complex solid wall boundaries respectively. All these tests gave accurate results, showing convergence to zero of the error with increasing the grid resolution. The results of these test demonstrated the robustness the code, its ability in handling high density and viscosity ratios and the capability of simulating flow at low capillary numbers even in presence of complex solid wall boundaries.

Figure 5.18. Static capillary pipe test: error in the drop curvature as a function of grid resolution for different values of the contact angle $\theta$. 

Chapter 6

Numerical simulations of two-phase flow

6.1 Introduction

In the last section of the previous chapter the numerical model has been validated with static benchmark problems. However, static or quasi-static conditions are rarely encountered in practical engineering problems involving two-phase flow in porous media. There are two types of displacement which can take place in two-phase systems: drainage, in which the wetting phase (water, in this work) is displaced by a non-wetting phase (for example \( \text{CO}_2 \)), and imbibition, in which it is the wetting phase that is adsorbed into the porous medium, displacing the resident non-wetting phase. In this chapter, both these two processes are simulated in porous systems of increasing complexity. First, the robustness of the code is tested in Sec. 6.2 by simulating imbibition in a circular pipe, for different flow conditions and high density and viscosity ratios. Then, the snap-off mechanism, which is the primary pore-scale event for capillary trapping in porous media, is studied in Sec. 6.3, and the influence of several parameters, including contact angle, capillary number and viscosity ratio, is examined. Finally, simulation results of two-phase flow on \( \mu \)-CT images of rock samples are presented in Sec. 6.4.

6.2 Imbibition in a circular capillary pipe

The movement of a bubble of water displacing either water or air in a circular pipe of radius \( R \) and length \( L = 8R \) is studied. The fluids physical properties are the same as in Test 5.5.2, with interfacial tension coefficient \( \sigma = 0.05 \text{ N/m} \), the static contact angle \( \theta = 45^\circ \) and the grid resolution \( R/\Delta x = 5 \). Previous results indicate that with this mesh
resolution the pipe is adequately resolved, and the computed curvature for this particular value of $\theta$ is sufficiently accurate (see Fig. 5.18). This test aims at investigating the stability of the numerical method for different flow conditions and assessing its capability to handle high density and viscosity ratios in dynamic conditions.

Boundary conditions consist of pressure at the outlet and a Poiseuille-like velocity distribution at the inlet $v_{in} \propto (r^2)$, where $r$ is the distance from the centre of the pipe. The different flow conditions can be represented by two dimensionless quantities, namely the Reynolds number and the capillary number. The Reynolds number $Re = \frac{\rho v D}{\mu}$ is the ratio between inertial and viscous forces, while the capillary number $Ca = \frac{\mu v}{\sigma}$ expresses the ratio between viscous and capillary forces. The Reynolds and capillary number are controlled by varying the mean inlet velocity $v_{in} = 0.1, 0.01$ and $0.001 \text{ m/s}$ and the pipe diameter $D = 25, 250, 2500 \mu m$, yielding a set of $3 \times 3$ possible flow conditions, with $Ca$ and $Re$ ranging between $2.0e^{-3}$ and $2.0e^{-5}$ and between $0.025$ and $250$ respectively.

Initially, the interface is placed at $L/4$ and a static simulation as in Test 5.5.3 is carried out in order to start the dynamic simulations from equilibrium conditions. $C_{de}$ is set equal to 1 for the water-water system and 0.5 for the water-air system. As for the static pipe, no smoothing is applied to the volume fraction. All the simulations are run until breakthrough or stopped after 200000 time steps.

The stability and accuracy of the simulations are evaluated using several parameters: the maximum difference in curvature $\epsilon_k$, the maximum difference in average interface velocity $\epsilon_v$, the relative standard deviation of the average interface velocity $RSD_v$, and the error in mass conservation $\epsilon_{mc}$. The maximum difference in curvature $\epsilon_k$ is the largest discrepancy between the drop curvature computed after each time step using eq. (5.65) and the exact one:

$$
\epsilon_k = \max \left( \frac{|k_{\text{min}} - k_{\text{exact}}|}{k_{\text{exact}}}, \frac{|k_{\text{max}} - k_{\text{exact}}|}{k_{\text{exact}}} \right),
$$

(6.1)

where $k_{\text{min}}$ and $k_{\text{max}}$ are the minimum and maximum curvature recorded during the simulation. The maximum difference in the average interface velocity $\epsilon_v$ is computed in the same way as

$$
\epsilon_v = \max \left( \frac{|\overline{v}_{\text{s,min}} - \overline{v}_{\text{in}}|}{\overline{v}_{\text{in}}}, \frac{|\overline{v}_{\text{s,max}} - \overline{v}_{\text{in}}|}{\overline{v}_{\text{in}}} \right),
$$

(6.2)

where $\overline{v}_{\text{s}}$ is the mean interface velocity, i.e. the average velocity calculated for the ”INT” and ”INT\_VOF” cells, after each time step. The relative standard deviation of the average interface velocity $RSD_v$ is a measure of the dispersion of the average interface velocity during the simulations. It is defined as the ratio between its standard deviation and mean value during the whole computation. For the evaluation of these three statistical
Table 6.1. Measures of error for different capillary and Reynolds numbers, and for different pair of fluids.

<table>
<thead>
<tr>
<th>$Ca$</th>
<th>$Re$</th>
<th>System</th>
<th>$\epsilon_k$</th>
<th>$\epsilon_v$</th>
<th>$RSD_v$</th>
<th>$\epsilon_{mc}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2e-3</td>
<td>2.5</td>
<td>w-w</td>
<td>0.061</td>
<td>0.23</td>
<td>0.041</td>
<td>5.95e-4</td>
</tr>
<tr>
<td></td>
<td></td>
<td>w-g</td>
<td>0.046</td>
<td>0.37</td>
<td>0.044</td>
<td>1.56e-3</td>
</tr>
<tr>
<td>2e-3</td>
<td>25</td>
<td>w-w</td>
<td>0.077</td>
<td>0.11</td>
<td>0.033</td>
<td>1.32e-3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>w-g</td>
<td>0.055</td>
<td>0.37</td>
<td>0.053</td>
<td>1.52e-3</td>
</tr>
<tr>
<td>2e-3</td>
<td>250</td>
<td>w-w</td>
<td>0.063</td>
<td>0.11</td>
<td>0.033</td>
<td>3.60e-3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>w-g</td>
<td>0.076</td>
<td>0.39</td>
<td>0.030</td>
<td>6.21e-3</td>
</tr>
<tr>
<td>2e-4</td>
<td>0.25</td>
<td>w-w</td>
<td>0.045</td>
<td>0.47</td>
<td>0.087</td>
<td>3.50e-5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>w-g</td>
<td>0.039</td>
<td>0.57</td>
<td>0.083</td>
<td>2.86e-5</td>
</tr>
<tr>
<td>2e-4</td>
<td>2.5</td>
<td>w-w</td>
<td>0.041</td>
<td>0.63</td>
<td>0.089</td>
<td>6.05e-5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>w-g</td>
<td>0.037</td>
<td>0.55</td>
<td>0.098</td>
<td>2.03e-3</td>
</tr>
<tr>
<td>2e-4</td>
<td>25</td>
<td>w-w</td>
<td>0.047</td>
<td>0.68</td>
<td>0.102</td>
<td>4.04e-5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>w-g</td>
<td>0.046</td>
<td>0.44</td>
<td>0.061</td>
<td>8.64e-3</td>
</tr>
<tr>
<td>2e-5</td>
<td>0.025</td>
<td>w-w</td>
<td>0.056</td>
<td>1.60</td>
<td>0.156</td>
<td>1.05e-3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>w-g</td>
<td>0.043</td>
<td>3.25</td>
<td>0.159</td>
<td>1.30e-3</td>
</tr>
<tr>
<td>2e-5</td>
<td>0.25</td>
<td>w-w</td>
<td>0.060</td>
<td>1.79</td>
<td>0.164</td>
<td>1.11e-3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>w-g</td>
<td>0.054</td>
<td>2.26</td>
<td>0.172</td>
<td>2.00e-3</td>
</tr>
<tr>
<td>2e-5</td>
<td>2.5</td>
<td>w-w</td>
<td>0.040</td>
<td>1.25</td>
<td>0.303</td>
<td>1.61e-3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>w-g</td>
<td>0.039</td>
<td>1.32</td>
<td>0.154</td>
<td>9.42e-3</td>
</tr>
</tbody>
</table>

parameters, the initial time steps were discarded to eliminate abnormal data. Finally, the mass conservation error is the relative difference between the total injected volume at the end of the simulation $V_{in} = (t_f - t_0) \int_{\partial A} v_{in} dA$ and the simulated change in volume of the injected phase $\Delta V = V_{\alpha f} - V_{\alpha 0}$:

$$\epsilon_{mc} = \frac{|\Delta V - V_{in}|}{V_{in}},$$

(6.3)

where $V_{\alpha f}$ and $V_{\alpha 0}$ are calculated from the initial and final volume fraction distributions in the computational domain.

As the computed parameters listed in Tab. 6.1 clearly indicate, all the simulations can be considered stable and accurate. The error in mass conservation is always below 1%, confirming the robustness of the code in handling high density and viscosity ratios even in dynamic conditions and at low capillary numbers. The largest maximum difference in curvature for all computations is 7.7 %. This means that the interface is pushed to
Figure 6.1. Time evolution of the volume fraction along the central plane (w-g system, $Ca = 2e^{-4}$, $Re=0.25$).
advance uniformly through the pipe while maintaining its equilibrium configuration (see Fig. 6.1). The maximum difference in average interface velocity is generally higher than the other indicators, due to the localized surface tension forces active in the interface transition region and their interplay with the viscous forces active at the wall. A small numerical error in forces is likely to generate some local perturbations of the interface front, resulting in changes of the pressure jump across the interface and thus changes of the velocity field. The influence of the different flow conditions on the velocity field is also more visible than their influence on the other two indicators. This is reasonable, as the curvature is primarily determined by the static contact angle \( \theta \), which is not influenced by the flow conditions (hysteresis and dynamic effects are not considered in the model), while the mass conservation is mainly a feature of the advection scheme. First thing to note is the dramatic increase \( \epsilon_v \) and \( RSD_v \) at low capillary numbers. Again this can be explained by the local perturbations of the interface front due to surface tension forces. At higher capillary numbers viscous forces are dominant, capillary forces are negligible and the displacement is stabilized by viscous effects. On the contrary, at low capillary numbers capillary forces are dominant, resulting in a more unstable interface advancing front. This difference is exacerbated at high viscosity ratios. This is made clearer by visualizing snapshots of the velocity field in a plane parallel to the flow direction passing through the centre of the pipe (see Fig. 6.2). Far from the interface, the velocity assumes the Poiseuille distribution for single-phase flow. In the transition region, the capillary forces are responsible of a deviation of the wetting fluid particles onto a direction along the interface. Evidence of these flow patterns was also shown by Molecular Dynamics (MD) simulations (Dimitrov et al., 2007). This results in a decrease in the velocity at the centre of the pipe compared to the Poiseuille distribution (see also Levine et al. (1980) for a study on the deviation from Poiseuille flow at the front meniscus). This in turn yields, for continuity, a higher velocity near the walls. In the water-air system this increase of the velocity at the contact line is more pronounced, giving rise to the formation of some vortices at the centre of the pipe (see Fig. 6.2b). However, it is likely that these vortices are provoked by numerical instabilities in the transition region caused by the high viscosity ratios.

6.2.1 Effect of time step

In order to reduce the magnitude of the velocity variations, a new set of simulations at low capillary numbers \( (Ca = 2.0e^{-5}) \) using the same numerical setup of Sec. 6.2 is carried out for different time steps, i.e. for values of \( C_d = 0.5, 0.25 \) and \( 0.1 \). The simulations are
Figure 6.2. Snapshots of the velocity field near the interface along the central plane for the w-w (left column) and w-g (right column) systems at different time steps. \( (Ca = 2e^{-4}, \text{Re} = 0.25) \).

Table 6.2. Measures of error for the w-g system for different time steps at different Reynolds number \((Ca = 2e^{-5})\).

<table>
<thead>
<tr>
<th>(C_t)</th>
<th>(Re=0.025)</th>
<th>(Re=0.25)</th>
<th>(Re=2.5)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(\epsilon_v)</td>
<td>(RSD_v)</td>
<td>(\epsilon_{mc})</td>
</tr>
<tr>
<td>0.5</td>
<td>3.25</td>
<td>0.159</td>
<td>1.30e-3</td>
</tr>
<tr>
<td>0.25</td>
<td>2.73</td>
<td>0.109</td>
<td>1.03e-3</td>
</tr>
<tr>
<td>0.1</td>
<td>2.30</td>
<td>0.131</td>
<td>1.03e-3</td>
</tr>
</tbody>
</table>
repeated for the corresponding three values of Reynolds numbers $Re=0.025, 0.25, 2.5$. Results are given in Tab. 6.2 in terms of $\epsilon_v$, $RSD_v$ and $\epsilon_{mc}$. The variability in average interface velocity considerably decreases when the time step decreases, and also mass conservation is better satisfied. However, using small time steps has the non-negligible drawback of increasing the computational time.

### 6.3 Snap-off in constricted tubes of variable cross-sections

Snap-off is a pore-scale mechanism occurring in porous media in which a bubble of non-wetting phase displacing a wetting phase, and vice-versa, can break-up into ganglia when passing through a constriction. This is the typical scenario of a pore-throat system in a reservoir rock. This mechanism is very important in foam generation processes, enhanced oil recovery techniques and capillary trapping of $CO_2$ bubbles during geological storage of $CO_2$ in saline aquifers. Several studies have been conducted to analyze this mechanism in order to establish a criterion for its occurrence. The first quasi-static criterion was derived by Roof et al. (1970) for circular pores and for perfectly wetting conditions ($\theta = 0^{\circ}$). The criterion states that snap-off occurs when the capillary pressure at the bubble front in the unconstricted pore becomes less than the local capillary pressure at the throat, i.e. when the following inequality is satisfied:

$$\frac{2}{R_p} \leq \frac{1}{R_t} + \frac{1}{R_{zt}}, \quad (6.4)$$

where $R_p$ and $R_t$ are the pore and throat radii and $R_{zt}$ is the longitudinal radius of curvature of the throat. Here, the l.h.s is the mean curvature of the bubble front in the unconstricted section of the pore while the r.h.s. is the local curvature of the throat.

Ransohoff et al. (1987) extended Roof’s criterion to variable cross-sections as follows:

$$\frac{\tilde{C}_p}{R_p} \leq \frac{1}{R_t} + \frac{1}{R_{zt}}, \quad (6.5)$$

where the coefficient $\tilde{C}_p$ depends on the shape of the cross-section ($\tilde{C}_p=2$ for circular, 1.89 for square and 1.77 for triangular), $\tilde{R}_t$ is the radius of the largest inscribed circle at the throat and the r.h.s. is the critical curvature for snap-off at the throat, corresponding to the point of instability where the curvatures at two corners of the cross-section meet. For long enough throats, the above criterion reduces to:

$$R_p \geq \tilde{C}_p \tilde{R}_t. \quad (6.6)$$
This is a purely geometric criterion stating that snap-off occurs when the contraction ratio $CR$, defined as

$$CR = \frac{R_p}{R_t},$$

satisfies certain conditions. Deng et al. (2014) simulated drainage and imbibition in diverse pore-throat systems of sinusoidal shape with different wavelengths and fixed contraction ratio. They then proposed a new criterion accounting also for the longitudinal radius of curvature of the pore $R_{zp}$ of the form

$$\tilde{C}_p \frac{1}{R_p} + \frac{1}{R_{zp}} \leq \tilde{C}_t \frac{1}{R_t} + \frac{1}{R_{zt}}.$$ (6.7)

Raeini et al. (2014a) investigated the existence of a threshold contraction ratio for snap-off for a single star-shaped pore-throat system of different aspect ratios $AR = \frac{L_t}{R_p}$, where $L_t$ is the length of the throat, and at different capillary numbers. Finally Armstrong et al. (2016) used Density Functional Hydrodynamics (DFH) tools to study geometry-constrained snap-off in pore doublets and simple systems of pores, demonstrating consistency of simulation results with theoretical criteria.

However, the last numerical studies assumed perfectly wetting behaviour between the two fluids, i.e. $\theta = 0^\circ$. Little effort has been devoted to quantifying the influence of contact angle on the occurrence of snap-off. Yu and Wardlaw (1986) carried out experiments under quasi-static conditions on a single pore-throat system of square cross-section. They found that the critical contraction ratio for snap-off increases only slightly from 1.5, when $\theta$ is equal to zero, to 1.75, when $\theta = 55^\circ$, however above $\approx 70^\circ$ snap-off never occurs. Pore-network studies (Blunt et al., 1997; Mogensen and Stenby, 1998) indicated that snap-off is inhibited above $Ca = 10^{-7}$ and for $\theta > 45^\circ$ when throats have a square cross-section. In the present study, the effects of contact angle and viscosity ratio on the occurrence of snap-off are examined.

### 6.3.1 Numerical setup

A single pore-throat constriction is studied for a range of capillary numbers between $10^{-4}$ and $10^{-6}$, and for different pore-throat geometries. The viscosity ratio $\mu$ is defined as the ratio between the viscosity of the injected non-wetting phase and the displaced wetting phase:

$$\mu = \frac{\mu_{nw}}{\mu_w}.$$
Figure 6.3. Cross-sections used in this study.

Figure 6.4. Initial conditions for the VOF indicator function (the non-wetting fluid is displayed in blue at the inlet) and the relevant geometrical parameters.
Table 6.3. List of parameters used in the simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(AR, CR)$</td>
<td>(1.5, 2), (1.5, 3), (5, 2), (5, 3)</td>
</tr>
<tr>
<td>$Ca$</td>
<td>$1.0e^{-4}, 1.0e^{-5}, 1.0e^{-6}$</td>
</tr>
<tr>
<td>$\bar{\mu}$</td>
<td>0.02, 1, 10, 20</td>
</tr>
<tr>
<td>$\theta$</td>
<td>All range of values starting from $0^\circ$ until snap-off is inhibited</td>
</tr>
</tbody>
</table>

Water is used as displaced wetting fluid. The viscosity ratio is varied considering different injected fluid: oil having the same density of water and supercritical CO$_2$ with density equal to 500 kg/m$^3$ and viscosity of $2e^{-5}$ Pa $\cdot$ s (reference values taken from Huppert and Neufeld (2014)). The interfacial tension coefficient is always equal to 0.05 N/m. Three cross-sections are considered (see Fig. 6.3): circular with unconstricted pore radius $R_p$ of 215 $\mu$m, square with largest inscribed circle in the unconstricted pore of radius equal to $R_p$ and isosceles triangle having base and height equal to 2$R_p$. This particular value of $R_p$ has been chosen to be consistent with the experimental apparatus of Yu and Wardlaw (1986). Initially, the non-wetting fluid is positioned just at the throat entrance, at a distance of 0.9$L_in$ from the inlet. This configuration allows for saving the computational time required for the bubble to reach the throat. Simulations results presented in previous section revealed that a bubble moves with constant curvature within a tube of constant cross-section. Moreover, preliminary simulations revealed that placing the initial interface far from the throat does not have significant effects on the predicted flow quantities relevant to this study. The outlet is sufficiently long to avoid boundary conditions effects. The entire geometry is therefore controlled solely by the two ratios $AR$ and $CR$, with $L_{in}$ and $L_{out}$ varying accordingly. A summary of the input data for the simulations is provided in Tab. 6.3, while the initial conditions for the VOF indicator function, as well as the various geometrical parameters involved, are displayed in Fig. 6.4. Boundary conditions are the same as for the dynamic capillary pipe test, with inlet velocity equal to 5 and 0.05 mm/s for the upper and lower capillary number respectively. Finally, values of $C_t = 1$ are used in all the simulations.

### 6.3.2 Description of the mechanism

The mechanism is illustrated in Fig. 6.5 for the case with square cross-section, $AR = 1.5$ and $CR = 2$. Two scenarios, with and without snap-off are presented, corresponding to values of $\theta$ equal to 30 and 35$^\circ$ respectively. As the bubble invades the throat (Fig.
Figure 6.5. Time evolution of the volume fraction for the case with square cross-section, $AR = 1.5$ and $CR = 2$ ($\bar{p} = 1$ and $Ca = 1.0e^{-4}$). Left column: $\theta = 30^\circ$, right column: $\theta = 35^\circ$. 
Figure 6.6. Visualization of the flow-back of the wetting phase along the corners of a square cross-section when the non-wetting phase invades the throat (Fig. 6.5a). (a) location of the cross-section, (b) volume-fraction distribution in the section and (c) axial velocity along the diagonal line (the x-axis is normalized against the diagonal half-length, where $R_t$ is the square half-side and $r$ is the distance from the origin, the latter positioned at the centre of the section).

Figure 6.7. Pressure drop between the inlet and the outlet as a function of time for different values of the contact angle $\theta$ (square cross-section, $AR = 1.5$, $CR = 2$, $\bar{\mu} = 1$ and $Ca = 1.0e^{-4}$).
6.5a), the mean curvature of the advancing front starts to increase as a result of the bubble squeezing into the throat. Since capillary pressure is directly proportional to the mean curvature according to the Young-Laplace equation, the capillary pressure in the throat also rises. This curvature (or pressure) drop between the interface advancing front just beyond the throat-pore junction and the initial unconstricted section of the pore causes faster interface speed within the throat than within the initial uncostricted section. This in turn initiates some amount of wetting phase to flow back along the corners of the cross-section, as shown in Fig. 6.6. If this drop in curvature is sufficiently large, enough wetting phase may accumulate in the throat to cause the interfaces from two corner regions to meet, and thus the flow to become unstable (Fig. 6.5c). This flow instability was distinctly observed during the simulations, and it was the critical condition leading to snap-off for long throats ($AR = 5$). Likewise, for shorter throats like the one in Fig. 6.5 ($AR = 1.5$), as the bubble reaches the throat exit (Fig: 6.5e), the interface starts to expand and the curvature decreases. Again, this drop in curvature causes a pressure gradient for the wetting phase driving a corner flow from the second pore back into the throat. At this point, snap-off occurs almost instantaneously. The wetting phase accumulating in the throat squeezes the collar of injected non-wetting phase (Fig. 6.5g) until it eventually breaks up, and two separate ganglia of non-wetting phase are formed (Fig. 6.5i). The newly-formed bubble will be floating within the second pore while the inlet-connected ganglion will re-start the mechanism from a configuration equivalent to (a). The case without snap-off does not present phenomena of flow instability. This is because when the bubble invades the second pore the entire cross-section of the throat is filled with the non-wetting phase, and thus the corner flowback of the wetting phase is prevented (see Fig. 6.5h). These steps are made clearer by plotting the pressure drop between the inlet and the outlet as a function of time (see Fig. 6.7) for both scenarios. For the case without snap-off, three stages are outlined. Initially, as the bubble of non-wetting phase invades the throat (Fig. 6.5d), the pressure rises as a result of the increase in the interface mean curvature. There is a peak in capillary pressure when the bubble assumes its max curvature, corresponding to the point the bubble starts filling the second pore (see Fig. 6.5f). Then, as the bubble invades the second pore (Fig. 6.5h), the interface mean curvature decreases and so does the pressure. Finally the capillary pressure approaches its theoretical value for a single unconstricted pipe.

The case with snap-off is characterized by flow instabilities and thus large drops and jumps in capillary pressure. When snap-off occurs, an instantaneous jump in pressure is observed as a result of the bubble break-up. The pressure at the inlet sharply increases,
Figure 6.8. Pressure drop between the inlet and the outlet as a function of time for different values of the contact angle $\theta$ (circular cross-section, $AR = 1.5$, $CR = 2$, $\mu = 1$ and $Ca = 1.0 e^{-4}$).

Figure 6.9. Volume fraction distribution at the time of instantaneous snap-off, when occurring, for different values of the contact angle $\theta$ (circular cross-section, $AR = 1.5$, $CR = 2$, $\mu = 1$ and $Ca = 1.0 e^{-4}$).
since the inlet-connected ganglion is back to the initial phase of invading the throat (see Figs. 6.5a and 6.5i), with consequent increase in curvature and capillary pressure. Besides, after snap-off (6.5i) there are two nw − w interfaces with a large curvature, and therefore a large pressure drop, instead than just one as in configuration 6.5a. In-between there is a w − nw interface with the opposite effect but with much smaller curvature. The localization of this pressure jump in the pressure vs time graph can therefore be used to find the exact location where snap-off occurs within the pore-throat system. An example of this is shown in Figs. 6.8 and 6.9 for a case with circular cross-section. For θ = 26°, the pressure drop rises dramatically as the non-wetting fluid invades the throat and the jump occurs at time t = 0.016 s before the curve approaches its descending branch, that is snap-off takes place at the throat. Conversely, for θ = 28°, the pressure jump occurs at time t = 0.09 s when the curve is in its descending branch, that is snap-off occurs after the non-wetting bubble has already invaded the second pore. Finally, for θ = 30°, snap-off does not occur.

### 6.3.3 Mesh sensitivity

Preliminary simulations were run in order to assess the role of some minor parameters such as the shape of the pore-throat junction, i.e. the angle ζ in Fig. 6.4, and the grid resolution $R_t/\Delta x$. While the shape of the pore-throat junction has no effect on the outcome of the simulations, the grid resolution strongly affects the dynamics of the flow. Fig. 6.10 shows the predicted pressure drop between the inlet and the outlet as a function of time, for different values of grid resolution $R_t/\Delta x=2, 4$ and 6, for two test-cases with square cross-section, $AR = 1.5$ and $CR = 2$. The two scenarios correspond to cases whether for the finer resolutions snap-off occurs or not, for values of θ equal to 28 and 32° respectively. As the figure clearly shows, the predicted pressure drop for the case with coarse resolution can be up to five times as the value predicted by the finer resolution models. These differences tend to diminish as the grid resolution increases, and the solution for the cases with $R_t/\Delta x=4$ and 6 are very similar for the case without snap-off. The same trend was observed also for other geometries, even in cases where using much higher contact angles snap-off was not recorded even for the coarser resolution (see Fig. 6.11). These unphysical pressure values may have an impact when running simulations on digital images of real rock samples. As a result of the segmentation process, the narrower throats, which are the ones determining the permeability of the medium, may potentially be resolved by very few elements, leading to inaccurate estimates of the capillary pressure and relative permeabilities-saturation curves. A possible remedy is to create finer grids such that the
Figure 6.10. Pressure drop between the inlet and the outlet as a function of time for different values of grid resolution and contact angle (square cross-section, $AR = 1.5$, $CR = 2$, $\bar{\mu} = 1$ and $Ca = 1.0e^{-4}$).
Figure 6.11. Pressure drop between the inlet and the outlet as a function of time for different values of the grid resolution (square cross-section, $AR = 5$, $CR = 2$, $\theta = 40^\circ$, $\mu = 1$ and $Ca = 1.0e^{-4}$).

narrower throats are resolved by more than 4 steps, in the same manner described in Sec. 4.4.3. However, this has two major consequences on the overall computational cost of the simulations. Firstly, increasing the size of the computational domain by a factor of at least 8 hugely increases the computational time required for performing each time step. Secondly, refining the original grid implies using a smaller grid size, leading to a time step smaller by a factor of at least $2^{3/2}$, as constrained by eq. (5.59).

Another preliminary study conducted for the selected benchmark geometry (square cross-section, $AR = 1.5$, $CR = 2$) revealed that there is also some sensitivity of mesh size on snap-off time. Fig. 6.12 shows that, although having the same trend, the time required for snap-off increases with increasing the mesh resolution. This gap is probably due to the additional time required for the bubble at the initial stage of the simulation to find its equilibrium configuration and to reach the throat, when the resolution is finer. The threshold contact angle value also slightly decreases from a value of 30 ($R_t/\Delta x=4$) to a value of 28° ($R_t/\Delta x=6$). These preliminary studies seem to suggest that a more resolved more space would be needed in order to have accurate predictions. However, this would have the cost of largely increasing the computational time needed to carry out the investigations. On the other hand, the focus here is to develop understanding of the mechanism rather that picking up the exact threshold contact angle value. In other words, the emphasis is put on capturing the correct physics of two-phase flow, and to determine the influence of the variation of the different quantities involved rather than
the exact quantification of their threshold values. Moreover, even if one would reach mesh independence and thus would be able to determine a sub-1° precision threshold contact angle value, this would have very limited practical relevance for engineering applications, as elementary geometries are used here. On the contrary, bearing in mind all these limitations, giving an overview of the influence of the different parameters involved is more valuable. For all these reasons a value of $\frac{R_t}{\Delta x} = 4$ seems adequate to the scope of the work, ensuring a good balance between computational effort and results accuracy, and therefore is used in all the following computations. More accurate simulations with higher resolutions are left for a later stage.

6.3.4 Effects of contact angle on the occurrence of snap-off

The threshold contact angle for snap-off, $\theta_{\text{thresh}}$, above which snap-off is inhibited, is computed using a systematic trial-error procedure by changing the static contact angle and repeating the simulations. Simulations are stopped when snap-off occurs or at breakthrough. In order to automatically detect snap-off, a function is implemented which measures how many separate ganglia of non-wetting fluid are present within the system. When the number of independent ganglia is greater than one, the simulation is terminated and the static contact angle is increased.

The time required for snap-off as a function of the contact angle for all the geometries considered is shown in Fig. 6.13. These graphs reveal two major things. Firstly, the time
Figure 6.13. Time required for snap-off as a function of the contact angle for all the geometries considered ($\overline{\mu} = 1$ and $Ca = 1.0e^{-4}$). Legend: Circle - $AR = 1.5$, $CR = 2$; asterisk - $AR = 1.5$, $CR = 3$; diamond - $AR = 5$, $CR = 2$; square - $AR = 5$, $CR = 3$;
required for snap-off increases with the contact angle. This can be easily explained by the fact that larger contact angles increase the flow resistance by forcing the interface towards the corners and thus reducing the available area for the flow back of the wetting phase (Legait, 1983; Ransohoff and Radke, 1988). Obviously, the time required for snap-off is generally much less for the simulations with $CR = 3$ that those with $CR = 2$. Less obviously, no significant changes in the time required for snap-off are observed for the case with longer throats. The second aspect to highlight is that $\theta_{\text{thresh}}$ constantly increases with diminishing the roundness of the cross-section, passing from a value of 28° for the circular cross-section to values of 30°–34° and up to 40° for the square and triangular cross-section respectively. This can be explained by using the concept of dimensionless flow resistance (Ransohoff and Radke, 1988). The dimensionless flow resistance is a parameter describing the wetting flow along the corners of a non-circular conduit and is determined solely by the geometry of the corner (half-angle and roundness). As the corner half-angle increases, i.e. from 30° of the equilateral triangular cross-section to 45° of the rectangular one, the area available for the wetting flow along the corner, for a given interface radius of curvature, decreases, resulting in a greater flow resistance. This greater flow resistance therefore acts as an impediment to the flow of the wetting phase, reducing the area available for the flow back along the corners of the cross-section, which is the origin of the snap-off mechanism. The circular cross-section can be seen as a limiting condition with an half-angle equal to 90°. However, with the approximations introduced when discretizing a circle using a structured cubic mesh, the circular cross section becomes in practice an irregular polygon. Nevertheless, since the aim here is to simulate pore-scale events taking place in real porous microstructures, the case with perfectly smoothed rounded capillary tubes of circular cross-section has no practical relevance.

### 6.3.5 Effects of viscosity ratio and capillary number on the occurrence of snap-off

Simulations are repeated for different viscosity ratio using as reference geometry the case with square cross-section, $AR = 1.5$ and $CR = 2$ ($Ca = 1.0e^{-4}$). The predicted values of the threshold contact angle $\theta_{\text{thresh}}$ as a function of the viscosity ratio are shown in Fig. 6.14. As the graph clearly shows, $\theta_{\text{thresh}}$ decreases with increasing the viscosity ratio. This is due to the increase in the viscous forces when $\mu$ increases. These forces oppose the flow of the injected more viscous phase but at the same time they also act as an impediment to the corner flow back of the resident wetting phase, as shown in Fig. 6.15.
Figure 6.14. Predicted values of the threshold contact angle as a function of the viscosity ratio (square cross-section, $AR = 1.5$, $CR = 2$ and $Ca = 1.0e^{-4}$).

As a result, when the non-wetting phase invades the throat, the interface assumes a stable configuration by filling the entire cross-section. Hence, smaller values of the contact angle, i.e. more bending of the interface, are necessary for increasing the area available for the wetting corner flow and therefore inducing the flow instability that leads to snap-off. Fig. 6.16 shows the time required for snap-off as a function of the viscosity ratio for a fixed value of $\theta = 24^\circ$, corresponding to the threshold value of the contact angle for which snap-off takes place for the whole range of viscosity ratios considered. This increase in time required for snap off for increasing viscosity ratios can be interpreted as an increase of the flow resistance due to the increase of the viscous friction, in agreement with the work of Legait (1983) for square cross-section.

Finally, simulations carried out at lower capillary numbers yield only a slight increase in $\theta_{thresh}$ from $30^\circ$ to $32^\circ$ for $Ca$ equal to $1.0e^{-4}$ and $1.0e^{-6}$ respectively.

### 6.3.6 Summary of key findings

To set context for the following studies in the real rock structures, the principal results of earlier studies are briefly summarized here:

- The code is capable of handling high density and viscosity ratios, and low capillary numbers. Computations are always stable and accurate, when the pore-space is sufficiently resolved. However, local numerical perturbations in form of vortices may arise in the transition region for high viscosity ratios (see Fig. 6.2b).
Figure 6.15. Axial velocity along the diagonal of a cross-section taken at the same position and at the same time step as in Fig. 6.6a, for different viscosity ratios (square cross-section, $AR = 1.5$, $CR = 2$, $\theta = 30^\circ$ and $Ca = 1.0e^{-4}$).

Figure 6.16. Time required for snap-off as a function of the viscosity ratio (square cross-section, $AR = 1.5$, $CR = 2$, $\theta = 24^\circ$ and $Ca = 1.0e^{-4}$).
Table 6.4. List of sub-samples used for the drainage simulations. *An initial 60x30x30-voxels sub-sample was cropped from the original sample and then refined by subdividing each voxel into 8 sub-voxels

<table>
<thead>
<tr>
<th>Original sample</th>
<th>Voxels</th>
<th>Size [mm$^3$]</th>
<th>$\phi$ [%]</th>
<th>$s_{nw}^0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CBsandstone1a</td>
<td>120x60x60*</td>
<td>0.054</td>
<td>31.5</td>
<td>0.11</td>
</tr>
<tr>
<td>Carb200</td>
<td>100x40x40</td>
<td>0.091</td>
<td>25.7</td>
<td>0.07</td>
</tr>
</tbody>
</table>

- When the geometry is more complex, as in the case of a pore-throat constriction, there is a non-physical building up of the pressure field when the pore space is not adequately resolved (see Sec. 6.3.3).

- When the injected fluid is up to two-order of magnitude less viscous than the resident fluid, as for the case with supercritical CO$_2$ and either water or brine, the dynamics of snap off does not significantly differ from the case with $\mu = 1$ (see Fig. 6.16). Hence, to avoid numerical instabilities induced by the high viscosity ratio, one may reasonably take the viscosity ratio equal to one as first approximation.

- In Ch. 3 an alternative formulation for the macroscopic capillary pressure was derived. It was then pointed out that this new formulation may be used for interpreting simulation results on digital images of real reservoir rocks and for providing more accurate $P_c - s_w$ curves.

### 6.4 Drainage simulations on rock samples

Drainage simulations are carried out on sub-samples cropped from the original $\mu$-CT images listed in Table 4.1. The new set of samples used for the simulations presented in this paragraph is listed in Table 6.4. For the sandstone, a sub-sample which is representative of the rock was taken. However, most of the throats in the original image were resolved by a single voxel only. Preliminary simulations carried out on the original image collapsed after few time steps, due to non-physical building up of the pressure field. Hence, the original image was refined by subdividing each voxel into 8 sub-voxels. For the carbonate sample instead, a sub-sample with porosity much higher than the measured one was selected, given the difficulties in finding sub-samples with connected pore-space, due to the high variability of the carbonate pore system configuration. Nevertheless, the carbonate sample did not need any grid refinement since the narrower throats were adequately resolved.
In order to simulate capillary trapping more realistically and to investigate the role of some relevant parameters, values of interfacial tension $\sigma$ and static contact angle $\theta$ for either supercritical $CO_2$-brine or supercritical $CO_2$-water systems are used. $\sigma$ is always taken equal to $0.04 \, N/m$ (Espinoza and Santamarina, 2010) while four different values of $\theta$ are used: $\theta = 40, 45$ and $50^\circ$ for the supercritical $CO_2$-brine system (Espinoza and Santamarina, 2010; Andrew et al., 2014), and $\theta = 30^\circ$ for the supercritical $CO_2$-water system (Espinoza and Santamarina, 2010). In order to speed-up the computations by using larger time-steps and avoid numerical instabilities, the viscosity ratio is kept equal to 1. This choice is justified by simulations results presented in the previous section. Boundary conditions are the same as for the snap-off test, with inlet velocity equal to 5 $mm/s$, corresponding to a capillary number $Ca$ equal to $1.0e^{-4}$. As initial conditions, the non-wetting phase fills the initial 10% of the image towards the inlet boundary. Finally, values of $C_t = 1$ are used in all the simulations.

The time evolution of the volume fraction for the carbonate sample can be visualized in Fig. 6.17 (final saturation at breakthrough of the injected non-wetting phase $s_{nw}^f = 0.6$). No significant differences in displacement patterns were observed for different values of $\theta$. The displacement of the injected $CO_2$ plume was always piston-like and no snap-off was recorded during the simulations for any of the contact angle values considered.

For the sandstone, the initial and final configurations are displayed in Figs. 6.18a and 6.18b respectively ($s_{nw}^f = 0.25$). A viscous-fingering pattern is clearly visible and several instances of snap-off were recorded. This is due to the higher complexity of the sandstone pore-space, where several pore-throat systems with high contraction ratios are easily encountered.

### 6.4.1 Comparison of different macroscopic capillary pressure measures

Following the theoretical developments presented in Ch. 3, a comparison of different measures of the macroscopic capillary pressure $P_c$ is carried out here. It is recalled that no universal definition of capillary pressure exists at the macro-scale, and $P_c$ is often defined by analogy with its microscopic definition, as in eq. (3.70). The relationship between $P_c$ and the shape of the various interfaces contained within the averaging volume $\forall$ was given by Whitaker (1986b) through eq. (3.71). It was then pointed out here that these traditional formulations present several inconsistencies, i.e. lack of rigour and ambiguity in averaging domain. Hence, to remove these inconsistencies, an alternative
Figure 6.17. Time evolution of the volume fraction for the carbonate sample ($\theta = 30^\circ$).
A new approach was developed, leading to a new definition of $\mathcal{P}_c$ as the macroscopic force due to capillary effects per unit averaging volume (eq. (3.92)).

Here, these different formulations of $\mathcal{P}_c$ are compared in the framework of the VOF method for interpreting the results of the simulations. The standard definition of $\mathcal{P}_c$ (eq. (3.70)), denoted as $\mathcal{P}_c^{standard}$, is computed as

$$\mathcal{P}_c^{standard} = \langle p_n \rangle^n - \langle p_w \rangle^w = \frac{\sum p_i(1 - \alpha_i)V_i}{\sum(1 - \alpha_i)V_i} - \frac{\sum p_i\alpha_iV_i}{\sum \alpha_iV_i}, \quad (6.8)$$

where the sum is over all the computational cells. The intrinsic surface average of the interface curvature (r.h.s. of eq. (3.71)), denoted as $\mathcal{P}_c^k$, is computed as

$$\mathcal{P}_c^k = \sigma \langle k_n \rangle^n = \sigma \frac{\sum k_i |\nabla \alpha_i|V_i}{\sum |\nabla \alpha_i|V_i}, \quad i \in "INT" \cup "INT\_WALL", \quad (6.9)$$

where the sum is now over the union of the cells containing an interface. The magnitude of the macroscopic capillary pressure force per unit interfacial area, denoted as $\mathcal{P}_c^{nw}$, is computed from the intrinsic surface averages of the pressures at the interface as follows

$$\mathcal{P}_c^{nw} = \frac{\sum p_i(1 - \alpha_i)V_i}{\sum(1 - \alpha_i)V_i} - \frac{\sum p_i\alpha_iV_i}{\sum \alpha_iV_i}, \quad i \in "INT" \cup "INT\_WALL". \quad (6.10)$$

Fig. 6.19 shows the different computed macroscopic capillary pressure measures as a function of time for the carbonate sample. Overall the three curves behave similarly.

With reference to Fig. 6.17, and sketching the preferential flow pattern as a network of five pores connected by four throats (see Fig. 6.20), the following trend is observed. Initially, as the bubble invades the first throat (Fig. 6.17b), the capillary pressure rises. Then there is a sudden drop corresponding to the injected fluid filling pore 1 (Fig. 6.17c).
Figure 6.19. Comparison of different macroscopic capillary pressure measures for the carbonate sample ($\theta = 30^\circ$)

Figure 6.20. Sketch of the carbonate pore-structure.
Likewise, another increase in capillary pressure is observed during invasion of throat 2 (Fig. 6.17d), followed by a second drop as the bubble starts filling pore 2 (see Figs. 6.17e and 6.17f, captured respectively soon before and after pore 2 is filled). A third drop in pressure occurs in the transition from throat 3 to pore 3 (see Figs. 6.17g and 6.17h). Finally, the capillary pressure increases again as the bubble moves within the last throat until breakthrough (Fig. 6.17i). However, a significant difference between the standard macroscopic capillary pressure, computed using eq. (6.8), and the other two measures, i.e. eqs. (6.9) and (6.10), is observed. This difference is due to the fact that $P_{c}^{\text{standard}}$ is computed from a discretization of the intrinsic volume average operator, while the other two measures are computed from discretized surface averages. This means that in real porous media the pressure within each phase is not constant. On the other hand, better agreement is observed between $P_{c}^{k}$ and $P_{c}^{nw}$. This confirms the argument made in Sec. 3.5.3 that use of surface averages for the pressures is more appropriate than that of volume averages when averaging the relevant surface microscopic balance equations.

The same analysis conducted for the sandstone sample produced results which are not likely to be physical (see Fig. 6.21), as the model resolution is not sufficient. For example, while for the carbonate $P_{c}^{\text{standard}}$ is roughly twice as much the other two measures, for the sandstone this ratio rises on average to 7 when $P_{c}^{\text{standard}}$ is compared to $P_{c}^{nw}$, and up
to 20 when it is compared to $P_c^k$. The latter discrepancy in particular can be explained by the fact that while $P_c^k$ is primarily determined by the shape and size of the pore space, $P_c^{\text{standard}}$ incorporates also all the dynamic effects caused by the local displacement mechanisms, such as snap-off. These mechanisms involve abrupt changes in velocity and sudden jumps in pressure, as discussed in the previous section. Besides, the poor resolution of the narrower throats is very likely to produce large inaccuracies in predicting the flow field, as reported in Sec. 6.3.3. Fig. 6.10 showed that an error up to a factor of five is produced when the throat is resolved with 4 steps along the effective diameter, even when simple polygonal cross-sections are employed. For this sandstone, the narrower throats are resolved by 2 elements only. Moreover, the pore-space is much more complex than the single pore-throat system used for the snap-off simulations. A better refinement of the original $\mu$-CT images is very likely to reduce the magnitude of these errors. However, even with the adopted subdivision into 2 sub-voxels per direction, the computational cost of the overall time-marching procedure was very high, with approximately 600 time steps/day performed versus roughly 3000 for the carbonate. Further increasing the subdivision to 4 voxels per direction would yield a computational domain 64 times larger that the original one (and 8 times the one used in these simulations). Besides, the additional constraint of adopting an even smaller time step, according to eq. (5.59), still applies. All this together would make the computations almost unpracticable at the current stage.

To conclude, when it is possible to select a sample with sufficiently resolved porous structure the model is able to produce physical results. Besides, by interpreting simulations results in the framework of a rigorous theory of porous media flows, accurate and more sound capillary pressure-saturation curves than those obtained with traditional coreflooding experiments, can be obtained. This demonstraes the potential of the model to be applied to complex geometries when mesh resolution is computationally achievable, and sets new perspectives for reservoir engineering applications. Conversely, results for the sandstone, where the pore size is too small to be captured at the resolutions used in this study, are not likely to be physical. In the future efforts should be devoted to optimize the code in order to make these complex $\mu$-CT meshes computationally achievable for two-phase flow simulations.

### 6.5 Summary

Simulations results of both drainage and imbibition on porous systems of increasing complexity have been presented. First, imbibition in a circular pipe has been simulated for
different flow conditions, i.e. varying $Re$ and $Ca$, and high density and viscosity ratios. Results confirmed the robustness of the code. The deviation from Poiseuille flow at the front meniscus has been shown, in agreement with MD simulations.

The snap-off mechanism, which is the pore-scale mechanism at the origin of capillary trapping, has then been studied. Single pore-throat systems of different geometry and different cross-section (circular, square and triangular) have been used to investigate the role of several parameters, including contact angle and viscosity ratio, on the dynamics of snap-off. Preliminary simulations revealed that poor resolution of the narrower throat can lead to a non-physical building-up of the pressure field. The threshold contact angle for snap-off, $\theta_{\text{thresh}}$, i.e. the value of the static contact angle above which snap-off is inhibited, has been computed for each case. Results showed that $\theta_{\text{thresh}}$ increases with diminishing the roundness of the cross-section, passing from a value of $28^\circ$ for the circular cross-section to values of 30-34° for the square cross-section, and up to 40° for the triangular cross-section. The analysis on the viscosity ratio has been restricted to the single case with square cross-section, $AR = 1.5$ and $CR = 2$. Increasing the viscosity of the injected phase resulted in a drop in $\theta_{\text{thresh}}$ from a value of $30^\circ$ when $\mu = 1$ to a value of $26^\circ$ when $\mu = 10$ and down to a value of $24^\circ$ when $\mu = 20$.

Finally, drainage simulations have been carried out on $\mu$-CT images of different rock samples. Results were shown to be physical when the pore space is sufficiently resolved. Comparison of different macroscopic capillary pressure measures revealed a significant difference between the standard definition of the macroscopic capillary pressure employing intrinsic volume averages for the pressures and other forms employing intrinsic surface averages. This confirms the argument that use of surface average for the pressures is more appropriate than that of volume average when averaging the relevant surface microscopic balance equations. This sets new perspectives for the evaluation of the capillary pressure-saturation curves, which are crucial relationships in reservoir engineering.
Chapter 7

Conclusions

The key findings and conclusions of this work, set against the objectives described in Sec. 1.2, are presented in the following.

Development of an in-house code for the computation of either single and two-phase flow at the pore-scale using conventional CFD techniques

A stable and accurate algorithm for modelling either single and two-phase flow at the pore-scale for applications in porous media flows has been developed.

For single-phase flow, the Stokes equations of creeping flow of an incompressible fluid are solved using the FV SIMPLE algorithm. The method has been validated with several benchmark cases, including the Stokes flow past a sphere problem, and then successfully applied to compute fluid flow on \( \mu \)-CT images of different rock samples. Furthermore, a new convergence criterion for the SIMPLE algorithm, and more generally for the family of pressure-correction methods, has been developed. This criterion is based on bulk momentum balance and is particularly useful for pore-scale modelling of reservoir rocks, especially when the predicted flow quantities are used for upscaling, e.g. Darcy’s law.

For two-phase flow, the algorithm is much more complex than for single-phase flow, due to the need of tracking the fluids within the computational domain and accounting for surface tension forces at the interfaces. The whole method consists of three main components: an interface-tracking algorithm, a model for the surface tension forces and a solver for the NS equations. The interfaces are tracked using the PLIC-VOF method and then evolved in time by solving an advection equation, with advection done through operator splitting. Surface tension forces are modelled using the FSF method of Raeini et al. (2012). Wettability conditions are enclosed in the model by means of a boundary condition at the wall, which gives the normal to the interface at a solid wall as a function of the static contact angle, the normal to the wall and the gradient of the VOF indicator.
function. Finally, the NS equations are solved using the PISO algorithm. The model has been extensively validated with several static and dynamic problems, for different flow conditions and for high density and viscosity ratios. All these tests gave accurate results and demonstrated the robustness of the code.

**Prediction of the petrophysical properties of rocks**

The petrophysical properties, namely REV, mean pore and grain size, and absolute permeability of two rock formations, one sandstone and one carbonate, have been successfully determined by applying an integrated approach comprising computer-tomography, statistical correlation, and numerical simulations. In particular, it has been shown that REV and mean pore and grain size are effectively estimated using the two-point spatial correlation function. Besides, rock homogeneity and anisotropy can also be assessed using spatial correlation tools. Absolute permeability is predicted from the computed flow field using Darcy’s law. The comparison between predicted permeability and the experimentally determined one showed good agreement for the carbonate but huge discrepancy up to 2 order of magnitude for the sandstone.

Typical two-phase relationships, such as relative permeability-saturation and capillary pressure-saturation, are more difficult to obtain from numerical simulations, due to uncertainties in the definition of some of these quantities, i.e. the macroscopic capillary pressure, and the non-physical building-up of the predicted pressure field when the narrower throats are not adequately resolved. However, it was shown that when is possible to extract an adequately resolved porous region of a reservoir rock, accurate capillary pressure-saturation curves can be computed.

**Understanding of the pore-scale mechanisms happening at conditions encountered in carbon sequestration**

The snap-off mechanism, which is at the origin of capillary trapping in porous rocks, has been studied. Numerical simulations were shown to be a powerful tool for understanding the origin of this mechanism, providing information on the instantaneous distribution of the relevant quantities otherwise impossible to access using traditional experiments. Snapshots of the velocity field clearly showed that snap-off is caused by local instability of the front meniscus, when the pore-throat constriction is such that a corner flow-back of the wetting phase is initiated. The effects of contact angle and viscosity ratio on the dynamics of snap-off have then been quantified by simulating drainage on single pore-throat constrictions of different geometry and for different shapes of the cross-section. Results
showed that the threshold contact angle for snap-off increases with diminishing the roundness of the cross-section, passing from a value of 28° for the circular cross-section to values of 30-34° for the square cross-section and up to 40° for the triangular cross-section. For a throat of square cross-section with CR = 2, increasing the viscosity of the injected phase resulted in a drop in the threshold contact angle from a value of 30° when \( \mu = 1 \) to a value of 26° when \( \mu = 10 \) and down to a value of 24° when \( \mu = 20. \)

**Critical analysis of the definition of the macroscopic capillary pressure in porous media flows**

A novel definition of the macroscopic capillary pressure as the macroscopic force due to capillary pressure acting on all the fluid-fluid interfaces per unit averaging volume has been presented. It was obtained through a rigorous spatial averaging procedure starting from the microscopic momentum balance for a surface. This procedure resolves most of the shortcomings of standard definitions, such as the lack of dynamic terms in the momentum balance, the accounting for the different orientation of the interfaces contained within the averaging volume and the averaging domain inconsistency. The latter refers to the incongruity in using intrinsic volume averages for the pressures when taking the average of a microscopic balance equation for a surface, and thus averaging quantities defined on that surface only. This inconsistency was highlighted by simulation results of drainage on \( \mu \)-CT images of rock samples. Comparison of different macroscopic capillary pressure measures showed a significant difference between the standard definition of the macroscopic capillary pressure employing intrinsic volume averages for the pressures and other forms employing intrinsic surface averages, i.e. the intrinsic surface average of the interface mean curvature and the magnitude of the newly defined macroscopic capillary pressure force per unit interfacial area. The latter two measures were instead in good agreement. This confirmed the argument that use of surface average for the pressure is more appropriate than that of volume average when averaging the relevant surface microscopic balance equation.

### 7.1 Future directions

The code developed as part of this project is possibly the major outcome of this work. It will form the basis for future extension to multiphysics modelling, i.e. heat transfer and reactive transport. A solver for the advection-diffusion equation, with temperature as unknown variable, was already implemented and validated independently within this
work. Inclusion in the model of equations of state and correlations for fluid properties such as density and viscosity, interfacial tension, and even contact angle, would certainly make the predictions more realistic, especially for the case of supercritical \(CO_2\). Likewise, inclusion of geochemical reactions would make the model particularly suitable for important environmental applications other than geological storage of \(CO_2\) such as groundwater flow pollution and contaminant transport. Another possible development is the extension to the case of compressible fluids. However, as mentioned in previous sections, the immediate development of the model is to optimize the existing code in order to handle larger computational domains with complex porous microstructure. This is of paramount importance if one wants to make the method fully applicable to real porous formations. Results presented in this Thesis also offer several suggestions for possible follow-up studies. These may include

- Collection of different reservoir rocks followed by their thorough characterization using samples of different scales.
- A numerical study on the different types of drags (viscous and form) and their relation with the rock pore-structure.
- Extension of the snap-off study to more complex pore-throat configurations, and even to representative porous regions extracted scanned images of real reservoir rocks.
- Extension of the theory of porous media flows to account for a thermodynamic description of the fluid-fluid-solid contact lines

Finally, potential applications of the new macroscopic capillary pressure formulation are to be explored. An example would be the development of a multi-scale approach where the absolute permeability and the \(P_c - s_w\) curves, which are input data for the reservoir-scale simulations, are obtained as output data of pore-scale simulations performed over volumes taken of size at least covering the REV for the rock. This would form an entirely computational approach which would overcome the practical difficulties and uncertainties of traditional experiments.
References


Challenges in modeling unstable two-phase flow experiments in porous micromodels. 


