

Imperial College London
Department of Earth Science and Engineering

Modelling two-phase flow at the micro-scale using a volume-of-fluid method

Mosayeb Shams

July 2018

Submitted in part fulfilment of the requirements for the degree of
Doctor of Philosophy in Department of Earth Science and Engineering of
Imperial College London
and the Diploma of Imperial College London

Abstract

We present a numerical scheme to model two-phase flow in porous media where capillary forces dominate over viscous effects. The volume-of-fluid method is employed to capture the fluid-fluid interface whose dynamics are described based on a finite volume discretization of the Navier–Stokes equations. Interfacial forces are calculated directly on reconstructed interface elements such that the total curvature is preserved. The computed interfacial forces are explicitly added to the Navier–Stokes equations using a sharp formulation which effectively eliminates spurious currents. The numerical model is validated in terms of physics, robustness, and mesh convergence, using an extensive hierarchy of static and dynamic test cases including wetting effects at the solid interface in two and three space dimensions.

Next we provide an extensive study of viscous coupling effects in porous media flows, where the flow of one phase in the centre of a pore affects the flow of phases in layers or corners and vice versa. We perform two-phase flow simulations for different fluid configurations in non-circular capillary tubes to investigate viscous coupling effects as a function of viscosity ratio, contact angle, wetting phase saturation and wettability. We demonstrate the accuracy of our code in determining fluid velocities and capillary pressures, even for slow flows, where previous approaches fail. We specifically show the dependence of velocity profile and consequently flow conductivities on viscosity ratio and interface boundary condition, by modelling immiscible two-phase flow through an equilateral triangular capillary tube with sandwiched layers. We also demonstrate that imposing no-flow or free-slip interface boundary conditions at a clean fluid-fluid interface with zero interfacial shear viscosity, may lead to under- or over-estimation of flow conductance in layers compared to the physically correct continuity boundary condition at the interface.

We use two-phase direct numerical simulation results in conjunction with basic arguments from fluid mechanics to present parametric models that estimate fluid conductivities as a function of the geometry and viscosity ratio. These scaling models, which take into account the flow coupling, can then be incorporated into pore-to-Darcy-scale flow models, for example two-phase pore-network models, to study the effects of viscous coupling on macroscopic flow properties such as relative permeabilities. These network models provide a much more computationally efficient framework for the simulation of flows to the centimetre or larger scales. Furthermore, in future work our methods can be used to assess local recovery and displacement mechanisms in multiphase flow using pore-scale images of different rocks.

Declaration

I declare that this thesis, titled “Modelling two-phase flow at the micro-scale using a volume-of-fluid method”, is entirely my own work under the supervision of Prof. Martin J Blunt and Dr Branko Bijeljic. All published and unpublished materials used in the thesis have been given full acknowledgement. This work has not been previously submitted, in whole or in part, to any other academic institution for a degree, diploma, or any other qualification.

Mosayeb Shams

Department of Earth Science and Engineering

Imperial College London

Copyright Declaration

The copyright of this thesis rests with the author and is made available under a Creative Commons Attribution Non-Commercial No Derivatives licence. Researchers are free to copy, distribute or transmit the thesis on the condition that they attribute it, that they do not use it for commercial purposes and that they do not alter, transform or build upon it. For any reuse or redistribution, researchers must make clear to others the licence terms of this work.

Acknowledgements

I would like to thank my supervisors, Prof. Martin J Blunt and Dr Branko Bijeljic, for their support and guidance during this study.

I would like to express my sincere gratitude to my PhD viva examiners, Prof. Stephane Zaleski and Prof. Stephen Neethling for their time and consideration.

I would like to thank my colleagues and friends at Imperial College London for their support and encouragement.

Last but not least, I owe my deepest gratitude to my family for their unconditional love, endless support, priceless care, and constant encouragement.

List of publications

M. Shams, A.Q. Raeini, M.J. Blunt, and B. Bijeljic. A numerical model of two-phase flow at the micro-scale using the volume-of-fluid method. *Journal of Computational Physics*, 357 (2018) 159-182.

M. Shams, A.Q. Raeini, M.J. Blunt, and B. Bijeljic. A study to investigate viscous coupling effects on the hydraulic conductance of fluid. *Journal of Colloid and Interface Science*, 522 (2018) 299-310.

Contents

1. Introduction	20
1.1. Background	21
1.2. Pore-scale modelling	23
1.2.1. Network modelling	23
1.2.2. Direct modelling	24
1.3. Grid-based methods: immiscible two-phase flow	26
1.3.1. Basic equations	26
1.3.2. Interface representation	30
1.3.3. Interfacial force representation	33
1.3.4. Contact line statics and dynamics	36
1.4. Thesis outline	39
2. Mathematical and numerical modelling	40
2.1. Mathematical model	41
2.2. Numerical method	43
2.2.1. Finite-volume discretization of the transport equations	43
2.2.2. Solution procedure of the discretized equations	45
2.2.3. Reconstructing the interface	47
2.2.4. Computing the interfacial force	52
2.3. Closure	55
3. Validation of the numerical method	56
3.1. Static test cases	57
3.1.1. Static droplet	57
3.1.2. Static contact-line	62
3.2. Dynamic test cases	64
3.2.1. Moving droplet	65
3.2.2. Moving contact-line	70
3.2.3. Corner flow	74
3.3. Closure	77
4. Viscous coupling	79
4.1. Introduction	80
4.2. Viscous coupling validation	82
4.3. Geometry configurations and coupled flow modelling	84

4.4. Scaling models and validation	94
4.4.1. Conventional (diagonal) terms	94
4.4.2. Coupling (off-diagonal) terms	98
4.5. Three-dimensional geometries with nonuniform cross-sections	101
4.6. Closure	103
5. Conclusions and future work	104
5.1. Conclusions	105
5.2. Future work	107
Bibliography	118
A. Semi-analytical solution of the velocity profile for two-phase flow through a uniform single tube	119

List of Tables

3.1. Effect of mesh resolution on the error in maximum velocity.	59
3.2. Errors in the maximum velocity and normalized error in the pressure jump across an interface in the corner of a star-shaped geometry for different mesh resolutions, corner angles, and equilibrium contact angles.	64
4.1. Fitted values for the parameters used to estimate the diagonal terms in the general mobility matrix for uniform and non-uniform wettability configurations. .	96
4.2. The mean relative errors in the predicted diagonal terms.	96
4.3. Fitted values for the parameters to estimate coupling terms in the general mo- bility matrix for uniform and nonuniform wettability configurations.	99
4.4. The mean relative errors in the predicted coupling terms.	100

List of Figures

1.1.	Illustration of a micro-CT pore-space image of a Ketton limestone rock sample, 2 mm across with a voxel size of $4\ \mu m$	22
1.2.	Illustration of stages involved in the post processing of micro-CT raw image data.	22
1.3.	A thin control volume, δV , with surface boundary δS_f and characteristic thickness ε . The control volume encloses an infinitesimal small interfacial element δS bounded by a closed contour C , on an interface S between two immiscible fluids.	27
1.4.	A schematic representation of a portion of a fluid-fluid interface and related methods used to model its shape and motion.	31
1.5.	Schematic representation of an interface between two fluids as a sharp boundary and a smooth transition zone using discontinuous and continuous indicator functions, respectively.	35
1.6.	Schematic representations of a static liquid-liquid interface at equilibrium on a solid surface with the equilibrium contact angle, θ_e , and contact angle hysteresis during the wetting phase advance (imbibition) and recession (drainage).	37
2.1.	A schematic of an infinitesimal control-volume, dV , containing two immiscible fluids separated by an interface, dS , and bounding contour C	42
2.2.	A three-dimensional hexahedral control-volume (or cell).	44
2.3.	A two-dimensional schematic of the steps in reconstructing the interface.	48
2.4.	Schematic representation of converting the smooth transition of the indicator function to a sharp profile.	49
2.5.	A schematic representation of a fluid-fluid interface adjacent to a solid surface and the correction of the normal vectors on the solid surface in accordance with the imposed contact angle, θ	51
3.1.	Dimensionless maximum velocity, the spurious current capillary number, Ca , as a function of dimensionless time for a two-dimensional static droplet.	58
3.2.	Velocity vector field and the indicator function contour ($\alpha = 0.5$) at dimensionless time $t_d = 0.25$, for a two-dimensional droplet in static equilibrium.	59
3.3.	Visualization of a reconstructed fluid-fluid interface of a three-dimensional static droplet on a uniform Cartesian mesh.	60
3.4.	Dimensionless maximum velocity, the spurious current capillary number, for a three-dimensional static droplet, when the interfacial force is modelled using the CSF, SSF and CLSF methods.	61

3.5. Computed pressure field for a three-dimensional static droplet (cut through the centre of the droplet), when the interfacial force is modelled using the CSF, SSF and CLSF methods.	61
3.6. Schematic visualizations of a two-dimensional star-shaped geometry and its uniform mesh.	63
3.7. Sample visualizations of the computed pressure field for an interface in the corner of a star-shaped geometry using using the CSF, SSF and CLSF methods.	63
3.8. Dimensionless average droplet velocity as a function of dimensionless time for a two-dimensional droplet moving in a uniform velocity field, simulated using the CSF, SSF and CLSF methods.	66
3.9. Velocity vector plots for a two-dimensional simulation of a droplet moving in a uniform velocity field, simulated using the CSF, SSF and CLSF methods.	67
3.10. A sample visualization of indicator function and computed pressure field for a two-dimensional droplet moving in a uniform velocity field, simulated using the CLSF method.	67
3.11. Dimensionless average droplet velocity as a function of dimensionless time for a three-dimensional droplet moving in a uniform velocity field, simulated using the CSF, SSF and CLSF methods.	68
3.12. A sample visualization of velocity vector field, indicator function and computed pressure field for a three-dimensional droplet moving in a uniform velocity field, simulated using the CLSF method.	69
3.13. Convergence study for a two- and three-dimensional moving droplet test cases, simulated using the CLSF method.	70
3.14. Plots of initial fluid configurations, velocity vector field and interface shape of a two-dimensional micro-channel, simulated using the CLSF method.	71
3.15. Plots of dimensionless average interface velocity as a function of dimensionless time for steady contact line displacement in a micro-channel.	71
3.16. L_2 error norm as a function of a dimensionless time for a steady contact line displacement in a micro-channel using different mesh resolutions, when simulated using the CLSF method.	72
3.17. A two-dimensional micro-channel with triangular roughness on its solid boundaries.	73
3.18. Spikes in the velocity field presented in terms of $L_2(Ca)$, Equation (3.10), as a function of the dimensionless time, t_d , for a steady contact line displacement through two-dimensional smooth and rough micro-channels on a grid of resolution $D/\delta x = 32$. The contact angle is $\theta = 30^\circ$ and the interfacial force is computed using the CLSF method.	73
3.19. A three-dimensional square micro-channel and the velocity vector field using the CLSF method.	74

3.20. Plots of the dimensionless average interface velocity and the related L_2 error norm for steady contact line displacement through a three-dimensional square micro-channel, computed using the CLSF method.	74
3.21. A square capillary tube with non-wetting phase in the centre and wetting phase in the corners.	75
3.22. Dimensionless flow resistance as a function of time in the corners of a square capillary tube with different mesh resolutions, computed using the CLSF method.	76
3.23. Comparison of dimensionless flow resistance in the corners of a gas-occupied and a liquid-occupied square capillary tube.	77
4.1. Schematic illustrations of a square capillary tube and cross-sectional configuration of wetting and non-wetting phases.	82
4.2. Axial velocity profiles for co-current two-phase flow along the diagonal of a square capillary tube.	83
4.3. The normalized error of computed velocity profile versus mesh resolution for two-phase flow with different viscosity ratios through a square capillary tube.	84
4.4. Schematic illustrations of fluid configurations for square, equilateral triangular and star-shape pore geometries with uniform and non-uniform wettability conditions.	85
4.5. Schematic illustrations of initial and stabilized form of fluid-fluid interfaces and corresponding geometric parameters for capillaries with uniform and non-uniform wettability conditions.	86
4.6. Visualizations of initialized and equilibrium configurations of sandwiched oil layers in the corners of an equilateral triangular capillary.	89
4.7. Steady-state velocity distribution across flowing fluids with different viscosity ratios in an equilateral triangular capillary.	90
4.8. Plot of dimensionless total hydraulic conductance of a sandwiched oil layer as a function of viscosity ratio, for different interface boundary conditions.	90
4.9. Comparison of contributing components to the total conductance of a sandwiched oil layer in a triangular capillary tube.	91
4.10. Comparisons of the dimensionless resistance for wetting phase flow along the sharp corners of a square capillary tube while the pressure gradient within the non-wetting phase in the centre is zero.	92
4.11. Comparisons of the dimensionless resistance for wetting phase flow along the sharp corners of a square capillary tube in a co-current flow.	93
4.12. Comparison of the predicted values of the scaling model with the simulated values of the diagonal terms.	97
4.13. Comparison of the predicted values of the scaling model with the simulated values of the coupling terms.	100

4.14. A visualization of a three-dimensional star-shaped pore-throat system used to simulate a snap-off process.	101
4.15. A visualization of the saturation profiles of the wetting phase (blue) and the nonwetting phase (red) at different time steps for an imbibition process in the three-dimensional nonuniform star-shaped geometry.	102
A.1. Schematic of a uniform polygonal tube geometry.	120

Nomenclature

Roman Symbols

A	Amplitude of a triangular roughness	m
a, b, c	Constant fitting parameters	
A_d	Diagonal elements of the coefficient matrix	
A_i	Area open to flow for region i	m ²
A_r	Relative thickness of a sandwiched layer	-
b	Inscribed radius	m
b_{12}	Meniscus-apex distance for interface Γ_{12}	m
b_{23}	Meniscus-apex distance for interface Γ_{23}	m
$\tilde{c}$	Smoothed colour function	-
c	Sharp colour function	-
C	Contour-line of an interfacial element	
C_α	Compression factor	-
Ca	Capillary number	-
Ca_{drop}	Capillary number of a moving droplet	-
Ca_{flow}	Capillary number of flow	-
Ca_{inj}	Capillary number of injection flow rate	-
$Ca_{\text{interface}}$	Capillary number of a moving interface	-
C_c	Clipping factor	
C_s	Smoothing relaxation factor	
D	Diameter of a droplet or width of a channel	m
$\mathbf{d}_i$	Distance vector between the centroid of face i	m
$d\ell$	the length of an increment along the perimeter of a contour line	m

$\mathbf{F}$	Body force per unit volume	N/m ³
$\mathbf{f}$	Body force per unit volume	N/m ³
$\mathbf{f}_c$	Curvature force	N
$\mathbf{f}_{\text{int}}$	Interfacial force acting on an interfacial element	N
f_{mix}	Mixed-face cut by an interface	
$\mathbf{f}_\sigma$	Interfacial force per unit area	Pa
$\mathbf{f}_{\sigma v}$	Interfacial force as a body force per unit volume	N/m ³
$\mathbf{G}$	An arbitrary vector or tensor field	
$\mathbf{g}$	Gravity	m/s ²
h	Face normal distance between the centroid of two cells	m
$\mathbb{I}$	Identity tensor	
L	Characteristic length	m
l	Distance between centre of interface Γ_{12} and the vertex of the related corner	m
L_2	L_2 error norm	
L_∞	L infinity error norm	
l_w	Wall length	m
$\mathbf{m}$	Tangent unit vector at the edge of an interfacial element	
M	Viscosity ratio	-
$\mathbf{n}$	Normal unit vector at a surface	
N_f	Total number of the faces that share the mesh point p	
$N_{f_{\text{mix}}}$	Total number of mixed-faces that belong to a cell	
N_p	Total number of the vertices of an interface element	
P	Period of a triangular roughness	m
p	Pressure field	Pa
p_w	Wetted perimeter	m
$[\tilde{q}]$	Column vectors of dimensionless volumetric fluxes	

q_i	Flow rate through region i	m^3/s
R	Radius of a droplet	m
r_{12}	Curvature radius for interface Γ_{12}	m
r_{23}	Curvature radius for interface Γ_{23}	m
R_l	Curvature radius	m
$\mathbf{s}$	Unit vector that is tangent to an interfacial element and normal to its edge	
s	Phase saturation	-
S	Fluid-fluid interface	
$\mathbf{S}_{\text{int}}$	Area vector of an interface element	m^2
S_i	Surface boundary of control-volume i	
$\mathbb{T}$	Stress tensor	Pa
t	Time	s
t_d	Dimensionless time	-
$\mathbf{u}$	Velocity vector field	m/s
$\mathbf{u}_r$	relative velocity	m/s
U	Velocity magnitude in flow direction	m/s
u_z	Velocity magnitude in z-direction	m/s
u_x	Velocity magnitude in x-direction	m/s
V_i	Volume of fixed control-volume i	m^3
$\mathbf{x}_{\text{int},c}$	Position vector of the centroid of an interface element	m
$\mathbf{x}_{\text{int},p}$	Position vector of the interface element point corresponding to mesh point p	m
$\mathbf{x}_p$	Position vector of mesh point p	m

Greek Symbols

α	Volume fraction	-
α_c	Sharp volume fraction	-
α_s	Smoothed volume fraction	-

β	Dimensionless flow resistance factor	-
δS	An interfacial element	
δS_f	Surface boundary of a control volume	
δV	A control volume	
Δ	Difference operator	
δ	Delta function	1/m
δ_x	Side length of uniform grid cells	m
ϵ	A very small scalar value	
η	Summation of contact and corner angles	[°]
ε	Thickness of the fluid-fluid interface	m
ϕ_f	Face-centred flux	
$\phi_{F,f}$	Interfacial force flux	
$\tilde{\phi}_f$	Intermediate face-centred flux	
$\tilde{\phi}_{r,f}$	Relative flux at face f	
γ	Corner angle	[°]
Γ_{12}	Fluid-fluid interface between flow regions 1 and 2	
Γ_{23}	Fluid-fluid interface between flow regions 2 and 3	
κ	Interface curvature	1/m
λ	Flow conductance	m ⁴ /(Pa.s)
$[\tilde{\lambda}_{ij}]$	Square matrix of dimensionless flow conductances	
μ	Dynamic viscosity	Pa.s
$\nabla \cdot$	Divergence operator	
∇	Gradient operator	
∇^2	Laplace operator	
$\nabla^\perp$	Normal gradient operator	
ω	Weighting factor	

ρ	Density	kg/m ³
σ	Interfacial tension coefficient	N/m
τ	Shear stress	Pa
θ	Contact angle	[°]
θ_{12}	Contact angle for interface Γ_{12}	[°]
θ_{23}	Contact angle for interface Γ_{23}	[°]
θ_a	Advancing contact angle	[°]
θ_e	Equilibrium contact angle	[°]
θ_r	Receding contact angle	[°]
$[\tilde{\xi}]$	Column vectors of dimensionless pressure gradients	
ξ_i	Pressure gradient in flow region i	Pa/m

Subscripts

Q_1	Q in fluid 1
Q_2	Q in fluid 2
Q_f	Q at surface face f
Q_p	Q at mesh point p
Q_s	Q at the fluid-fluid interface
Q_{cv}	Q at the control-volume centre

Superscripts

Q^h	Numerical approximation of Q
Q^T	Transpose of Q
Q^{-1}	Inverse of tensor Q

Oversymbols

$\dot{Q}$	Flow rate of Q
$\overline{Q}$	Average of Q
$\tilde{Q}$	Dimensionless Q

Other symbols

$\frac{D}{Dt}$ Material derivative

$\langle \rangle_c$ Face to cell average

$\langle \rangle_f$ Cell to face interpolation

$n_{outerLoop}$ Number of outer-corrector loop iterations

n_{PISO} Number of PISO correction iterations

1. Introduction

1.1. Background

Multiphase flow through porous media can occur in a variety of environmental, industrial and engineering processes such as contaminant cleanup (Mercer and Cohen, 1990; Mulligan et al., 2001), fluid separation in fuel cells (He et al., 2000; Srinivasan, 2006), enhanced oil recovery (Lake, 1989), and carbon dioxide storage in geological porous media (Marini, 2006). A considerable body of literature, including experimental, analytical and numerical studies, indicates that accurate quantification and interpretation of the physics of such flows is of great importance to design and control these processes optimally and safely (Blunt, 2017).

The broad term “multiphase flow” can be used to address a large variety of flow patterns and regimes involving flow of two or more phases; in this work, as a specific class of multiphase flow through porous media, we focus on immiscible liquid-liquid two-phase flow at the micro-scale in geological porous media. In this type of flow, the two phases are distinctively separated by liquid-liquid interfaces which can also form solid-liquid-liquid contact lines with the rock surface. The variety of possible topological configurations for the interfaces, different degree of affinity for fluids to cover the rock surface, i.e. different wettabilities, and the inherent complexity of the flow path in natural geological porous media, makes the prediction of the flow behaviour a very challenging task.

The overall efficiency of many engineering processes involving two-phase flow at the mega-scale (on the order of 10^6 m), for example geological storage of carbon dioxide inside deep brine-saturated rock formations, is governed by the pore-scale (on the order of 10^{-6} m) behaviour of the flow (Blunt, 2017). Understanding and analysis of this pore-scale behaviour can provide direct insight into micro-scale processes and link them with phenomenological flow properties such as relative permeability and capillary pressure, which are crucial for field-scale simulations.

Recent advances and developments in non-destructive X-ray computed tomography (micro-CT) has provided a reliable way to obtain high-resolution three-dimensional images of the rock pore space, Figure 1.1, with pore-scale resolution at which individual grains, pores and fluid-fluid interfaces can be resolved (see Ketcham and Carlson (2001) and references therein). The direct output from a micro-CT scanner is normally a grey-scale image that is post processed by performing filtering and segmentation techniques, as illustrated in Figure 1.2, to identify discrete material phases in the image. Quantitative analyses then can be performed on the segmented images to extract different rock and fluid features such as porosity, fluid saturations, fluid distributions, and fluid-fluid interfacial characteristics (Wildenschild and Sheppard, 2013; Blunt et al., 2013).

The availability of high-resolution pore-space images has given new impetus to pore-scale modelling. Pore-scale modelling has proved to be a reliable approach to identify and characterize pore-scale displacement mechanisms and their impact on averaged flow properties, such as relative permeability and capillary pressure, at the next larger scale - from cm to m. Therefore, as a natural extension of pore-scale imaging, there is a need to develop pore-scale numerical

methods that can accurately model the dynamics of flow on the pore-space images. Moreover, these pore-scale modelling tools are highly valuable to simulate and probe phenomena which are impossible or extremely difficult to be obtained by laboratory experiments.

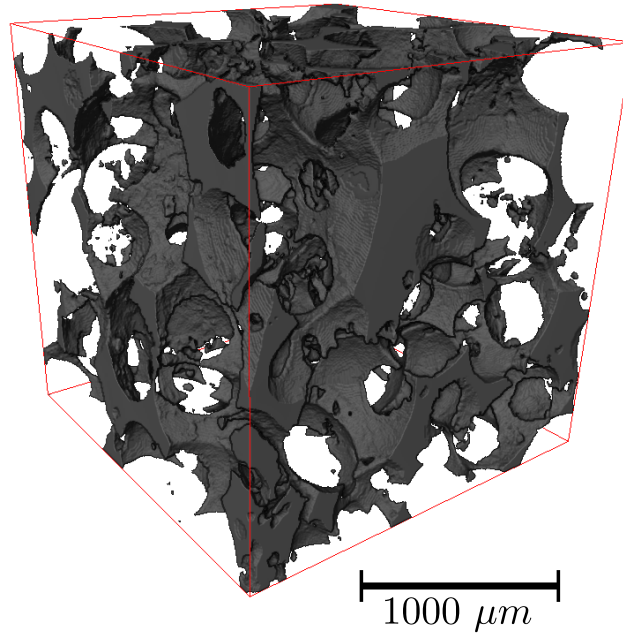


Figure 1.1. Illustration of a micro-CT pore-space image of a Ketton limestone rock sample, 2 mm across with a voxel size of $4\ \mu\text{m}$ (Singh and Blunt, 2018).

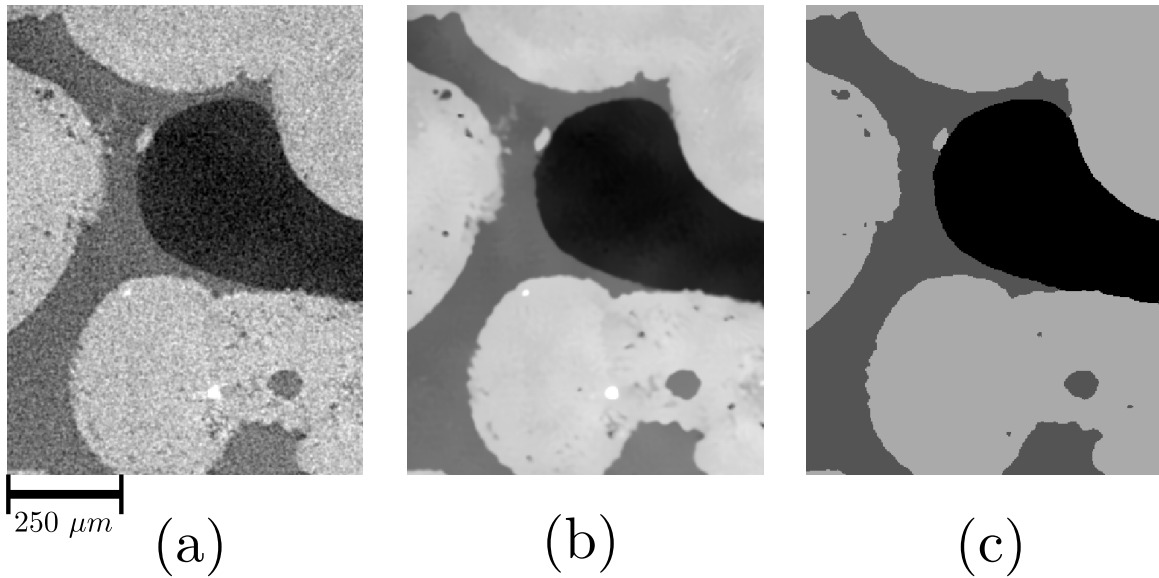


Figure 1.2. Illustration of stages involved in the post processing of micro-CT raw image data: (a) a grey-scale image of a Ketton rock sample, saturated with oil and brine, obtained from the micro-CT scan, (b) the corresponding filtered image, and (c) the corresponding segmented image; the black is oil, the dark grey is brine and the light grey is rock (Singh and Blunt, 2018).

In this study, we focus on developing a numerical scheme to model two-phase flow for porous media applications where capillary effects dominate at the micro-scale. Typical field-scale values for capillary number, which is defined as the ratio of viscous to capillary forces, in porous media applications such as waterflooding can be in the range of 10^{-7} to 10^{-9} (Blunt, 2017). At the pore level, since the pore velocity can be about two orders of magnitude higher than the Darcy velocity, we can safely assume a range of 10^{-5} to 10^{-7} for the micro-scale capillary number (Singh et al., 2017). Then for a viscosity of 10^{-3} Pa.s and an interfacial tension of 10 mN/m, this range of the capillary number is associated with a physical pore velocity in the range of 10^{-4} m/s to 10^{-7} m/s. This implies that direct simulation methods, which solve the Navier-Stokes equations while accounting for interfacial forces, must compute the velocity field with, at least, an accuracy of $O(10^{-5})$ to $O(10^{-8})$.

One of the main difficulties of direct numerical simulation of two-phase flow is the procedure to handle the interfacial force between the two immiscible fluids. The interfacial force model must estimate the pressure jump across the fluid-fluid interface accurately, and its implementation in the Navier-Stokes equations has to be carried out in a well-balanced fashion (Francois et al., 2006; Popinet, 2018). Otherwise, the error may manifest itself as nonphysical velocity currents known as spurious currents, which can be higher than physical velocity field and introduce large errors in two-phase flow simulations (Jamet et al., 2002).

This study addresses this issue by introducing a new numerical solution technique to describe the arrangement and displacement of two Newtonian incompressible immiscible fluid phases at the pore-scale. The numerical scheme efficiently reduces spurious currents, and is able to accurately predict jump conditions across the interface, while the interface is moving through complex geometries such as porous media. The numerical scheme is implemented within a finite-volume volume-of-fluid framework, and validated for immiscible two-phase flow at relatively low capillary numbers, $Ca = 10^{-4}$ to 10^{-5} .

In the rest of this chapter, we first introduce two common computational classes for modelling two-phase flow at the pore-scale. Then, we present an overview of the physical problem and modelling challenges in the computational approach that is extensively used and developed further in this study. Finally, we present an outline of the contents of Chapters 2 to 5.

1.2. Pore-scale modelling

There are two common ways to model two-phase flow at the pore scale: direct modelling and network modelling. In the following sections, we briefly discuss both approaches and present a review of the relevant literature.

1.2.1. Network modelling

In the network modeling approach, pioneered by Fatt (1956), a network of pores connected by throats is extracted from the underlying micro-CT pore-space image. Then, flow equations are

solved, usually semi-analytically, through the network elements (Blunt and King, 1991; Bakke and Øren, 1997; Blunt, 2001; Øren and Bakke, 2003; Raeini et al., 2017, 2018).

A key step in this methodology is extracting physically realistic networks from pore-space images. There are several algorithms employed to partition the pore space into pore- and throat-bodies, and determine their connectivity. These algorithms extract the topological skeleton mainly using one of the following approaches: (a) the medial axis based method (Lindquist et al., 1996), (b) the maximal ball method (Silin and Patzek, 2006), and (c) the grain recognition based method (Thompson et al., 2008). Each of these approaches come with their own advantages and limitations (Dong and Blunt, 2009; Blunt et al., 2013). Even though these approaches may not be able to generate a unique representation of the pore space due to inherent approximations and dependency on image resolution, they should produce representative networks that preserve pore- and throat-size distributions and make reasonable estimates of single- and multi-phase transport properties such as permeability, formation factor and relative permeabilities.

Network modelling has been successfully employed to study transport mechanisms in two- and three-phase flow, non-Newtonian displacement, wetting layer flow, reactive transport and non-Darcy flow. Examples of such studies can be found in Valvatne and Blunt (2004), Piri and Blunt (2005b,a), Lopez et al. (2003), Raoof et al. (2013), and Balhoff and Wheeler (2009). In addition, recently developed dynamic network models (e.g. Tørå et al., 2012), by taking into account the effects of viscous forces, have made it possible to accurately simulate displacements with high flow rates such as surfactant flooding and flow in fractures. The superior computational efficiency of network models has made them probably the most potent method for large pore-space geometries - from mm to cm. They can serve as efficient and accurate tools to investigate pore-scale to continuum-scale coupled flow problems, and analyze the impact of pore-scale heterogeneity on macroscopic flow properties.

The computational efficiency gain, however, comes at the price of simplifying the geometry of the pore space and relying on semi-analytical relations to estimate flux within network elements. These inherent simplifications may have an adverse impact on the outcome of network models and add to the uncertainty of the predicted results. Moreover, network models are not able to implicitly capture pore and sub-pore displacement mechanisms and physical processes, unless all relevant details are identified beforehand and explicitly included in the models. In other words, whether predicted transport properties by a network model are accurate and reliable depends on whether the network model accommodates the pertinent physics.

Direct modelling can overcome these limitations and relax a number of approximations inherent to network modelling. In the following section, we present a brief overview on direct numerical methods.

1.2.2. Direct modelling

In the last few decades, with improvements in computing power and numerical methods, different computational schemes have been developed for direct numerical simulations of multiphase

flows. Popular approaches to simulate multiphase pore-scale processes directly on pore-space images include (a) lattice Boltzmann models (Shan and Chen, 1993; Pan et al., 2004; Ahrenholz et al., 2008), (b) mesh-free Lagrangian particle methods such as smoothed particle hydrodynamics (Monaghan, 1994; Tartakovsky and Meakin, 2006), and (c) grid-based approaches (Tanguy et al., 2007; Ferrari and Lunati, 2013; Raeini et al., 2014). See Meakin and Tartakovsky (2009) for a review of these methods.

Lattice Boltzmann methods

The lattice Boltzmann method solves the Boltzmann transport equation along with an appropriate collision operator to recover the Navier-Stokes equations over a discrete lattice mesh (Chen et al., 1992). Each fluid in the system is represented by a collection of fictitious particles confined to the fixed nodes of the lattice, and the flow of the fluid is modelled through the propagation and collision of these particles. For immiscible two-phase flow, these particles represent fluid elements of two different phases that interact with each other with an equivalent interfacial tension. The algorithm of the lattice Boltzmann method is relatively simple, easy to code and highly parallelizable. Moreover, the method does not require explicit and complicated interface tracking algorithms, and can naturally deal with the interfacial boundary through the particle dynamics. Because of these advantages, the method has been extensively used to compute single and multiphase flow directly on pore-space images, to provide detailed analyses of pore-scale dynamics and to help develop improved theories of porous media flow (Chen and Doolen, 1998; Pan et al., 2004; Ramstad et al., 2010).

In spite of the increasing popularity of the lattice Boltzmann method for studying multiphase flow in complex geometries, and with complex and moving fluid interfaces, this approach has some limitations. Numerical instabilities may arise when this method is used to simulate multiphase flows with large density and viscosity ratios (Meakin and Tartakovsky, 2009). Moreover, multiphase lattice Boltzmann models notoriously introduce unphysical velocities, so-called parasitic or spurious currents, which can severely limit the applicability of these models for multiphase simulations where the capillary number is relatively low (less than 10^{-4}) (Shan, 2006).

Smoothed particle hydrodynamics

Smoothed particle hydrodynamics is a mesh-free Lagrangian particle-based computational method, where the fluid is represented by a set of fixed-mass particles that move with the fluid velocity and carry averaged (smoothed) physical fluid properties such as density (Liu and Liu, 2010). This method and its variants are intrinsically mass-conservative, non-dissipative, simple to implement, robust, easy to parallelize, and able to handle complex boundary conditions through implementing appropriate forces between boundary and fluid particles. The method is readily extended to multiphase flow by the use of an indicator function to characterize different phases in the system. The fluid-fluid interface is represented naturally without the need for explicit

and complicated interface tracking algorithms (Tartakovsky and Meakin, 2005). These features make the method well suited for simulating flows with moving interfacial boundaries in complex geometries. However, this method can be computationally demanding to simulate large three-dimensional systems with a reasonable temporal and spatial resolution, due to the need for a large number of particles and small time steps (Zhu et al., 1999). The applicability of this approach for pore-scale modelling of multiphase flow and reactive transport in porous media has been reviewed by Tartakovsky et al. (2016).

Grid-based methods

Grid-based methods approximate the continuum Navier-Stokes equations using an appropriate discretization technique such as finite difference method, finite volume method, finite element method or a combination of them. The resulting system of algebraic equations then is coupled and solved using a computational algorithm based upon direct or iterative solvers. Grid-based methods, due to their computational efficiency and ability to simulate fluid flow with large density and viscosity ratios, are conventionally considered as the preferred approach for most applications (Meakin and Tartakovsky, 2009). The major challenge in modelling flows with moving interfaces in grid-based methods, however, is the need for an algorithm to model the interface including its location, shape and evolution with time. Therefore, grid-based methods are often used in conjunction with various algorithms to model fluid–fluid interfaces, such as front-tracking (Glimm et al., 1999; Popinet and Zaleski, 1999), level-set (Sussman et al., 1994; Osher and Sethian, 1988), phase-field (Anderson et al., 1998; Alpak et al., 2016), and volume-of-fluid models (Hirt and Nichols, 1981; Raeini et al., 2012).

In this work we develop our direct modelling method based on a grid-based approach. In the following we describe two-phase grid-based methods in more details.

1.3. Grid-based methods: immiscible two-phase flow

In multiphase grid-based methods, the governing equations are derived based on the continuum assumption, where intermolecular forces are neglected, and under the hypothesis of sharp (zero-thickness) fluid–fluid interfaces (Tryggvason et al., 2011). In the following sections, we address the basic concepts of immiscible two-phase flow modelling using grid-based methods.

1.3.1. Basic equations

The governing equations, can be written and solved separately for each fluid in the domain while the solutions are coupled across the fluid–fluid interface using appropriate jump conditions imposed on the interface, which is treated as a moving boundary (Ferziger and Peric, 2012). The equations of motion, the Navier-Stokes equations for isothermal incompressible Newtonian flow, are as follows,

$$\nabla \cdot \mathbf{u} = 0, \tag{1.1}$$

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \mathbf{f} + \mu \nabla^2 \mathbf{u}, \quad (1.2)$$

where, $\frac{D()}{Dt} = \frac{\partial()}{\partial t} + \mathbf{u} \cdot \nabla()$ is the material derivative, ρ is the fluid density, μ is the fluid viscosity, $\mathbf{u}$ is the velocity vector, p is pressure and $\mathbf{f}$ denotes any body force, for example the gravity force, $\rho \mathbf{g}$. This set of equations is solved separately in the bulk of each phase and the solutions are coupled using appropriate boundary conditions, jump conditions, at the interface.

Figure 1.3 depicts a thin control volume δV , enclosing a small interfacial element δS bounded by a closed counter C on a sharp (zero-thickness) fluid-fluid interface S separating two immiscible fluids. The characteristic thickness (length scale) of the control volume is ε and the control volume coincides with δS as ε approaches to zero. Therefore, the jump conditions at the interface can be obtained by applying mass- and momentum-conservation principles on this control volume in the limit of $\varepsilon \rightarrow 0$ (Tryggvason et al., 2011).

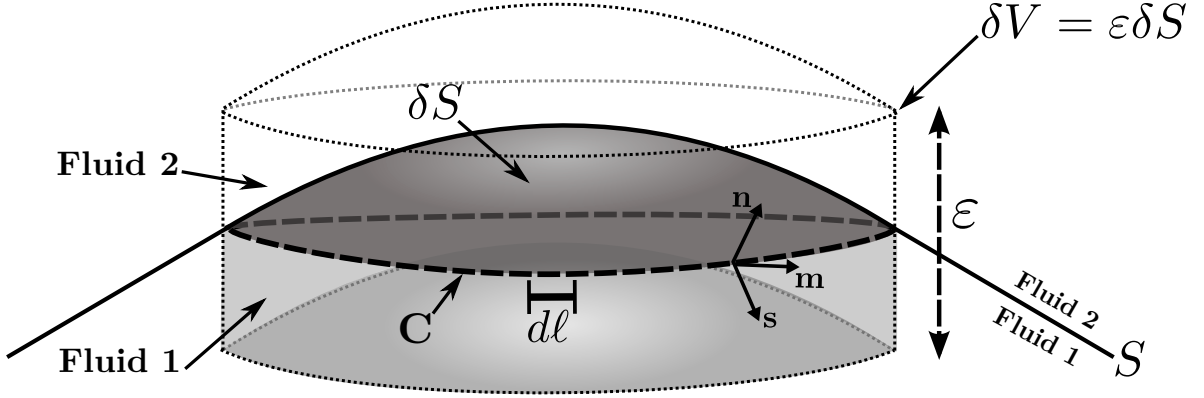


Figure 1.3. A thin control volume, δV , with surface boundary δS_f and characteristic thickness ε . The control volume encloses an infinitesimal small interfacial element δS bounded by a closed contour C , on an interface S between two immiscible fluids. Local vectors $\mathbf{m}$, $\mathbf{s}$ and $\mathbf{n}$ are unit vectors defined on the edge of the interfacial element; $\mathbf{m}$ is tangent to C , $\mathbf{s}$ is perpendicular to C but tangent to δS , and $\mathbf{n} = \mathbf{s} \times \mathbf{m}$ is the unit normal vector perpendicular to the surface element.

The mass conservation equation for the control volume is

$$\frac{d}{dt} \int_{\delta V} \rho dv = - \oint_{\delta S_f} \rho \mathbf{u} \cdot \mathbf{n} ds_f, \quad (1.3)$$

where δS_f is the closed surface boundary of the control volume, and $\mathbf{n}$ is the unit vector normal to δS_f . Since ε is assumed to be zero, δS_f coincides with δS and mass can not accumulate inside the control volume, i.e.

$$\oint_{\delta S_f} \rho \mathbf{u} \cdot \mathbf{n} ds_f = 0. \quad (1.4)$$

This implies that inflow balances outflow, i.e.

$$\int_{\delta S} \rho_1(\mathbf{u}_1 - \mathbf{u}_s) \cdot \mathbf{n} ds = \int_{\delta S} \rho_2(\mathbf{u}_2 - \mathbf{u}_s) \cdot \mathbf{n} ds = \dot{m}, \quad (1.5)$$

By taking the limit $\delta S \rightarrow 0$, we have the following expression that holds at each point on the interface

$$\rho_1(\mathbf{u}_1 - \mathbf{u}_s) \cdot \mathbf{n} = \rho_2(\mathbf{u}_2 - \mathbf{u}_s) \cdot \mathbf{n} = \lim_{\delta S \rightarrow 0} \frac{\dot{m}}{\delta S}, \quad (1.6)$$

where $\mathbf{u}_1$ is the velocity of fluid 1 at the interface, $\mathbf{u}_2$ is the velocity of fluid 2 at the interface, $\mathbf{u}_s$ is the velocity of the interface and $\dot{m}$ is the mass flow rate across the interface. In the absence of phase change at the interface, $\dot{m} = 0$, Equation (1.6) leads to the following kinematic condition,

$$\mathbf{u}_s \cdot \mathbf{n} = \mathbf{u}_2 \cdot \mathbf{n} = \mathbf{u}_1 \cdot \mathbf{n}, \quad (1.7)$$

or

$$\mathbf{u}_2 \cdot \mathbf{n} - \mathbf{u}_1 \cdot \mathbf{n} = 0, \quad (1.8)$$

stating that the interface allows no flow through it, and the fluids at interface have the same velocity equal to the normal velocity of the interface.

At the molecular level, the interface is under tension due to unbalanced intermolecular (adhesion/cohesion) forces near the interface. This interfacial tension, however, does not arise naturally from the continuum description of the interface as a zero-thickness surface element. Alternatively, at the continuum scale, it is modelled as a force per unit length acting on C to pull on the interface in the $\mathbf{s}$ -direction, perpendicular to C and tangent to the interfacial element (Tryggvason et al., 2011). Its magnitude is σ , which is a material property referred to as the interfacial tension coefficient.

The curvature force on the interfacial element δS , $\mathbf{f}_c$, is equal to the line integral of the interfacial tension, $\sigma \mathbf{s}$, over the element perimeter, i.e.

$$\mathbf{f}_c = \int_{\delta S} \mathbf{f}_\sigma ds = \oint_C \sigma \mathbf{s} d\ell, \quad (1.9)$$

where $\mathbf{f}_\sigma$ is interfacial force per unit area, and $d\ell$ is the length of an increment along the perimeter of the contour line, and $\mathbf{s}$ is unit vector which is perpendicular to C but tangent to δS . For constant interfacial tension coefficient, based on Equation (1.9), one can write (Tryggvason et al., 2011)

$$\mathbf{f}_\sigma = \sigma \lim_{\delta S \rightarrow 0} \frac{1}{\delta S} \oint_C \mathbf{s} d\ell. \quad (1.10)$$

It can be shown that

$$\kappa \mathbf{n} = \lim_{\delta S \rightarrow 0} \frac{1}{\delta S} \oint_C \mathbf{s} d\ell, \quad (1.11)$$

where

$$\kappa = -\nabla \cdot \mathbf{n}, \quad (1.12)$$

is the curvature of the interface.

Then the interfacial force per unit area, $\mathbf{f}_\sigma$, can be written as

$$\mathbf{f}_\sigma = \sigma \kappa \mathbf{n}. \quad (1.13)$$

The momentum conservation equation for the control volume reads

$$\int_{\delta V} \rho \frac{D\mathbf{u}}{Dt} dv = \int_{\delta V} \mathbf{f} dv + \oint_{\delta S_f} \mathbb{T} \cdot \mathbf{n} ds_f + \int_{\delta S} \mathbf{f}_\sigma ds, \quad (1.14)$$

where

$$\mathbb{T} = -p\mathbb{I} + \mu[\nabla \mathbf{u} + (\nabla \mathbf{u})^T]. \quad (1.15)$$

Here $\mathbf{f}$ is any body force acting on the control volume, $\mathbb{T}$ is the stress tensor acting on the surface boundary of the control volume, p is local pressure and $\mathbb{I}$ is the identity tensor. Since ε is taken to be zero, Equation (1.14) is reduced to

$$\int_{\delta S} (\mathbb{T}_2 - \mathbb{T}_1) \cdot \mathbf{n} ds + \int_{\delta S} \mathbf{f}_\sigma ds = 0. \quad (1.16)$$

Therefore at any interface point, we have

$$\mathbb{T}_1 \cdot \mathbf{n} - \mathbb{T}_2 \cdot \mathbf{n} = \mathbf{f}_\sigma. \quad (1.17)$$

Substituting Equation (1.13) into Equation (1.17) yields the stress balance equation at the interface

$$\mathbb{T}_1 \cdot \mathbf{n} - \mathbb{T}_2 \cdot \mathbf{n} = \sigma \kappa \mathbf{n}. \quad (1.18)$$

Finally, this dynamic condition can be written in terms of normal and tangential stress balances (Tryggvason et al., 2011)

$$\begin{aligned} \mathbf{n} \cdot \mathbb{T}_1 \cdot \mathbf{n} - \mathbf{n} \cdot \mathbb{T}_2 \cdot \mathbf{n} &= \sigma \kappa, \\ \mathbf{s} \cdot \mathbb{T}_1 \cdot \mathbf{n} - \mathbf{s} \cdot \mathbb{T}_2 \cdot \mathbf{n} &= 0, \\ \mathbf{m} \cdot \mathbb{T}_1 \cdot \mathbf{n} - \mathbf{m} \cdot \mathbb{T}_2 \cdot \mathbf{n} &= 0. \end{aligned} \quad (1.19)$$

These imply that, for a constant σ , the jump in the normal stress across the interface is balanced by the curvature force, while the jump in the tangential stress is zero.

The equations of motion for each bulk phase, Equations (1.1) and (1.2), together with the kinematic and dynamic jump conditions at the interface, Equations (1.8) and (1.19), and other flow boundary conditions, form a complete set to model isothermal immiscible two-phase flow of incompressible Newtonian fluids with a constant interfacial tension coefficient, σ .

In another approach, often referred to as “single-fluid” or “one-fluid” formulation, the whole system is treated as one single continuum. Therefore one set of governing equations is written and solved for the whole domain while the interface is modelled implicitly as a discontinuity

in the fluid properties (Tryggvason et al., 2011). In the single-fluid approach, extra singular terms must be added to the equations to take into account the curvature forces at the interface. This can be done by adding a body force representing the interfacial force to the momentum equation and concentrating it on the interface using a delta-function.

Following the single-fluid approach, the Navier-Stokes equations for an isothermal, incompressible two-phase flow of Newtonian fluids are written for the whole flow field as (Tryggvason et al., 2011)

$$\nabla \cdot \mathbf{u} = 0, \quad (1.20)$$

$$\frac{D}{Dt}(\rho \mathbf{u}) = -\nabla p + \mathbf{f} + \nabla \cdot (\mu[\nabla \mathbf{u} + (\nabla \mathbf{u})^T]) + \mathbf{f}_{\sigma v}, \quad (1.21)$$

where ρ and μ are the local density and viscosity, respectively, which may change abruptly at the interface. Here $\mathbf{f}_{\sigma v}$ is a body force representing interfacial force effects,

$$\mathbf{f}_{\sigma v} = \mathbf{f}_{\sigma} \delta_s, \quad (1.22)$$

where δ_s is a delta function concentrated on the interface, i.e. is non-zero only at the interface points. For constant interfacial tension, using Equation (1.13), we can write

$$\mathbf{f}_{\sigma v} = \sigma \kappa \mathbf{n} \delta_s. \quad (1.23)$$

One major challenge in modelling flows with moving interfaces in grid-based methods, however, is the need for an algorithm to model the interface including its location, shape and evolution with time. Moreover, in the single-fluid approach, an accurate and robust representation of the interfacial force as a volume force, which is incorporated into the momentum equation, can be a challenging task. Another modelling challenge is the difficulty of dealing with contact line statics and dynamics where the interface meets a solid boundary. A brief overview of these challenges is given in the following sections.

1.3.2. Interface representation

Different numerical techniques have been developed to find the interface shape while moving through the flow domain. They can be broadly classified into three main groups: (a) interface-tracking, (b) interface-capturing, and (c) hybrid methods.

In interface-tracking methods the interface is modelled as a sharp boundary between the two fluids and its motion is explicitly tracked through the domain. This can be accomplished using (a) moving mesh (Ryskin and Leal, 1984; Fyfe et al., 1988) or (b) front-tracking techniques (Glimm et al., 1986, 1999). In the moving mesh methods each phase is meshed using separate boundary-fitted grids, and the interface is described as the boundary between the grids, see Figure 1.4b. Since the interface location changes with time, the boundary, interface-fitted mesh points, must move with the same flow velocity, dictated by the kinematic boundary condition,

Equation (1.7), to accommodate the changing interface. The remaining points, namely the non-interface points, can move with the flow velocity, i.e. a purely Lagrangian method, or with arbitrary velocities that lead to Lagrangian-Eulerian methods.

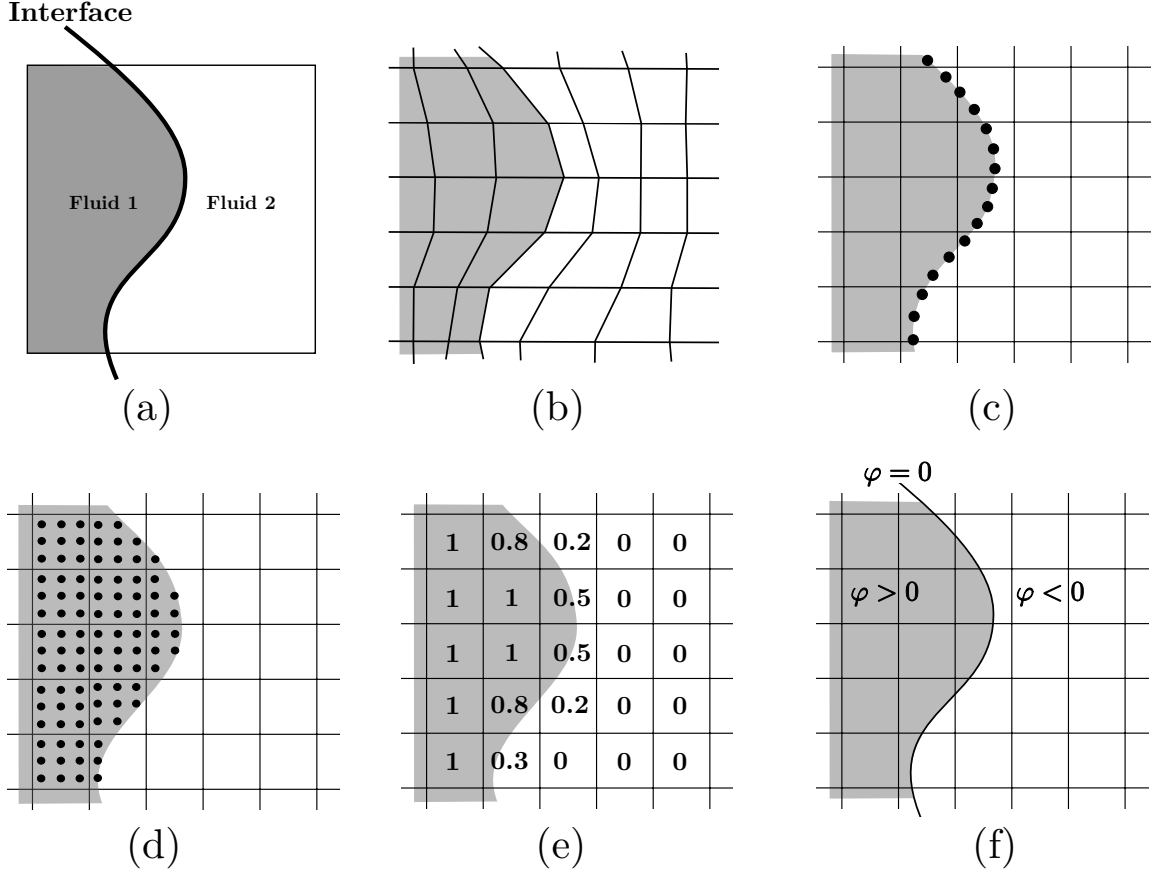


Figure 1.4. A schematic representation of a portion of a fluid-fluid interface and related methods used to model its shape and motion. (a) Interface between two fluids. Interface-tracking methods such as (b) the interface-fitted moving mesh method, and (c) the front-tracking method. Interface-capturing methods such as (d) the marker-and-cell method, (e) the volume-of-fluid method, and (f) the level-set method.

Mesh moving methods have the main advantage of making the interface a sharp discontinuity, which can lead to an accurate representation of jump conditions at the interface (Ferziger and Peric, 2012). However, explicit tracking of the interfaces that undergo large deformations may lead to strong mesh distortions. This can be handled to some extent through re-meshing that adds to the complexity of the computational algorithm as well as numerical errors due to transferring the solution from the old mesh to the new (re-meshed) one.

On the other hand, the front-tracking methods offer a more flexible way to track the interface by computing the flow on a stationary grid while the dynamic evolution of the interface (front) is explicitly tracked using Lagrangian-based approaches. The interface can be represented as connected mass-less particles, see Figure 1.4c, and advected by following the motion of these particles while the stationary background grid is only adjusted near the interface to coincide

with the interface; see Glimm et al. (1986). Front-tracking methods, similar to the mesh-moving methods, offer a sharp resolution of the interface. However, the accuracy and robustness of these approaches can be highly dependent on the adaptive grid strategy employed to align the computational grid to the interface (Glimm et al., 1986). Implementing a mesh alignment strategy which provides a robust and effective way to handle interfaces with complex motions as well as interface topological changes, can be a challenging task. Moreover, housekeeping operations on the interface, namely deleting, inserting and re-ordering the interface particles, to preserve the resolution of the interface, can add to the complexity and the computational cost of the method.

In general, despite offering highly accurate solutions to resolve the position of the interface, the interface-tracking methods are limited to relatively simple problems where the interface does not experience severe deformations. These methods are not able to automatically resolve topology changes in the interface, for example when liquid films rupture or coalesce. Therefore, additional operations are required to explicitly handle the topological changes. Another difficulty with the interface-tracking methods is that special care is required to enforce strict mass conservation as the mesh movement may violate volume (geometric) conservation resulting in mass-balance errors.

Interface-capturing methods represent the interface implicitly on a regular fixed grid by marking the fluids on both sides of the interface, using either virtual particles (marker-and-cell methods), or an indicator function such as a volume fraction (volume-of-fluid methods), a signed distance function (level-set methods) or an order parameter (phase-field methods), see Figure 1.4d-f. One key advantage of these methods as opposed to interface-tracking is that they do not require complicated interface tracking algorithms. This is important for modelling two-phase flows through complex geometries such as three-dimensional micro-CT images of porous media in which we usually have large interface motions and interactions.

In the marker-and-cell method, mass-less particles are used to mark the fluids while advected with the flow velocity (Harlow and Welch, 1965; McKee et al., 2008). The marker-and-cell method provides a robust representation of complex interface motions and preserves strict mass conservation. The main difficulty with this method, however, is the high cost of using particles, their computation and storage, in simulating relatively large systems (Meakin and Tartakovsky, 2009).

The volume-of-fluid method captures the interface using an indicator function that physically represents volume fractions of one of the two fluids. The indicator function often has a value of one in one fluid and zero in the other fluid. The volume-of-fluid method, is intrinsically mass conservative and highly flexible for treating complex interface configurations. This method, due to the fact that only one indicator function is required to be advected through the computational domain, is more computationally efficient compared to the marker-and-cell method. However, in the volume-of-fluid method, an accurate representation of the interface as a sharp boundary between the fluids can be quite challenging because of the numerical diffusion of the indicator

function, which tends to smear the interface sharpness through time (Meakin and Tartakovsky, 2009).

The level-set method uses a level-set function, often in the form of a signed distance function, to represent the interface as a sharp boundary between fluids. It captures the interface more accurately compared to the volume-of-fluid method. However, the main disadvantage of this method is that it is not inherently mass-conservative and additional effort is required to enforce strict mass conservation (Osher and Fedkiw, 2001).

Phase-field models flexibly capture complex interface motions and related physical phenomena by describing the interface as a thin transition region based on thermodynamic arguments. However, resolving the diffusive interface while convecting it in a mass-conservative fashion can be numerically challenging and computationally expensive (Liu and Yu, 2016).

In interface-capturing methods, the advantage of flexibility is offset by the disadvantage of having the interface smeared. To make use of the respective advantages of interface-tracking and interface-capturing methods, hybrid methods offer computational algorithms to use a combination of both methods (Unverdi and Tryggvason, 1992; Tryggvason et al., 2001). In these methods the interface is explicitly tracked, as in the front-tracking methods, on a fixed computational mesh where the fluid properties are smeared close to the interface, as in interface-capturing methods. Exchange of data between the interface and the fixed grid, mainly velocity information from grid to interface and curvature information from interface to grid, is necessary to satisfy the kinematic and dynamic constraints. However, as for the front-tracking methods, an accurate representation of the interface comes at the cost of additional computational effort to preserve the resolution of the interface while it evolves (Tryggvason et al., 2001). In addition, a well-balanced and conservative estimation of the interfacial force term, see Equation (1.21), based on the interface normal and curvature data from the front, requires special interpolation and discretization techniques near the interface (Popinet and Zaleski, 1999).

1.3.3. Interfacial force representation

Different methods have been employed to compute interfacial forces using implicit data from the interface-capturing methods on a fixed grid such as the volume-of-fluid method. Continuum models such as the continuous surface force (CSF) method (Brackbill et al., 1992) and the continuous surface stress (CSS) method (Gueyffier et al., 1999) are among the most widely used techniques that treat the singular interfacial force as a body force and concentrate it in the region of the interface using a delta function, Equation (1.23). A recent review of the accuracy and robustness of numerical models of interfacial force implemented within different frameworks such as volume-of-fluid, level-set, height function and mixed methods, is given by Popinet (2018). A brief discussion of the CSF method within the volume-of-fluid approach and the related challenges are given next.

Figure 1.5 illustrates two fluids marked by the colour or indicator function c , which has a value of one in the first fluid (fluid 1) and zero in the second fluid (fluid 2), as in the volume-of-

fluid method. As shown in Figure 1.5b, the indicator function changes abruptly at the interface and its one-dimensional profile as a function of the normal interface distance, n , is the Heaviside step function.

In the CSF method, the sharp indicator function, c , is replaced with a smoothed one, $\tilde{c}$, replacing the discontinuous interface with a continuous transition zone, which covers a band of width $\varepsilon/2$ around the interface, Figure 1.5c-d. The smoothed indicator function, $\tilde{c}$, is chosen in a way that

$$\lim_{\varepsilon \rightarrow 0} \tilde{c} = c. \quad (1.24)$$

Thus, the CSF method models the interfacial force as a body force applied in the transition zone where $0 < \tilde{c} < 1$.

The Equation (1.23) is approximated to obtain the body force as

$$\mathbf{f}_{\sigma v} = \sigma \kappa \mathbf{n} \delta_s \approx \sigma \kappa |\nabla \tilde{c}|, \quad (1.25)$$

where

$$\kappa = -\nabla \cdot \mathbf{n}, \quad (1.26)$$

and

$$\mathbf{n} = -\frac{\nabla \tilde{c}}{|\nabla \tilde{c}|}. \quad (1.27)$$

Here κ is the interface curvature and $\mathbf{n}$ is the interface unit normal vector which points from fluid 1 to fluid 2. Equation (1.25) is numerically approximated for those grid cells that fall into the transition zone, interface cells, and is zero for the rest, the cells filled with only one fluid (Brackbill et al., 1992).

The CSS method offers a momentum conservative approach to estimate the interfacial force as the divergence of a stress tensor, $\mathbb{T}_s = \sigma(\mathbb{I} - \mathbf{n}\mathbf{n})$ (Tryggvason et al., 2011)

$$\mathbf{f}_{\sigma v} = \nabla \cdot (\mathbb{T}_s \delta_s) \approx \nabla \cdot (\mathbb{T}_s |\nabla \tilde{c}|). \quad (1.28)$$

where $\mathbf{n}$ is obtained from Equation (1.27).

The main problem with these models, however, is that they suffer from spurious currents near the interface especially when it comes to simulating flows in which the capillary force is dominant over viscous and gravity effects (Lafaurie et al., 1994; Jamet et al., 2002). Another fundamental drawback is that, due to the lack of a sharp boundary between different fluids, these methods may not be able to ensure a zero net capillary force on closed interfaces (Tryggvason et al., 2001). The adverse effects of failing to impose this force conservation property have been reported in modelling of free rising bubbles in quiescent liquids and moving droplets in uniform velocity fields (Rusche, 2002; Raeini et al., 2012).

These issues have been addressed in many studies. Tryggvason et al. (2001) employed a front-tracking method to reconstruct a sharp interface from volume fractions to compute a more accurate interfacial force on fixed grids. Scardovelli and Zaleski (1999) used an interface

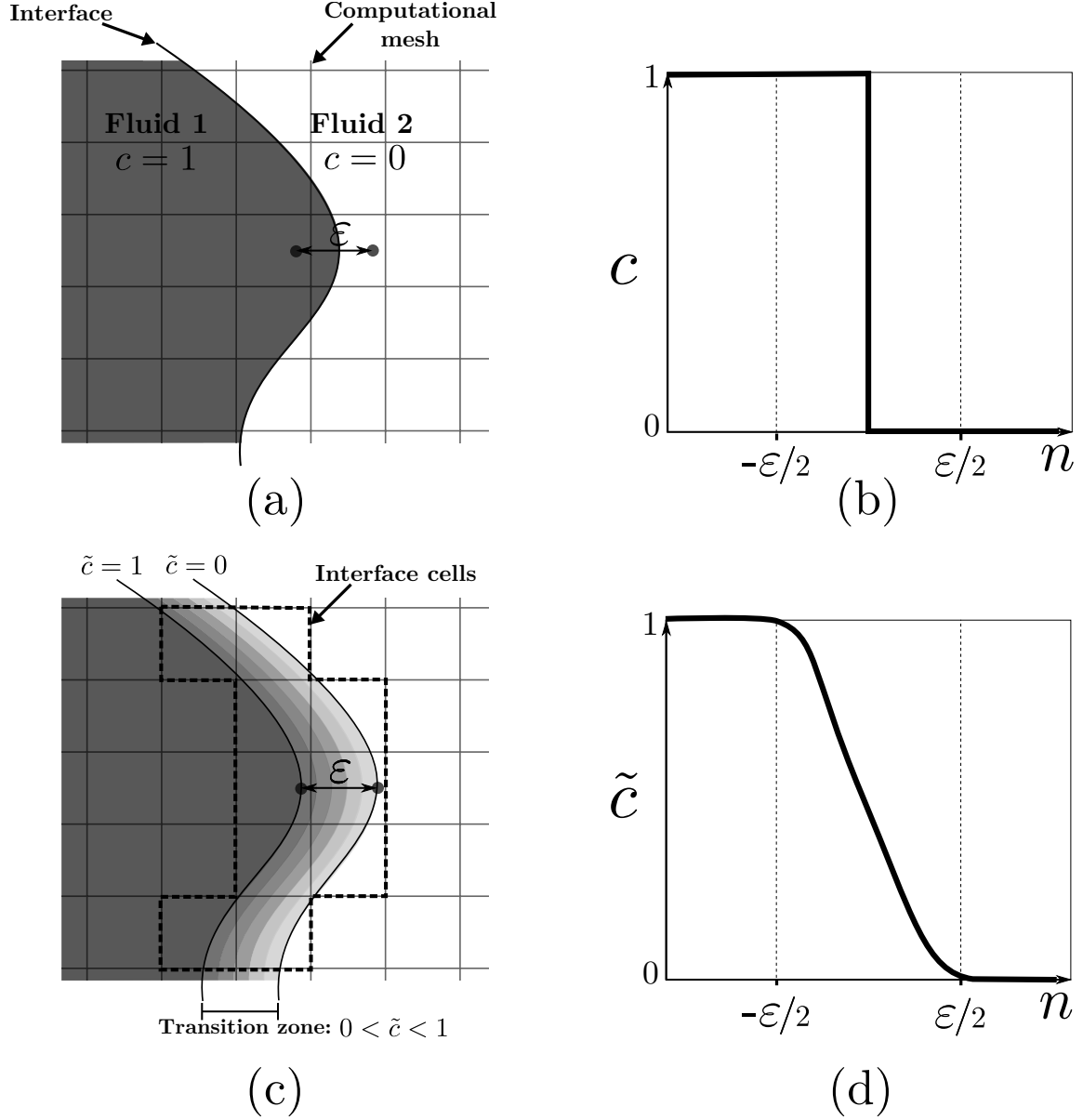


Figure 1.5. Schematic of: (a) the sharp representation of an interface between two fluids using a discontinuous indicator function, c , and (b) the one-dimensional profile of the function c as a function of the local normal distance from the interface; (c) continuous representation of the interface using a continuous smoothed indicator function, $\tilde{c}$, and (d) the one-dimensional profile of the smoothed function $\tilde{c}$ as a function of the local normal distance from the interface.

tracking algorithm based on the piecewise linear interface construction method (PLIC) and a Lagrangian advection scheme to balance interfacial forces more accurately and reduce spurious currents to machine accuracy for two-dimensional calculations. Renardy and Renardy (2002) developed a parabolic reconstruction of surface tension (PROST) algorithm for three-dimensional cases to model the volume force due to interfacial tension, which effectively reduced spurious currents in comparison to CSF and CSS. Jamet et al. (2002) implemented an energy conserving

discretization scheme, similar to the phase-field implementation of Jacqmin (1999), to achieve a physical equilibrium state without spurious currents. He argued that conserving energy to round-off errors makes it possible to model fluid interfaces accurately, eliminating non-physical currents to machine accuracy, even if momentum is not strictly conserved.

Raeini et al. (2012) introduced a filtered surface force (FSF) model to remove spurious currents from numerical simulations at the micro-scale, where the capillary forces are dominant. They successfully applied the method to simulate two-phase flow on micro-CT pore-space images claiming that the method is able to efficiently eliminate the non-physical behaviour from the numerical results (Raeini et al., 2014, 2015). However, there are two major issues with the model: (a) the method is strongly dependent on various numerical filtering parameters. One needs to find an appropriate set of filtering parameters for each numerical test case using a trial-and-error approach, which is quite cumbersome; and (b) the filtering techniques themselves may introduce non-physical behaviour that can adversely affect pore-scale phenomena such as capillary trapping. In this study, we borrow the idea of sharpening the indicator function from their work (Raeini et al., 2012) to develop a new interface reconstruction based surface force model. We show that the new surface force model, so-called contour level surface force (CLSF) model, can efficiently reduce spurious currents without requiring the need of applying numerical filtering techniques; see Chapter 3.

1.3.4. Contact line statics and dynamics

Another challenge in modelling two-phase flow in the presence of a solid phase is the need to introduce appropriate contact angle boundary conditions to describe the physics of the contact line, where the fluid-fluid interface meets the solid boundary. The static force balance at a contact point is controlled by wettability effects, which is often quantified by a contact angle. The contact angle is a key parameter that can have a significant impact on the arrangement of fluids as well as contact line dynamics in two-phase flow through porous media.

The equilibrium (static) contact angle, θ_e , resulting from the force balance of interfacial tensions at the contact line on a perfectly flat surface in thermodynamic equilibrium, can be determined using the Young equation (Young, 1805), Figure 1.6a,

$$\sigma_{s1} = \sigma_{s2} + \sigma_{12} \cos \theta_e, \quad (1.29)$$

where σ_{s1} , σ_{s2} and σ_{12} are, respectively, the solid-fluid1, the solid-fluid2 and the fluid1-fluid2 interfacial tensions.

The Young equation assumes that the surface is perfectly smooth and chemically homogenous. However, most natural surfaces, for example porous rocks, do not meet the requirements of the Young equation and the contact angle on these surfaces may be affected by surface roughness and heterogeneity. Consequently, the surface wetting behaviour can not be quantified using a single contact angle, and hysteresis in contact angle, θ , is expected. On a non-ideal solid

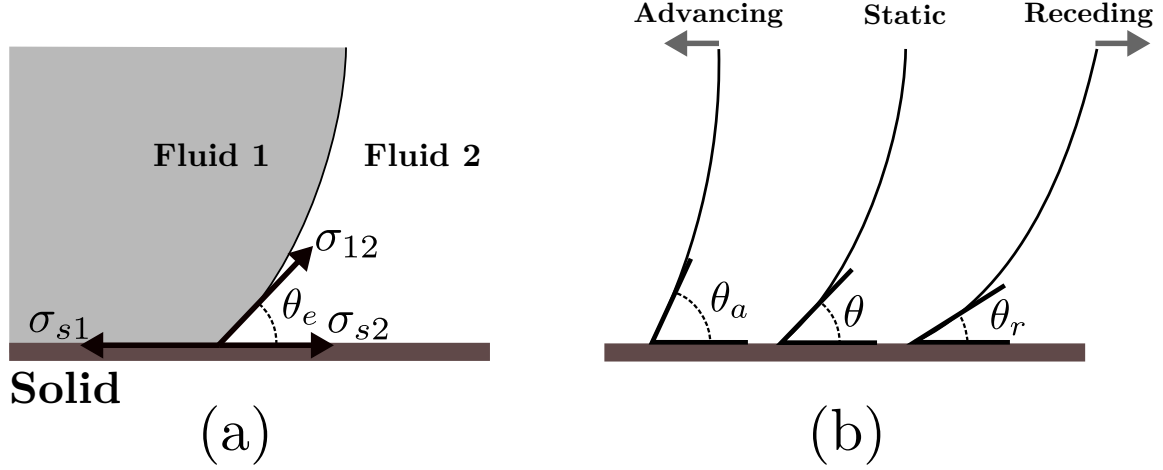


Figure 1.6. Schematic representations of (a) a static liquid-liquid interface on a solid surface with the equilibrium contact angle θ_e and (b) contact angle hysteresis during the wetting phase (fluid 2) advance and recession. The receding contact angle, θ_r , and the advancing contact angle, θ_a are, respectively, the threshold minimal and maximal contact angles at which the contact line starts to move.

surface, due to pinning and immobility of the contact line, the interface can be in a metastable state with a static contact angle, θ , which falls into an interval around θ_e (Gao and McCarthy, 2006),

$$\theta_r \leq \theta \leq \theta_a. \quad (1.30)$$

Here θ_a is the threshold maximal contact angle, the advancing contact angle, at which the contact line begins to move during wetting phase advance (imbibition), and θ_r is the threshold minimal contact angle, the receding contact angle, at which the contact line begins to move during wetting phase recession (drainage), Figure 1.6b. The interval $\theta_a - \theta_r$ is called the contact angle hysteresis and can be affected by different contributing factors such as surface roughness, chemical contamination (heterogeneity), and the presence of liquid solutes, for example surfactants and polymers. Even though contact angle hysteresis has been the subject of significant literature, it is still difficult to establish quantitative correlations between factors affecting wetting behaviour and contact angle on solid surfaces; see Dussan (1979) and Eral et al. (2013) for reviews on the subject.

Accurate modelling and implementation of the contact angle boundary condition in grid-based methods is of great importance to capture wetting effects while simulating two-phase flow with moving contact lines through porous media. However, developing a numerical technique for modelling flows with moving contact lines that accounts for the effects of (a) inertia, namely a relation to describe the dependency between contact line speed and contact angle, (b) contact angle hysteresis, and (c) contact line slip along the solid boundary, can be a challenging task. The main reason for this is the widely different length- and time-scales involved in moving contact line phenomena.

Renardy et al. (2001) implemented two formulations to model two-dimensional contact line phenomena in a piecewise linear interface construction based on the volume-of-fluid method by (a) extrapolating the indicator function beyond the solid surface in a way that its gradient at the contact line was in accordance with the prescribed contact angle, and (b) treating the contact line as a three-phase region and balancing interfacial forces similar to Young equation. They suggested that the extrapolation method leads to better results compared to a Young-like formulation, which introduces relatively high spurious currents at the contact line. However, in their approach, a fixed-dynamic contact angle, i.e. independent of the contact line speed, is assumed while the contact line stress singularity is handled implicitly by spatial discretization errors, which introduce an effective slip proportional to grid spacing.

Afkhami and Bussmann (2008) employed height functions within a volume-of-fluid framework to estimate curvature and consequently interfacial forces at the contact line more accurately, compared to the work of Renardy et al. (2001), and applied the contact angle as a boundary condition at the contact line in the same fashion as in the work of Renardy et al. (2001). Afkhami and Bussmann (2009) extended their previous work, which was limited to two-dimensional volume-of-fluid simulations, to model three-dimensional contact line phenomena and studied various examples of static and dynamic contact line problems. Afkhami et al. (2009) performed a mesh sensitivity analysis to investigate the convergence behaviour of two different boundary conditions at the solid surface within a volume-of-fluid framework: (a) the no-slip boundary condition with implicit effective slip introduced by the spatial discretization, and (b) the Navier-slip boundary conditions with an explicit slip length applied to remove the singularity of the contact line. They demonstrated that both boundary conditions lead to mesh-dependent solutions of moving contact line phenomena, and the results of simulations do not converge when the no-slip boundary condition is applied. Therefore, based on an analogy with the Cox theory (Cox, 1986), they developed a new numerical contact angle model to compute the contact angle boundary condition at the contact line (numerical contact angle) as a function of a prescribed contact angle (apparent contact angle), capillary number and mesh size. They suggested that the new contact angle boundary condition yields mesh-independent solutions for moving contact lines at the solid surface with a no-slip boundary condition. Afkhami et al. (2017) introduced a specific boundary condition at the contact line that employs a scaling factor to handle the moving contact line singularity in dynamic simulations, which can lead to grid-independent simulations.

A review of different numerical models for the simulation of moving contact lines within the framework of the volume-of-fluid method can be found in Legendre and Maglio (2015). They investigated the accuracy of different contact angle models, namely static and dynamic contact angles, and different boundary conditions, namely no-slip and slip boundary conditions, in predicting experimental results for a spreading drop.

Spelt (2005) proposed a level-set based computational scheme that takes into account the effects of inertia and contact angle hysteresis as well as slip boundary conditions in the flow

simulations with moving contact lines.

Jacqmin (2000) investigated the applicability of a free energy based diffusive interface model, in which the contact line is equilibrated through chemical potential gradients, to describe the dynamics of moving contact lines. He showed that the diffusive model can naturally resolve the stress singularity of the contact line on a solid surface with no-slip boundary conditions, without any need to introduce an effective slip along the surface.

1.4. Thesis outline

The structure of this thesis is as follows: Chapter 2 describes the governing mathematical equations as well as the numerical implementation of these equations, the interface reconstruction algorithm and the proposed interfacial force model in detail. Chapter 3 is dedicated to verification studies to ensure the correctness of the proposed numerical approach. Chapter 4 presents an investigation of viscous coupling effects in two-phase flow through non-circular capillary tubes with uniform and non-uniform wettability conditions. In this chapter, we put forward simple hydraulic conductance relations that can be incorporated into pore-network models, which are more computational efficient compared to direct numerical simulation approaches, to study the effects of viscous coupling on macroscopic flow properties in relatively large pore-space images. Finally, Chapter 5 gives a summary of conclusions, a discussion of contributions, and potential areas for future work.

2. Mathematical and numerical modelling

In this chapter, we describe the numerical scheme to model two-phase flow in porous media at the micro-scale where capillary forces dominate over viscous effects. The volume-of-fluid method is employed to capture the fluid-fluid interface whose dynamics is explicitly described based on a finite volume discretization of the Navier–Stokes equations. Interfacial forces are calculated directly on reconstructed interface elements such that the total curvature is preserved. The computed interfacial forces are explicitly added to the Navier–Stokes equations using a sharp formulation which effectively eliminates spurious currents.

In Section 2.1, we present the governing mathematical equations. In Section 2.2, we present the numerical implementation of the governing transport equations, the interface reconstruction algorithm and the interfacial force model in detail.

2.1. Mathematical model

The equations of motion for an isothermal, incompressible two-phase flow of Newtonian fluids, are written using the single-fluid continuum approach, as discussed in Section 1.3,

$$\nabla \cdot \mathbf{u} = 0, \quad (2.1)$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \rho \mathbf{g} + \nabla \cdot \mathbb{T} + \mathbf{f}_{\sigma v}, \quad (2.2)$$

where $\mathbf{u}$ is the velocity vector, p is pressure, $\mathbf{g}$ is the gravitational acceleration, $\mathbf{f}_{\sigma v}$ is the interfacial force concentrated on the interface, $\mathbb{T} = \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ is the viscous stress tensor, and ρ and μ are the fluid density and viscosity, respectively, defined as

$$\begin{aligned} \rho &= \alpha \rho_1 + (1 - \alpha) \rho_2, \\ \mu &= \alpha \mu_1 + (1 - \alpha) \mu_2. \end{aligned} \quad (2.3)$$

Here α is an indicator function (physically representing the volume fraction of one phase) that has a value of one in the first fluid (subscript 1) and zero in the second fluid (subscript 2). In the volume-of fluid method, α represents volume fractions of one of the two fluids and varies smoothly between 0 and 1. The interface can be defined as the surface where the value of α is equal to 0.5.

The indicator function is evolved using the following advection equation:

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{u}) = 0. \quad (2.4)$$

The interfacial force per unit area, $\mathbf{f}_\sigma$, at any point on the interface, assuming the interfacial tension, σ , is constant, can be obtained as (Tryggvason et al., 2011)

$$\mathbf{f}_\sigma = \sigma \kappa \mathbf{n}, \quad (2.5)$$

where

$$\kappa \mathbf{n} = \lim_{dS \rightarrow 0} \frac{1}{dS} \oint_C \mathbf{m} d\ell, \quad (2.6)$$

for an infinitesimal volume element dV enclosing an interface dS bounded by a closed contour C (Figure 2.1). Here κ is the local interface curvature, $\mathbf{n}$ is the local unit vector normal to the interface, $d\ell$ is the length of an increment along the perimeter of the contour line, C , and the vector $\mathbf{m} = \mathbf{t} \times \mathbf{n}$ lies on the interface and is perpendicular to both the normal vector, $\mathbf{n}$, and the unit vector $\mathbf{t}$ tangent to the interface along C .

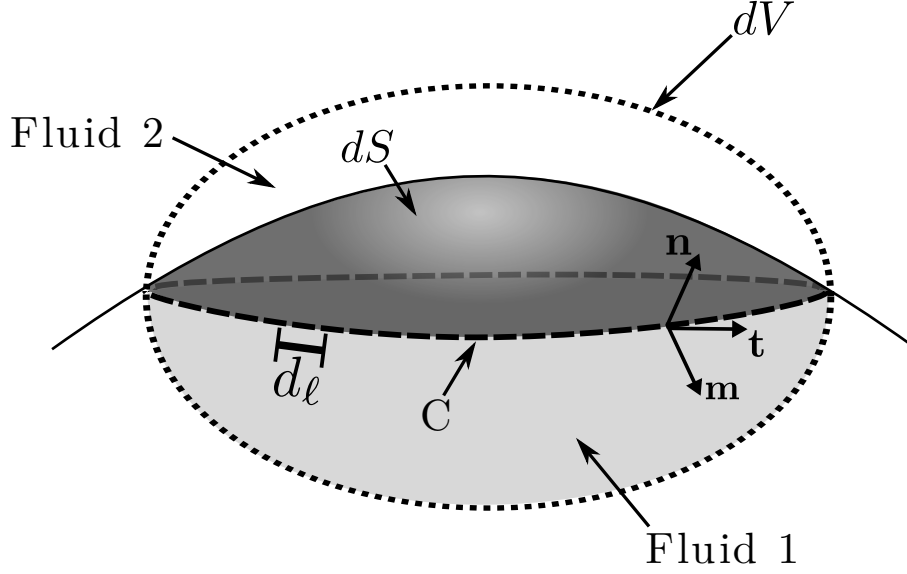


Figure 2.1. A schematic of an infinitesimal control-volume, dV , containing two immiscible fluids separated by an interface, dS , and bounding contour C .

Finally, the interfacial force per unit volume, $\mathbf{f}_{\sigma v}$, can be computed as

$$\mathbf{f}_{\sigma v} = \mathbf{f}_{\sigma} \delta_s \quad (2.7)$$

where δ_s is a delta function concentrated on the interface, i.e. is non-zero only at the interface points.

In the single-fluid approach, the fluid–fluid interface is treated as a discontinuity in fluid properties rather than an explicit boundary. Therefore we do not need to prescribe kinematic and dynamic boundary conditions explicitly at the fluid–fluid interface (Ferziger and Peric, 2012). In our study, apart from bulk phase viscosity, μ , Equation (2.3), we do not consider any additional hydrodynamic resistance to flow at the fluid–fluid interface, i.e. zero interfacial shear viscosity (Gupta and Wasan, 1974).

In contact line regions, where the fluid–fluid interface joins a solid boundary, wetting effects must be taken into account. This is achieved by modifying unit vectors normal to the interface at the solid boundary in accordance with a prescribed contact angle, θ . The contact angle is an input parameter and, in our numerical tests, it is set equal to the equilibrium contact angle.

2.2. Numerical method

The finite volume method, with a collocated arrangement of variables at centres of discrete non-overlapping control-volumes (Jasak, 1996; Weller et al., 1998), is used to numerically solve the governing equations of flow. The flow algorithm in conjunction with a volume-of-fluid based interface tracking method, is taken from the interFoam solver of OpenFOAM (OpenFOAM, 2016). In this section, first the finite-volume discretization procedure is briefly described; more details can be found in Jasak (1996) and Rusche (2002). Then, the algorithm employed in interFoam to solve and couple the discretized transport equations is described; see Deshpande et al. (2012) and references therein for more details. Next, we present a new numerical algorithm to reconstruct the location of the interface. Finally, the computation of the interfacial force on the reconstructed interface and its transfer to the underlying fixed mesh are discussed.

2.2.1. Finite-volume discretization of the transport equations

The finite volume method is based on evaluating the volume integral of the transport equations over discrete control-volumes (cells), which surround computational node points on a mesh. By taking the volume integral over the total volume V_i of a fixed control-volume i , the governing equations, Equations (2.1), (2.2) and (2.4), become

$$\int_{V_i} \nabla \cdot \mathbf{u} \, dV_i = 0, \quad (2.8)$$

$$\frac{\partial}{\partial t} \int_{V_i} \rho \mathbf{u} \, dV_i + \int_{V_i} \nabla \cdot (\rho \mathbf{u} \mathbf{u}) \, dV_i = \int_{V_i} (-\nabla p) \, dV_i + \int_{V_i} \nabla \cdot \mathbb{T} \, dV_i + \int_{V_i} \mathbf{F} \, dV_i, \quad (2.9)$$

$$\frac{\partial}{\partial t} \int_{V_i} \alpha \, dV_i + \int_{V_i} \nabla \cdot (\alpha \mathbf{u}) \, dV_i = 0. \quad (2.10)$$

where $\mathbf{F}$ is any body force (in our case, only interfacial forces).

The divergence theorem is applied to the volume integrals of divergence terms to convert them to surface integrals over the surface boundary of the control-volume, i.e

$$\int_{V_i} \nabla \cdot \mathbf{G} \, dV_i = \oint_{S_i} \mathbf{G} \cdot \mathbf{n} \, dS_i, \quad (2.11)$$

where $\mathbf{G}$ denotes a vector or tensor field, S_i is the surface boundary of the control-volume, and $\mathbf{n}$ is the outward-pointing unit vector normal to S_i

The integrations over the volume of the control-volume are approximated by the product of the value of the integrand at the cell centre and the volume of the cell, i.e.

$$\int_{V_i} Q \, dV_i \approx Q_{cv} V_i, \quad (2.12)$$

where Q denotes an arbitrary variable integrated over the volume of the control-volume and Q_{cv} represents the value of Q at the control-volume centre.

By applying Equations (2.11) and (2.12) to the transport equations, then we can write

$$\oint_{S_i} \mathbf{u} \cdot \mathbf{n} dS_i = 0, \quad (2.13)$$

$$\frac{\partial}{\partial t}(\rho \mathbf{u})_{cv} + \frac{1}{V_i} \oint_{S_i} (\rho \mathbf{u} \mathbf{u}) \cdot \mathbf{n} dS_i = (-\nabla p)_{cv} + \frac{1}{V_i} \oint_{S_i} \mathbb{T} \cdot \mathbf{n} dS_i + \mathbf{F}_{cv}, \quad (2.14)$$

$$\frac{\partial \alpha_{cv}}{\partial t} + \oint_{S_i} (\alpha \mathbf{u}) \cdot \mathbf{n} dS_i = 0. \quad (2.15)$$

The discretized form of these equations over the control-volume i can be written as

$$\sum_{f \in S_i} \mathbf{u}_f \cdot \mathbf{S}_f = 0, \quad (2.16)$$

$$\partial_t^h(\rho \mathbf{u})_{cv} + \frac{1}{V_i} \sum_{f \in S_i} (\rho \mathbf{u} \mathbf{u})_f \cdot \mathbf{S}_f = (-\nabla^h p)_{cv} + \frac{1}{V_i} \sum_{f \in S_i} \mathbb{T}_f \cdot \mathbf{S}_f + \mathbf{F}_{cv}, \quad (2.17)$$

$$\partial_t^h \alpha_{cv} + \sum_{f \in S_i} (\alpha \mathbf{u})_f \cdot \mathbf{S}_f = 0. \quad (2.18)$$

where $\mathbf{n}_f$ is the outward-pointing unit normal on the surface face S_f , as shown in Figure 2.2, $\mathbf{S}_f = S_f \mathbf{n}_f$ is the area vector, the superscript h denotes an appropriate numerical approximation, and the subscript f means belong to or evaluated at the surface face f .

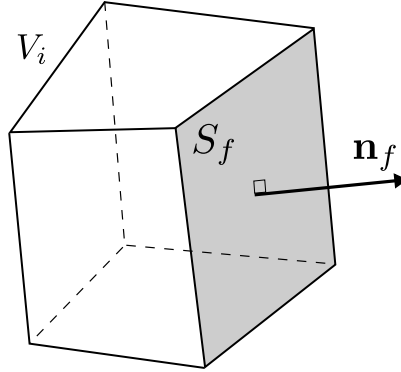


Figure 2.2. A three-dimensional hexahedral control-volume (cell i), with volume V_i and total closed surface boundary S_i , surrounding a computational node point. The normal vector $\mathbf{n}_f$, pointing outward, is defined on the surface face, S_f .

2.2.2. Solution procedure of the discretized equations

The linearized discretized form of the momentum equation, for the set of control-volumes in a computational mesh, can be written as

$$A_d \mathbf{u} = \mathbf{H}(\mathbf{u}) - \nabla^h p + \mathbf{F}, \quad (2.19)$$

where A_d is a scalar field containing the diagonal elements of the coefficient matrix, corresponding to a system of linear algebraic equations resulting from the discretization of the momentum equation, Equation (2.2), the term $\mathbf{H}(\mathbf{u})$ accounts for off-diagonal elements of the coefficient matrix and also all source terms apart from pressure gradients and body forces.

The discretization procedure for each control-volume is based on Equation (2.17) when a first-order, forward Euler method is used for the temporal discretization, $\partial_t^h()$, while second-order finite volume schemes, based on Gauss theorem, are used for the spatial discretizations. The bounded self-filtered central differencing (SFCD) scheme is used to interpolate velocity and the indicator function from cell centres to face centres in the convective terms. Central differencing is used to compute required gradients normal to the cell faces.

By rearranging Equation (2.19), we have

$$\mathbf{u} = \frac{\mathbf{H}(\mathbf{u}) + \mathbf{F}}{A_d} - \frac{1}{A_d} \nabla^h p. \quad (2.20)$$

Imposing the continuity condition, Equation (2.1), upon this velocity field, after discretization, leads to the following equation for the pressure:

$$\sum_{f \in S_i} \frac{S_f}{\langle A_d \rangle_f} \nabla_f^\perp p = \sum_{f \in S_i} \tilde{\phi}_f, \quad (2.21)$$

where

$$\tilde{\phi}_f = \left\langle \frac{\mathbf{H}(\mathbf{u})}{A_d} \right\rangle_f \cdot \mathbf{S}_f + \frac{\phi_{F,f}}{\langle A_d \rangle_f}. \quad (2.22)$$

Here, $\tilde{\phi}_f$ can be considered as an intermediate face-centred flux field that lacks the pressure gradient effect, $\mathbf{S}_f$ and S_f are, respectively, the outward-pointing area vector of face f and its magnitude, $\langle \rangle_f$ denotes the face-centred field interpolated from the corresponding cell-centred field, $\nabla_f^\perp$ denotes face normal gradient evaluated as a scalar field directly at the face centres, and $\phi_{F,f} = \mathbf{F}_f \cdot \mathbf{S}_f$ is the interfacial force flux computed directly at the face f , which is the focus of discussion in Section 2.2.4.

Once the pressure field is obtained, a corrected face-centred flux field, ϕ_f , is computed using the following equation:

$$\phi_f = \tilde{\phi}_f - \frac{S_f}{\langle A \rangle_f} \nabla_f^\perp p. \quad (2.23)$$

Finally, the cell-centred velocity vector for each cell i , $\mathbf{u}_{cv}$, can be reconstructed in a conserved

way from its face fluxes, ϕ_f , as follows:

$$\mathbf{u}_{cv} = \mathcal{S}^{-1} \cdot \sum_{f \in S_i} \mathbf{n}_f \phi_f, \quad (2.24)$$

where $\mathcal{S}^{-1}$ is the inverse of the following second rank symmetric tensor:

$$\mathcal{S} = \sum_{f \in S_i} \mathbf{n}_f \mathbf{S}_f. \quad (2.25)$$

Here $\sum_{f \in S_i}$ is a sum operator over all faces belonging to the cell i .

The major problem with advecting the indicator function using Equation (2.4), is numerical diffusion, which tends to smear the interface sharpness through time. To alleviate this problem, an additional artificial convection term is added to the advection equation:

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{u}) + C_\alpha \nabla \cdot [\alpha(1 - \alpha) \mathbf{u}_r] = 0, \quad (2.26)$$

where C_α is a compression factor, set to 1 in our simulations, and $\mathbf{u}_r$ is the relative velocity vector (Rusche, 2002; Deshpande et al., 2012). The fluid–fluid interface is advected by solving the system of linear algebra arising from the discrete form of Equation (2.26) for each cell c :

$$\partial_t^h \alpha + \frac{1}{V_i} \sum_{f \in S_i} [\langle \alpha \rangle_f \phi_f + C_\alpha \langle \alpha \rangle_f (1 - \alpha)_f \phi_{r,f}] = 0. \quad (2.27)$$

Here ∂_t^h represents the first-order Euler method for the temporal discretization, ϕ_f is the volumetric flux at face f computed using Equation (2.23), and $\phi_{r,f}$ is a relative volumetric flux at face f defined as

$$\phi_{r,f} = |\phi_f| \langle \mathbf{n}_s \rangle_f \cdot \mathbf{n}_f, \quad (2.28)$$

where $\mathbf{n}_f = \mathbf{S}_f / S_f$ is the unit normal to the face f , and $\mathbf{n}_s$ is the unit normal to the interface defined as

$$\mathbf{n}_s = \frac{\nabla \alpha}{|\nabla \alpha|}. \quad (2.29)$$

Equations (2.21), (2.23) and (2.27) are solved iteratively in two loops: (a) an outer-corrector loop to semi-implicitly couple the interface evolution and consequently the interfacial forces with the velocity field, and (b) an inner-PISO loop, to couple pressure and velocity fields, based on the pressure implicit with splitting of operator (PISO) method of Issa (1986). The solution algorithm from time step n to time step $n + 1$ can be summarized as follows:

1. Outer-corrector loop ($n_{outerLoop}$ iterations):
 - a. Advect the indicator function to update the interface profile at time $n+1$ (Eq. (2.27)), using the fluxes at time n for the first iteration.
 - b. Update fluid properties, viscosity and density (Eq. (2.3)).

- c. Reconstruct the interface by linear approximation of the $\alpha = 0.5$ contour, and compute interfacial forces at face centres (details in Sections 2.2.3 and 2.2.4).
 - d. Inner-PISO loop (n_{PISO} iterations):
 - i. Compute the intermediate volumetric flux field, $\tilde{\phi}_f$ (Eq. (2.22)).
 - ii. Solve the pressure equation to update the pressure field (Eq. (2.21)).
 - iii. Correct the volumetric flux field (Eq. (2.23)).
 - iv. Reconstruct the cell-centred velocity field (Eq. (2.24)).
 - e. End of inner-PISO loop
2. End of outer-corrector loop

We use two iterations in both the outer-corrector and the inner-PISO loops, $n_{outerLoop} = n_{PISO} = 2$, in our simulations.

2.2.3. Reconstructing the interface

Our motivation in reconstructing the interface is to reduce spurious velocities and calculate the pressure jump across the fluid–fluid interface more accurately within a finite-volume volume-of-fluid framework. The proposed algorithm is face-based, robust and easy to implement. We define the interface as face-based surface elements that consist of connected points where the value of α is equal to 0.5.

Figure 2.3 schematically illustrates the interface reconstruction process which consists of three steps:

1. Defining a sharp indicator function, α_c , based on volume fractions (the smooth indicator function), α .
2. Using the sharp profile of α_c to indicate mixed-faces, i.e. the faces that are cut by the interface.
3. Identifying the interface location, i.e. where $\alpha = 0.5$, using a simple linear extrapolation from the the vertices of the mixed-faces.

For the purpose of constructing a sharp interface, we first introduce a new indicator function by clipping α and rescaling it between 0 and 1 as follows (Raeini et al., 2012):

$$\alpha_c = \frac{1}{1 - C_c} \left[\min \left(\max \left(\alpha, \frac{C_c}{2} \right), 1 - \frac{C_c}{2} \right) - \frac{C_c}{2} \right], \quad (2.30)$$

where the clipping factor, C_c , controls the sharpness of α_c in the vicinity of $\alpha = 0.5$. In this study, this factor is set to 0.98. Then, we declare a cell face to be a mixed-face, f_{mix} , when for that face the following condition is satisfied (Figure 2.4):

$$|\nabla_f^\perp \alpha_c| > \frac{\epsilon}{h}, \quad (2.31)$$

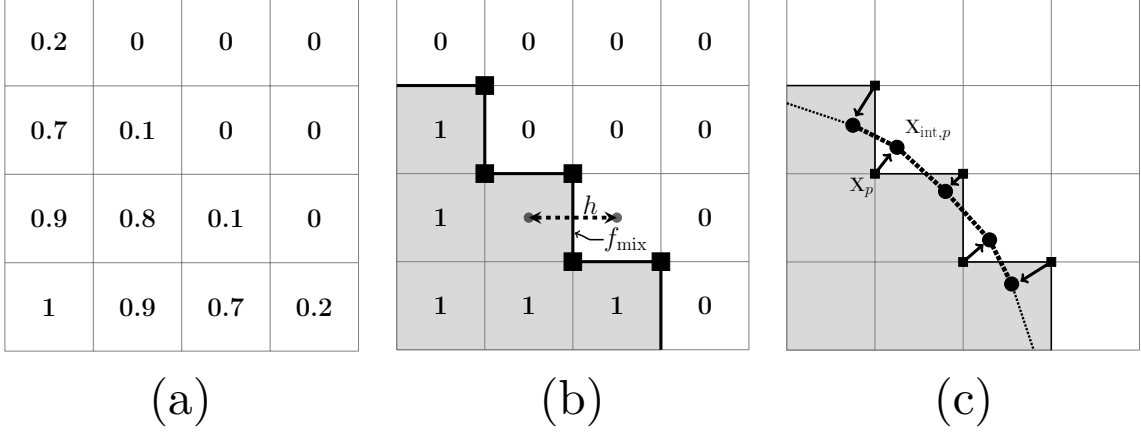


Figure 2.3. A two-dimensional schematic of the steps in reconstructing the interface: (a) the indicator function, α , (b) the sharp indicator function, α_c , used to mark mixed-faces and their corner points (shown as filled black squares), and (c) linear reconstruction of the interface (dashed line), where $\alpha = 0.5$.

where ϵ is a small number set to 10^{-8} and h is the face normal distance between the centroid of the two cells that share the face f .

This technique converts the smooth profile of the indicator function, α , into a sharp discontinuity, α_c , as illustrated in Figure 2.4, without distorting the location of $\alpha = 0.5$. The sharpness of the discontinuity can be controlled using the clipping factor, C_c . As the clipping factor approaches 1, the discontinuity becomes sharper and the profile of α_c becomes closer to a stair-stepped approximation. Employing the face normal gradient of α_c , instead of α , to mark mixed-faces, Figure 2.4, i.e. the only faces on which the interfacial force is non-zero, increases the interface locality. Consequently, this improves the balance of the interfacial forces with the pressure gradient which can effectively eliminate spurious currents, as shown for static test cases in Chapter 3.

The smooth profile of α may get distorted due to the artificial compression of the interface during the advection process, Equation (2.27), especially for dynamic test cases. This can adversely affect the accuracy of the interface normal vector computations which require a smooth change in the gradient of the indicator function. Therefore, we define a smoothed indicator function, α_s , by interpolating α from cells to faces and back to faces, recursively, for four iterations ($i = 0-3$):

$$\alpha_{s,i+1} = C_s \langle \langle \alpha_{s,i} \rangle_f \rangle_c + (1 - C_s) \alpha_{s,i}, \quad \alpha_{s,0} = \alpha, \quad (2.32)$$

where $\langle \rangle_c$ denotes the cell-centred field interpolated from the corresponding face-centred field, and C_s is the smoothing relaxation factor, which is set to 0.6 in our simulations. This smoothed indicator function is then used to obtain the interface normal vectors. This step may also

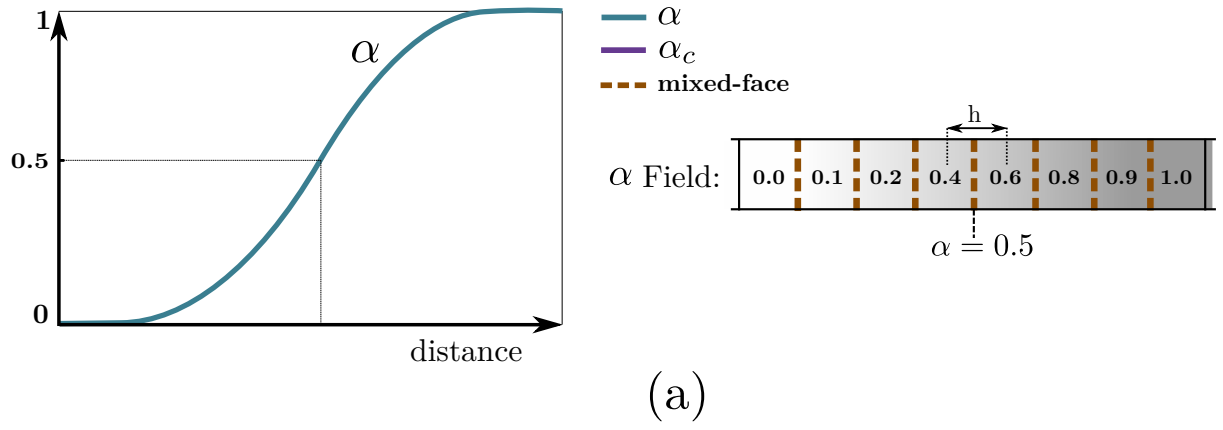
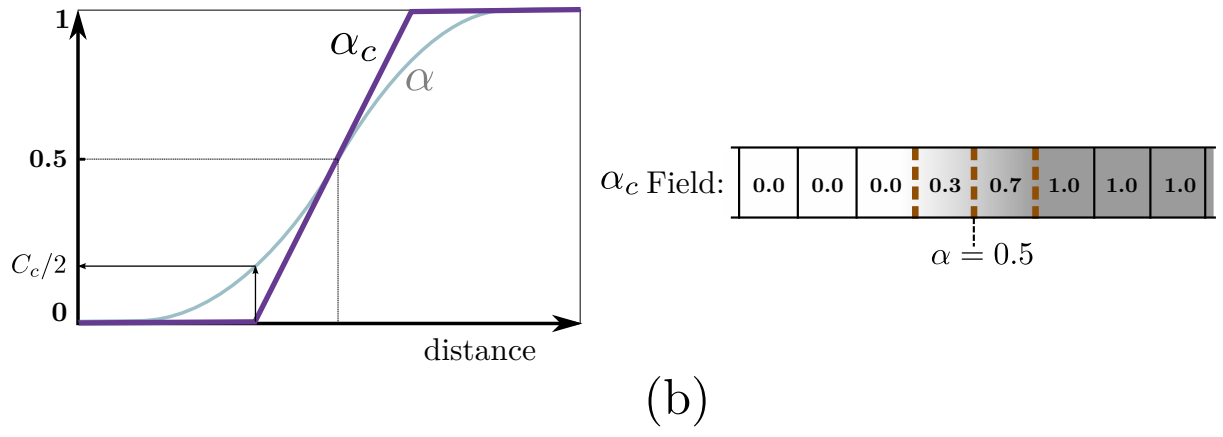
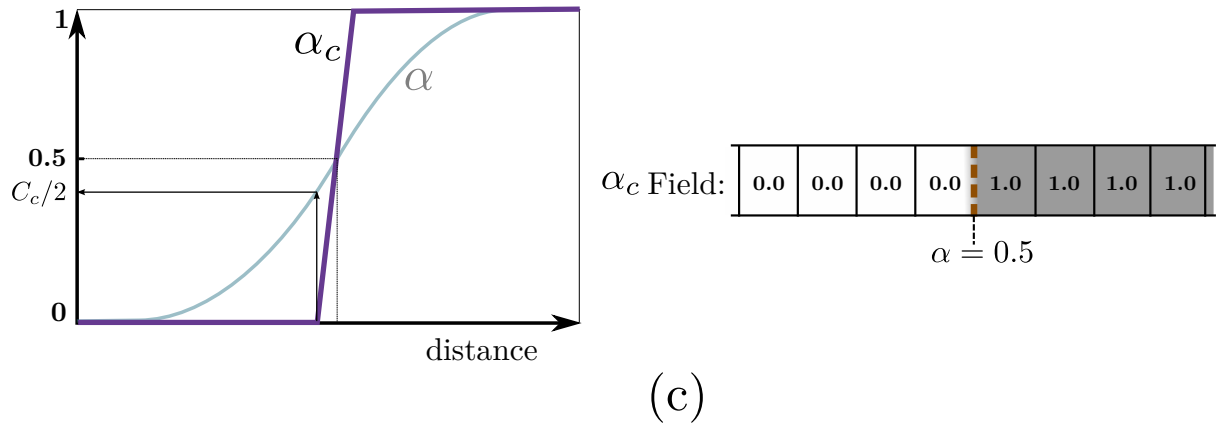


Figure 2.4. Schematic representation of converting the smooth transition of the indicator function, α , to a sharp profile, α_c , using Equation (2.30). (a) The clipping factor, C_c , is equal to zero, therefore α_c has a similar profile to α . (b) C_c is increased to a value between zero and one, hence α_c exhibits sharper discontinuity at the interface. (c) As C_c approaches to one the α_c profile becomes closer to a stair-stepped function around $\alpha = 0.5$.

include an optional prior clipping of α to exclude localized unphysical variations in α close to 0 or 1 in the vicinity of the interface zone,

$$\alpha_{s,0} = \min(\max(C_{c,0}(\alpha - 0.5) + 0.5, 0), 1), \quad (2.33)$$

where $C_{c,0}$ is a constant controlling the length of the clipping that is set to 1.02.

A second order least-squares method is used to estimate the gradient of α_s at mesh points, p , which form the mixed-faces:

$$(\nabla \alpha_s)_p = \sum_{i=1}^{N_f} \omega_i^2 \mathcal{G}_p^{-1} \cdot \mathbf{d}_i (\Delta \alpha_s)_i, \quad (2.34)$$

where $\mathcal{G}_p^{-1}$ is the inverse of the following symmetric tensor:

$$\mathcal{G}_p = \sum_{i=1}^{N_f} \omega_i^2 \mathbf{d}_i \mathbf{d}_i^T, \quad (2.35)$$

and

$$(\Delta \alpha_s)_i = \alpha_{s,i} - \alpha_{s,p}. \quad (2.36)$$

Here N_f is the number of faces that share the point p , $\mathbf{d}_i$ is the distance vector between the centroid of face i and the location of point p , ω_i is the inverse distance weighting factor calculated as $\omega_i = 1/|\mathbf{d}_i|$, $\alpha_{s,i}$ is the interpolated value of the smoothed indicator function, α_s , at face i , and $\alpha_{s,p}$ is the interpolated value of α_s at the point p , computed using the following inverse-distance-weighting interpolation method:

$$\alpha_{s,p} = \frac{\sum_{i=1}^{N_f} \omega_i \alpha_{s,i}}{\sum_{i=1}^{N_f} \omega_i}. \quad (2.37)$$

Using a least-squares method to estimate $(\nabla \alpha_s)_p$ is preferable because it only uses the values of immediate neighbour cells of point p , hence preserving its locality to a greater extent than the wide stencil finite difference approximations at cell centres followed by interpolation. Localized estimations of $(\nabla \alpha_s)_p$ are crucial to compute the interface location, $\alpha = 0.5$, accurately.

Finally, the interface unit normal for each corner point p is defined as follows:

$$\mathbf{n}_p = \frac{(\nabla \alpha_s)_p}{|(\nabla \alpha_s)_p|}. \quad (2.38)$$

For the points on solid boundaries, fluid–fluid–solid contact points, however, the direction of $\mathbf{n}_p$ must be modified in accordance with the contact angle, θ , to obtain interface unit normal vectors at the contact line, $\mathbf{n}_p|_w$ (Figure 2.5). The interface normals at contact line, $\mathbf{n}_p|_w$, is

obtained as a linear combination of $\mathbf{n}_p$ and the unit normal vector to the solid wall, $\mathbf{n}_w$,

$$\mathbf{n}_p|_w = (\cos \theta - \frac{\sin \theta \cos \theta'}{\sin \theta'}) \mathbf{n}_w + \frac{\sin \theta}{\sin \theta'} \mathbf{n}_p, \quad (2.39)$$

where

$$\theta' = \cos^{-1}(\mathbf{n}_w \cdot \mathbf{n}_p). \quad (2.40)$$

Here $\mathbf{n}_w$ is obtained by interpolating face unit normal vectors of the solid boundary to the mesh points. In the case of stair-like solid boundaries, used in Section 3.1.2, $\mathbf{n}_w$ is smoothed by recursively interpolating from the mesh points to their adjacent solid boundary faces and back to the mesh points (Raeini et al., 2012), four times in this work.

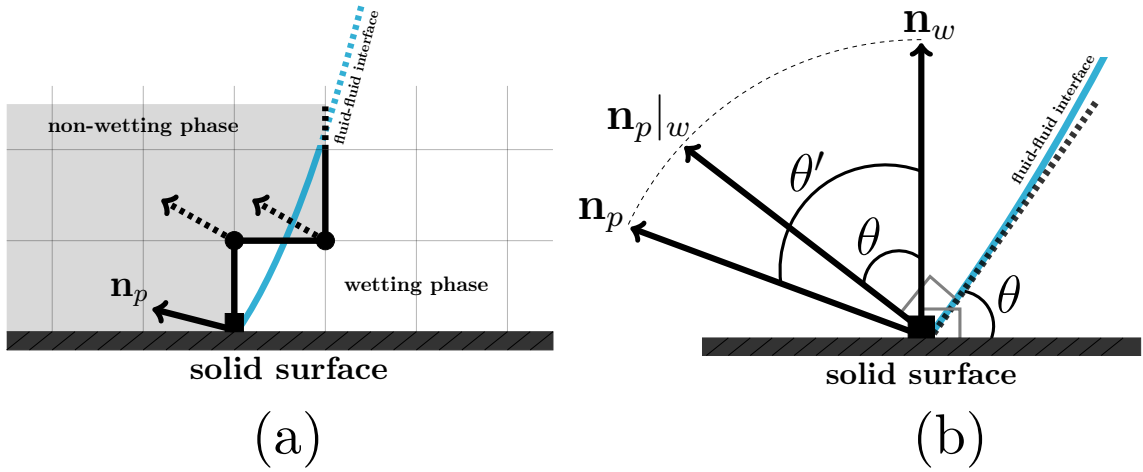


Figure 2.5. A schematic representation of (a) unit normal vectors, $\mathbf{n}_p$, Equation (2.38), to a fluid–fluid interface (dotted arrow) and to its contact point (solid arrow), on a solid surface, and (b) the modified interface unit normal vector at the wall, $\mathbf{n}_p|_w$, Equation (2.39), which is in accordance with the imposed contact angle, θ .

For every mixed-face, an interface element is considered so that a one-to-one correspondence is established between the points of the mixed-face and the interface points. The location of the interface points, where $\alpha = 0.5$, is calculated from a simple linear extrapolation (see Figure 2.3c)

$$\mathbf{x}_{\text{int},p} = \mathbf{x}_p + \frac{0.5 - \alpha_{s,p}}{|(\nabla \alpha_s)_p|} \mathbf{n}_p, \quad (2.41)$$

where $\mathbf{x}_{\text{int},p}$ is the position vector of the interface points, and $\mathbf{x}_p$ is the position of point p on the mixed-face.

Once the locations of the interface points are computed, the area vector of each interface

element, $\mathbf{S}_{\text{int},f}$, is calculated using the following sum over its points:

$$\mathbf{S}_{\text{int},f} = \frac{1}{2} \sum_{i=1}^{N_p} [(\mathbf{x}_{\text{int},p_{i+1}} - \mathbf{x}_{\text{int},p_i}) \times (\mathbf{x}_{\text{int},c} - \mathbf{x}_{\text{int},p_i})], \quad (2.42)$$

where N_p is the total number of the corner points that form the interface element, and $\mathbf{x}_{\text{int},c} = \frac{\sum_{i=1}^{N_p} \mathbf{x}_{\text{int},p_i}}{N_p}$ is the centroid of the interface element. The interface element points are ordered in a way that the computed area vector always points towards the same fluid (fluid 1).

Employing the least-squares method to estimate the interface normal at corner points alongside the one-to-one correspondence between corner points of interface elements and mixed-faces results in a simple and robust face-based methodology for reconstructing the interface. All that is required is a set of discrete marked faces described by their corner points. We stress that the clipped and smoothed indicator functions, α_c and α_s , are only used to reconstruct the interface elements, without affecting the original indicator function, α . Moreover, the indicator function, α , is advected in a conservative control-volume framework that guarantees mass conservation to round-off in all test cases; see the dynamic test cases presented in Chapter 3.

2.2.4. Computing the interfacial force

In this section, we introduce our algorithm for computation of interfacial forces directly on the reconstructed interface using a sharp surface force model. Herein, the term contour-level surface force (CLSFS) method is used to refer to the proposed approach for the treatment of the interfacial force. Then, we briefly describe the previously-published continuous surface force (CSF) (Brackbill et al., 1992) and sharp surface force (SSF) Raeini et al. (2012) models. We later in Chapter 3 compare the accuracy of the CLSF, CSF and SSF algorithms.

Contour-level surface force (CLSFS) model

The interface is reconstructed and explicitly represented as face-based discrete elements. The interfacial force for each interface element, $\mathbf{f}_{\text{int},\sigma}$, can be written as an integral of $\mathbf{f}_\sigma$, Equation (2.5), over the surface of the element and converted to a line integral using the Stokes theorem (Tryggvason et al., 2001):

$$\mathbf{f}_{\sigma,\text{int}} = \int_{S_{\text{int}}} \mathbf{f}_\sigma ds = \sigma \int_{S_{\text{int}}} \kappa \mathbf{n} ds = \sigma \oint_{C_{\text{int}}} \mathbf{m} d\ell, \quad (2.43)$$

where C_{int} is the closed boundary along the edges of the interface elements. The interfacial force for each element is computed using this line integral over the edges of the interface element. This offers the unique advantage of not needing to calculate the interface curvature at cell centres and then interpolating them to faces, which improves the balance of forces in the momentum equation (Tryggvason et al., 2001).

On the discrete level, the interfacial force on an interface element corresponding to face f ,

$\mathbf{f}_{\sigma,\text{int},f}$, is obtained by estimating Equation (2.43) using the following sum over the corner points of the element:

$$\mathbf{f}_{\sigma,\text{int},f} = \sigma \sum_{i=1}^{N_p} \left[(\mathbf{x}_{\text{int},p_{i+1}} - \mathbf{x}_{\text{int},p_i}) \times \frac{(\mathbf{n}_{p_{i+1}} + \mathbf{n}_{p_i})}{2} \right]. \quad (2.44)$$

The computed interfacial forces then are smoothed by looping over corresponding mixed-faces to equally distribute $\mathbf{f}_{\sigma,\text{int},f}$ between the two grid cells that share the mixed-face, and then interpolate the cell values back to the mixed-face based on an area-weighting method,

$$\mathbf{f}_{\sigma,\text{int},f} = \sum_{i=1}^2 \omega_i \mathbf{f}_{\sigma,i}, \quad (2.45)$$

where

$$\omega_i = \frac{S_{\text{int},f}}{\sum_{j=1}^{N_{f,\text{mix}}} |\Delta\alpha_c|_f S_{\text{int},f_j}}, \quad (2.46)$$

and

$$\mathbf{f}_{\sigma,i} = \frac{1}{2} \sum_{j=1}^{N_{f,\text{mix}}} |\Delta\alpha_c|_f \mathbf{f}_{\sigma,\text{int},f_j}. \quad (2.47)$$

Here, ω_i is the area-based interpolation weighting for cell i , $N_{f,\text{mix}}$ is the number of mixed faces belong to cell i , and $|\Delta\alpha_c|_f$ is the magnitude of the difference of α_c between the two cells that share the mixed-face f . This smoothing step is essential to keep the conservation of the net capillary force on closed surfaces within an acceptable limit for our dynamic test cases, when applying the interfacial forces onto the underlying fixed grid.

Finally, the interfacial force flux term, $\phi_{F,f} = \mathbf{F}_f \cdot \mathbf{S}_f$, Equation (2.22), is approximated on the fixed grid faces as follows:

$$\phi_{F,f} = \mathbf{f}_{\sigma,\text{int},f} \cdot \langle \mathbf{n}_s \rangle_f \nabla_f^\perp \alpha_c, \quad (2.48)$$

where $\mathbf{n}_s$ is the interface normal computed using Equation (2.29).

The steps taken in the CLSF method to compute the face-based interfacial force at each time step, can be summarized as follows:

1. Compute a sharp indicator function, α_c (Equation (2.30)).
2. Find all mixed-faces, i.e. faces in the boundary between the two fluids, for which $\nabla_f^\perp \alpha_c$ is nonzero (Equation (2.31)).
3. Compute a smoothed indicator function, α_s (Equation (2.32)).
4. Compute interpolated values of α_s at the mesh points (Equation (2.37)).
5. For each mixed-face, do the following:
 - a. Compute the gradient of α_s at the face vertices using a second order least-squares method (Equation (2.34)).

- b. Obtain the interface normals at the vertices using the computed gradients (Equation (2.38)). Modify the normal vectors on solid boundaries to include wettability effects (Equation (2.39)).
 - c. Estimate the location of the fluid–fluid interface, where $\alpha = 0.5$, in the direction of the interface normal vectors (Equation (2.41)).
 - d. Form interfacial surface elements using the computed interface location coordinates by holding a one-to-one correspondence between the mixed-faces and their interface elements (Equation (2.42)).
 - e. Compute the interfacial force on the interface elements (Equation (2.44)).
6. Smooth the computed interfacial forces (Equation (2.45)).
 7. Use the computed interfacial forces to estimate the interfacial force flux on the corresponding mixed-faces on the fixed grid (Equation (2.48)).

In the CLSF model, interfacial forces are computed using a sharp surface force model that can efficiently eliminate the problem of spurious currents. The explicit representation of the interface used to compute interfacial forces leads to an accurate estimation of capillary pressure even for low grid resolutions. This can be very important to model multiphase flows directly on micro-CT images of porous media for which simulations with a very fine grid resolution are prohibitively expensive using currently available computational resources.

Continuous surface force (CSF) model

In the CSF model, the interfacial force is estimated as

$$\mathbf{f}_{\sigma v} = \sigma \kappa \mathbf{n}_s \delta_s, \quad (2.49)$$

where δ_s is a delta function concentrated on the interface, $\mathbf{n}_s$ is the unit normal interface, and $\kappa = -\nabla \cdot \mathbf{n}_s$ is the interfacial curvature.

On the discrete level, to have a balanced-forced flow algorithm similar to Francois et al. (2006), Equation (2.49) is used to approximate the interfacial force flux term, $\phi_{F,f}$, on the faces of the fixed-grid, as follows:

$$\phi_{F,f} = \sigma (\langle \kappa \mathbf{n}_s \rangle_f \cdot \mathbf{S}_f) \delta_{sf}, \quad (2.50)$$

where interfacial unit normals, $\mathbf{n}_s$, are computed at cell centres using Equation(2.29), and δ_{sf} is approximated as

$$\delta_{sf} \approx \nabla_f^\perp \alpha. \quad (2.51)$$

Sharp surface force (SSF) model

In the SSF model, the same approach is employed as the CSF model, Equation (2.49), however, the delta function in Equation (2.50), δ_{sf} , is approximated using the normal gradient of the

sharp indicator function, α_c , Equation (2.30), rather than α (Raeini et al., 2012):

$$\delta_{sf} \approx \nabla_f^\perp \alpha_c. \quad (2.52)$$

This implies that the SSF method employs a more compact delta function in comparison to the CSF method, while the interfacial normal vectors, $\mathbf{n}_s$, and consequently the interfacial curvature, κ , are estimated with a wide stencil as in the CSF method. We show that even though this approach may help to reduce spurious currents in some static test cases, it has the same limitations as CSF: large errors in pressure jump and consequently an unbalanced (non-zero) interfacial force on closed surfaces (Rusche, 2002; Raeini et al., 2012).

2.3. Closure

A simple numerical approach is proposed for computing immiscible two-phase flow at the micro-scale. A modified fully sharpened indicator function is used to present the fluid–fluid interface as a sharp discontinuity. A simple and effective algorithm is devised to reconstruct the interface from volume fractions only at the cell faces for which the gradient of the sharpened indicator function is non-zero. The reconstructed interface is then employed to compute the interfacial force at the centre of cell faces to give a balanced-force algorithm. The method is implemented within a finite-volume volume-of-fluid framework, based upon interFoam solver in OpenFOAM.

3. Validation of the numerical method

In this chapter we use several two- and three-dimensional test cases to validate our numerical method. We first consider examples where the two phases are in static equilibrium (Section 3.1). Then, the accuracy of the method is examined using dynamic test cases (Section 3.2). Finally, to explore applications in porous media, corner flow through a three-dimensional non-circular capillary tube is investigated (Section 3.2.3).

In all simulations presented herein, for liquid–liquid systems we use two liquids, both with viscosities of 10^{-3} Pa·s and densities of 1000 kg/m^3 and for gas–liquid systems a gas phase with a viscosity of 10^{-5} Pa·s and a density of 1 kg/m^3 . The interfacial tension is constant and taken to be $\sigma = 0.03 \text{ N/m}$. We compare the results of the CLSF model to analytical solutions and also CSF and SSF models.

3.1. Static test cases

A common test to validate two-phase flow models with interfacial tension, is simulating fluid–fluid systems at static equilibrium conditions where the velocity field must remain zero (Popinet and Zaleski, 1999; Renardy and Renardy, 2002). The discrete balance of the pressure gradient with the interfacial force can be examined by measuring the value of the maximum velocity in the computational domain. In addition, the accuracy of the interfacial force model can be quantified by measuring the error in pressure jump across the interface.

3.1.1. Static droplet

First, we simulate a two-dimensional circular droplet in the absence of gravity as either (a) a gas–liquid system (gas is surrounded by liquid) or (b) a liquid–liquid system. A static droplet with a radius of $R = 10 \text{ }\mu\text{m}$ is centred in a rectangular domain having side lengths of $L = 40 \text{ }\mu\text{m}$. The computational domain is discretized using a uniform Cartesian grid with a resolution of $R/\delta x = 8$, where δx is the side length of uniform grid cells. Since the interfacial force is treated explicitly, small time steps, δt , are taken to satisfy the time step constraint,

$$\delta t \leq \left[\frac{\bar{\rho} \delta x^3}{2\pi\sigma} \right]^{1/2}, \quad (3.1)$$

where $\bar{\rho} = \frac{\rho_1 + \rho_2}{2}$ (Brackbill et al., 1992).

Figure 3.1 shows comparisons of calculated dimensionless measures of the maximum magnitude of the spurious current. The spurious current capillary number, $Ca = |\mathbf{u}|_{\max} \mu / \sigma$, for the gas–liquid and liquid–liquid systems is shown as a function of a dimensionless time scale,

$$t_d = \frac{\mu t}{\rho D^2}, \quad (3.2)$$

where μ and ρ are, respectively, viscosity and density of the liquid, and D is the diameter of the droplet.

It can be observed that Ca reduces to machine precision, 10^{-15} , in both systems using the CLSF method. For the SSF method, the velocity field also dies out to machine precision but with a slower convergence rate. On the other hand, for the CSF method, the maximum dimensionless error in the velocity field remains of order 10^{-3} for the gas–liquid and the liquid–liquid systems, which obviously is unfavourable when using the numerical method to model multiphase flow at low capillary numbers.

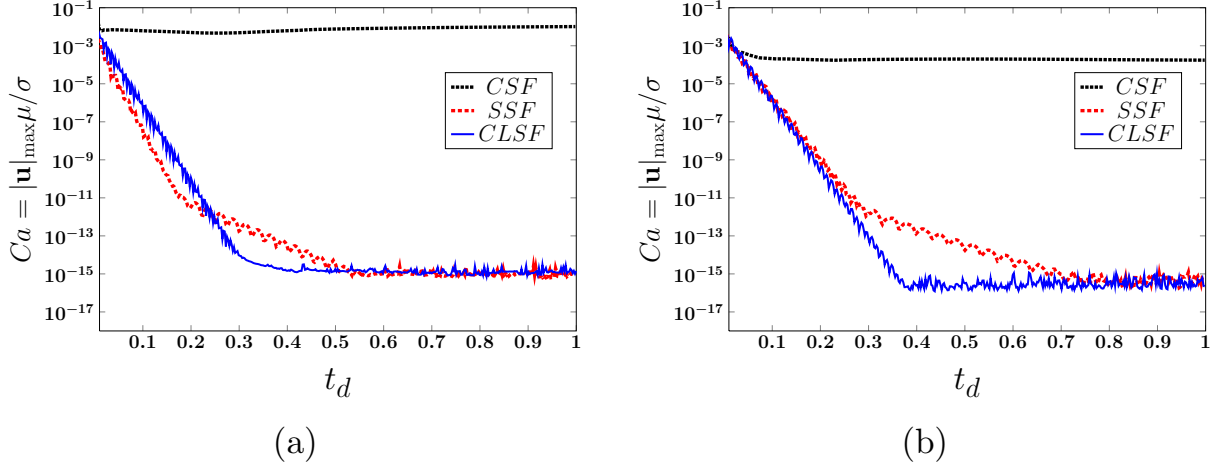


Figure 3.1. Dimensionless maximum velocity, the spurious current capillary number, Ca , as a function of dimensionless time, Equation (3.2), for a two-dimensional static droplet: (a) gas–liquid system, and (b) liquid–liquid system. The radius of the droplet is discretized by 8 uniform grid cells, i.e. $R/\delta x = 8$.

Figure 3.2 shows the velocity vectors and droplet shapes ($\alpha = 0.5$ contour-line) at $t_d = 0.25$ for the liquid–liquid system using the three formulations. The velocity vectors are scaled by different factors to make them visible. The magnitude of the error in maximum velocity, Equation (3.3), is given in Table 3.1. One can see that the structure and location of spurious vortices for the CSF method are different from those of the SSF and CLSF methods. For the SSF and CLSF methods, the spurious currents spread over a smaller area of the domain, due to employing a more compact delta function approximation than the CSF method, and are insignificant away from the interface to such an extent that they are effectively not present. This clearly shows the importance of implementing the interfacial force with a sharp force model to eliminate spurious currents efficiently.

The error in velocity is measured using the following L_∞ error norm:

$$L_\infty(\mathbf{u}) = |\mathbf{u}|_{\max}, \quad (3.3)$$

while the relative error of the pressure jump is estimated as

$$E(\Delta P) = \left| \frac{\Delta P_{\text{numerical}} - \Delta P_{\text{exact}}}{\Delta P_{\text{exact}}} \right|. \quad (3.4)$$

The pressure jump across the droplet, according to the Young–Laplace equation, is $\Delta P_{\text{exact}} = \sigma/R = 3000$ Pa.

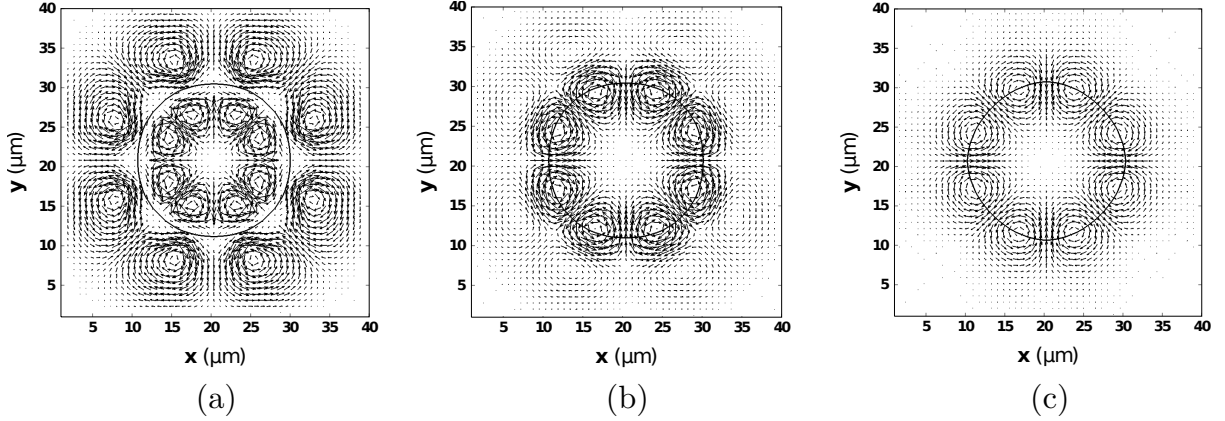


Figure 3.2. Velocity vector field and the indicator function contour ($\alpha = 0.5$) at dimensionless time $t_d = 0.25$, Equation (3.2), for a two-dimensional droplet in static equilibrium (the liquid–liquid system): (a) the CSF method, (b) the SSF method, and (c) the CLSF method. The mesh resolution is $R/\delta x = 8$. Vector plots are scaled differently to be visible.

Table 3.1.

Effect of mesh resolution on the error in maximum velocity, $L_\infty(\mathbf{u})$, Equation (3.3), and pressure jump across the interface, $E(\Delta P)$, Equation (3.4), for the liquid-liquid two-dimensional static droplet at a dimensionless time $t_d = 0.25$, Equation (3.2), using the CSF, SSF and CLSF methods.

$R/\delta x$	CSF		SSF		CLSF	
	$L_\infty(\mathbf{u})$ (m/s)	$E(\Delta P)$	$L_\infty(\mathbf{u})$ (m/s)	$E(\Delta P)$	$L_\infty(\mathbf{u})$ (m/s)	$E(\Delta P)$
4	1.28×10^{-2}	0.170	1.09×10^{-7}	0.160	5.14×10^{-9}	0.013
8	5.29×10^{-3}	0.170	1.12×10^{-9}	0.160	3.76×10^{-10}	0.012
16	4.05×10^{-3}	0.130	8.80×10^{-11}	0.054	2.49×10^{-10}	0.011
32	8.04×10^{-3}	0.102	4.98×10^{-11}	0.033	8.48×10^{-11}	0.009

In Table 3.1, we report the results for the error in maximum velocity, $L_\infty(\mathbf{u})$, and pressure jump, $E(\Delta P)$, Equations (3.3) and (3.4) respectively, as a function of mesh resolution for the two-dimensional static droplet (liquid–liquid system) at $t_d = 0.25$. These results show that the CLSF method can predict the pressure jump accurately, with about 1% error, even at low resolutions, $R/\delta x = 4$ and $R/\delta x = 8$, while for the CSF and SSF methods the error is about 16% for these cases. This accuracy at low resolution is essential for modelling large problems and specially for three-dimensional calculations where the resolution may be low due to constraints imposed by high simulation costs. Further refinement to $R/\delta x = 16$ and $R/\delta x = 32$ lead to

further reduction of the error in pressure jump for all methods. However, the magnitude of the error is still high, above 10%, for the CSF method. For the SSF method the error in pressure jump decreases dramatically from about 16% to 5% as the interface is resolved to $R/\delta x = 16$, whereas for the CSF method the reduction in the error is not that significant. It can also be observed that mesh refinement does not decrease the L_∞ norm of the spurious currents significantly in the CSF method, while for the SSF and CLSF methods spurious currents reduce to very small values, $O(10^{-11})$.

Next, we consider a three-dimensional droplet of radius $R = 10 \mu\text{m}$ positioned in the centre of a uniform cubic mesh of resolution $R/\delta x = 8$. The system is taken to be the liquid–liquid system and the theoretical pressure jump across the interface is $\Delta P_{exact} = 2\sigma/R = 6000 \text{ Pa}$.

Figure 3.3 shows a visualization of the final shape of reconstructed fluid–fluid interface used to compute interfacial forces. Note that each interface element corresponds uniquely to one mixed-face on the fixed grid.

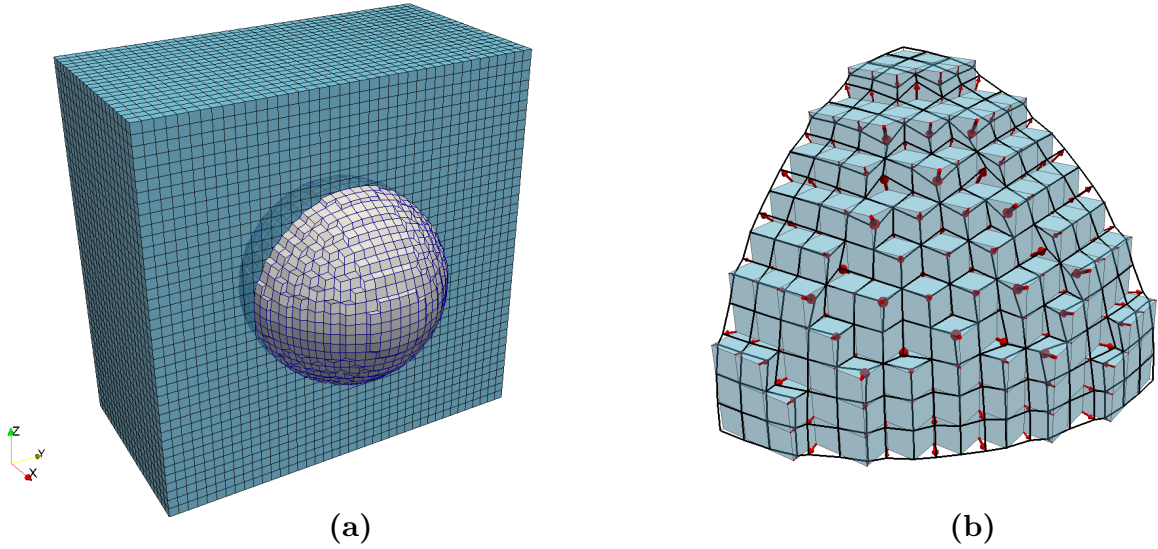


Figure 3.3. Visualization of (a) reconstructed fluid–fluid interface of a three-dimensional static droplet on a uniform Cartesian mesh of resolution $R/\delta x = 8$, at $t_d = 1.5$, and (b) the one-to-one correspondence between mixed-faces and reconstructed quadrilateral interface elements, shown for a quarter of the droplet. Arrows in (b) are the distant vectors from the mixed-face vertices to the corresponding interface element vertices.

Figure 3.4 depicts the evolution of the dimensionless maximum velocity for the three-dimensional test case using the CSF, SSF and CLSF methods. The spurious current capillary number is reduced efficiently to a very small value, $O(10^{-13})$, with the SSF and CLSF methods. On the other hand, similar to the two-dimensional case, Ca persists at the order of 10^{-3} , for the CSF method.

The pressure profile for a cross-section passing through the centre of the droplet for the three methods are shown in Figure 3.5. Improvements in both the accuracy and profile of the computed pressure with the CLSF method are evident. It yields a sharp pressure profile

with a relative pressure jump error of 2%, while the CSF method leads to a smooth pressure distribution with a high relative pressure jump error of approximately 12%. For the SSF method, the pressure profile is not quite sharp; some transitional grid cells can be observed in comparison to the CLSF method, and the pressure jump error is 8%.

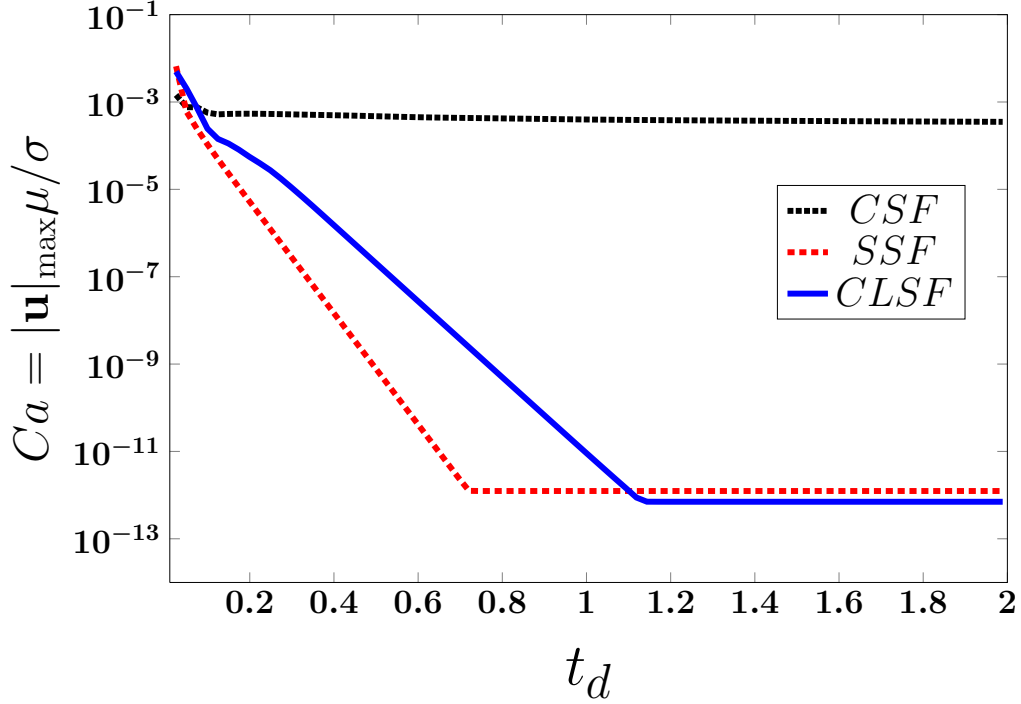


Figure 3.4. Dimensionless maximum velocity, the spurious current capillary number, as a function of dimensionless time, Equation (3.2), for a three-dimensional static droplet when the interfacial force is modelled using the CSF, SSF and CLSF methods. The mesh resolution is $R/\delta x = 8$.

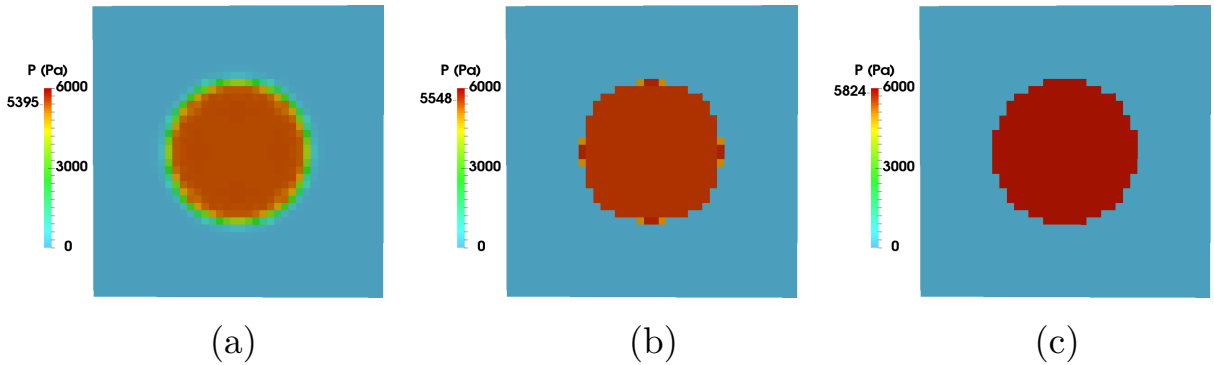


Figure 3.5. Computed pressure field for a three-dimensional static droplet (cut through the centre of the droplet) at dimensionless time $t_d = 2$: (a) the CSF method, (b) the SSF method and (c) the CLSF method. The computed pressure jumps across the interface for the CSF, SSF and CLSF methods are 5395 Pa, 5548 Pa and 5824 Pa, respectively. The analytical value of the pressure jump across the interface for this case is 6000 Pa.

These results suggest that the CLSF method can predict the sharp pressure jump across the interface accurately, even for low resolution grids. In addition, it can virtually eliminate spurious currents in a stable manner for both the two- and three-dimensional static droplets.

3.1.2. Static contact-line

A two-dimensional domain with a star-shaped solid boundary is considered in this subsection. The domain is partially filled with a non-wetting phase while a wetting phase with the same fluid properties resides in the corners (Figure 3.6). The grid cells which lie in a circle of radius $40 \mu\text{m}$, centred in the computational domain, are initialized with the non-wetting phase while the rest (corner cells) contain the wetting phase. The aim is to test the ability of our model to simulate static immiscible fluid–fluid interfaces in contact with staircase-like solid walls, on a uniform mesh, with different corner and equilibrium contact angles, 2γ and θ , respectively. The accuracy and stability of the method are quantified in terms of the infinite error norm in velocity field and the normalized error in the pressure jump across the interface,

$$E_n(\Delta P) = \left| \frac{\Delta P_{\text{numerical}} - \Delta P_{\text{exact}}}{\Delta P_{\text{exact}, \theta=0}} \right|, \quad (3.5)$$

where ΔP_{exact} can be calculated from

$$\Delta P_{\text{exact}} = \frac{\sigma}{R_l}, \quad (3.6)$$

where R_l is the radius of the interface curvature in the corners. The wetting phase cross-sectional area, A_l , as a function of R_l (Figure 3.6c) is:

$$A_l = \left[\left(\sin \eta + \frac{\cos \eta}{\tan \gamma} \right) \cos \eta - \left(\frac{\pi}{2} - \eta \right) \right] R_l^2, \quad (3.7)$$

where $\eta = \theta + \gamma$. The layer area, A_l , is estimated numerically and plugged in Equation (3.7) to obtain R_l , which is in turn used in Equation (3.6) to obtain ΔP_{exact} .

Figure 3.7 shows a sample visualization of the computed pressure field for the geometry with a corner angle of $2\gamma = 45^\circ$, an equilibrium contact angle of $\theta = 30^\circ$, and a mesh resolution of $L/\delta x = 8$. The improvement in the profile and magnitude of the pressure jump across the interface with our proposed method is clear.

Table 3.2 lists the simulation results for the CSF, SSF and CLSF methods at $t_d = 2.5$, for different mesh resolutions, $L/\delta x$, where L is the characteristic length of the geometry, see Figure 3.6, which is taken to be $20 \mu\text{m}$. One can observe that the errors resulted from the CSF and SSF methods do not follow a consistent behaviour. The accuracy of the results for these two methods is unacceptably high, and apparently dependent on the values of the corner and equilibrium contact angles, which dictate the final configuration of the contact line with respect to the solid wall. On the other hand, the CLSF method reduces the spurious currents

to machine accuracy and predicts the pressure jump across the interface to better than 8% in all cases.

These results clearly show that the CLSF method is able to model a static contact line accurately in a liquid–liquid–solid system even with a stair-case-like discretization of solid boundaries.

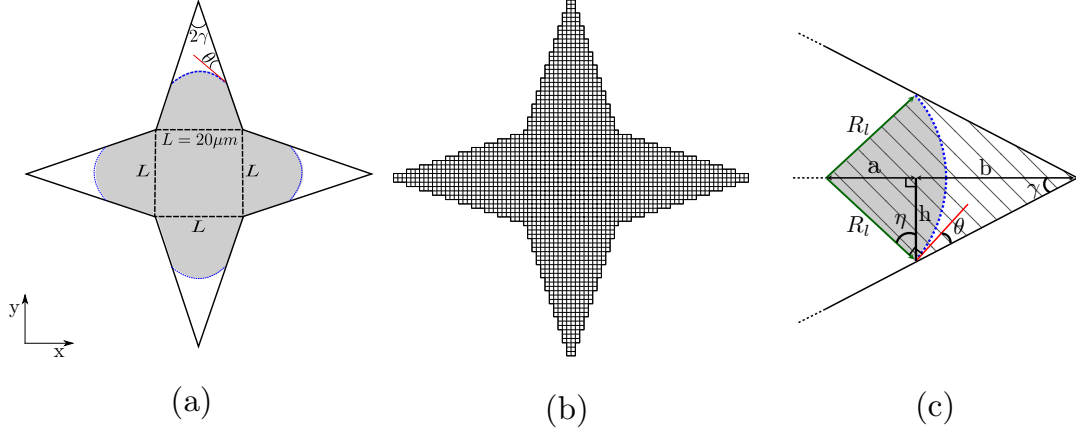


Figure 3.6. A schematic visualization of a two-dimensional star-shaped geometry: (a) non-wetting phase (grey) fills the centre while the wetting-phase (white) resides in corners; (b) uniform mesh of resolution $L/\delta x = 22$ with staircase-like modelling of the solid boundary, and (c) wetting layer parameters used to obtain an analytical equation for the wetting layer area, A_l . It is obtained by subtracting the grey area from the shaded area, Equation (3.7). $a = R_l \sin \eta$, $b = R_l \cos \eta / \tan \eta$, $h = R_l \cos \eta$ and $\eta = \theta + \gamma$. The corner angle, 2γ , is the same for all corners. θ is the equilibrium contact angle and L is the characteristic length (fixed and equal to $20 \mu\text{m}$) for the geometry.

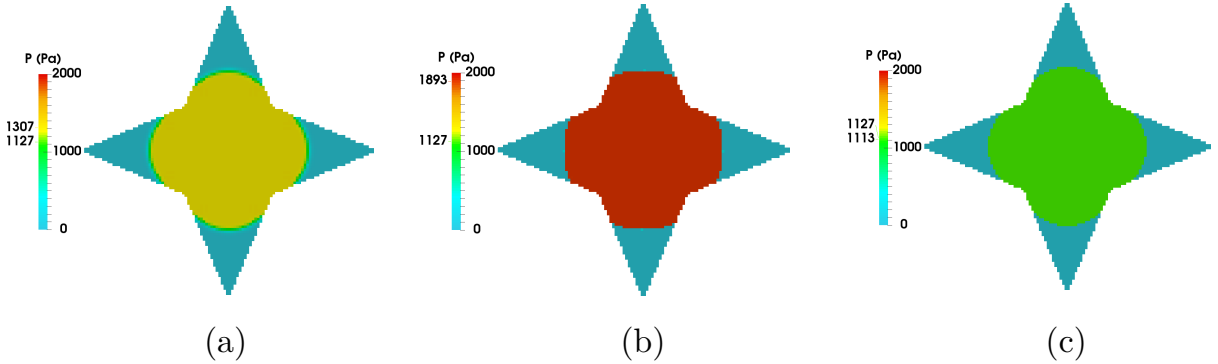


Figure 3.7. Sample visualizations of the computed pressure field at dimensionless time $t_d = 2.5$, Equation (3.2), for a corner angle of $2\gamma = 45^\circ$, an equilibrium contact angle of $\theta = 30^\circ$, and a mesh resolution of $L/\delta x = 8$: (a) the CSF method, (b) the SSF method, and (c) the CLSF method. The computed pressure jumps across the interface for the CSF, SSF and CLSF methods are 1307 Pa, 1893 Pa and 1113 Pa, respectively. The analytical value of the pressure jump across the interface for this case is 1127 Pa.

Table 3.2.

Errors in the maximum velocity, $L_\infty(\mathbf{u})$, Equation (3.3), and normalized error in the pressure jump across the interface, $E_n(\Delta P)$, Equation (3.5), for different mesh resolutions ($L/\delta x$), corner angles (2γ), and equilibrium contact angles (θ).

$\frac{L}{\delta x}$	$2\gamma(^{\circ})$	$\theta(^{\circ})$	CSF		SSF		CLSF	
			$L_\infty(\mathbf{u})$ (m/s)	$E_n(\Delta P)$	$L_\infty(\mathbf{u})$ (m/s)	$E_n(\Delta P)$	$L_\infty(\mathbf{u})$ (m/s)	$E_n(\Delta P)$
4	45	30	1.01×10^{-2}	0.199	4.78×10^{-10}	0.696	5.84×10^{-14}	0.073
4	45	60	2.48×10^{-3}	0.432	4.11×10^{-6}	0.161	1.52×10^{-14}	0.049
4	60	30	9.90×10^{-3}	0.225	3.47×10^{-2}	0.574	1.34×10^{-14}	0.071
4	60	60	2.55×10^{-3}	0.454	5.78×10^{-3}	0.848	1.29×10^{-14}	0.042
8	45	30	1.63×10^{-2}	0.120	4.45×10^{-11}	0.325	8.96×10^{-14}	0.062
8	45	60	3.02×10^{-3}	0.344	8.57×10^{-11}	0.372	5.09×10^{-14}	0.018
8	60	30	1.39×10^{-2}	0.178	3.51×10^{-6}	0.317	6.59×10^{-14}	0.068
8	60	60	2.51×10^{-3}	0.494	5.46×10^{-11}	0.460	1.62×10^{-14}	0.027
16	45	30	1.54×10^{-2}	0.108	1.12×10^{-3}	0.527	7.47×10^{-14}	0.008
16	45	60	6.99×10^{-3}	0.227	3.28×10^{-11}	0.282	4.89×10^{-14}	0.001
16	60	30	2.30×10^{-2}	0.026	9.13×10^{-5}	0.247	8.13×10^{-14}	0.055
16	60	60	7.89×10^{-3}	0.511	2.37×10^{-11}	0.399	1.06×10^{-14}	0.012
32	45	30	9.34×10^{-2}	0.045	1.25×10^{-11}	0.018	4.59×10^{-14}	0.006
32	45	60	1.44×10^{-2}	0.356	1.23×10^{-11}	0.372	3.18×10^{-14}	0.011
32	60	30	8.56×10^{-2}	0.058	2.12×10^{-2}	0.043	6.93×10^{-14}	0.007
32	60	60	1.46×10^{-2}	0.505	1.79×10^{-11}	0.430	1.78×10^{-14}	0.006

3.2. Dynamic test cases

To complete our numerical investigations, we study two sets of dynamic test cases including (a) a moving droplet in a uniform velocity field (in two and three dimensions), and (b) two-dimensional moving contact lines in micro-channels.

The moving droplet test case is selected to test the ability of our method to conserve zero total force on a closed interface as the indicator function is advected through the domain. This property is crucial, especially for capillary-dominated flows, where even a small error in the computation of interfacial forces can lead to a non-physical solution.

The moving meniscus test case is considered to check the accuracy and stability of the new method to model the dynamics of immiscible fluid displacement in the presence of a moving contact line.

3.2.1. Moving droplet

We model the steady movement of a liquid droplet of radius $R = 10 \mu\text{m}$ in a uniform velocity field and with zero gravity. Theoretically, the droplet should move with the same velocity as the underlying uniform velocity field, and the pressure jump across the interface is $\Delta P = \sigma/R = 3000 \text{ Pa}$ and $\Delta P = 2\sigma/R = 6000 \text{ Pa}$ for two and three dimensions, respectively.

First, we investigate the effect of the velocity field, U_{flow} , on the movement of the droplet in a two-dimensional domain with a uniform grid of resolution $R/\delta x = 16$.

Figure 3.8 depicts the predicted dimensionless droplet velocity, $Ca_{\text{droplet}} = U_{\text{droplet}}\mu/\sigma$, for different dimensionless flow velocities, $Ca_{\text{flow}} = U_{\text{flow}}\mu/\sigma$, as a function of a dimensionless time, t_d :

$$t_d = \left(\frac{\mu U}{\rho D^3} \right)^{0.5} t, \quad (3.8)$$

here $U = U_{\text{flow}}$ and D is the diameter of the droplet. It is clear that the CLSF method is able to predict the movement of the droplet accurately for capillary numbers as low as 10^{-5} . Some relatively small fluctuations in the droplet velocity can be observed for $Ca_{\text{flow}} = 10^{-4}$ and $Ca_{\text{flow}} = 10^{-5}$. $Ca_{\text{flow}} = 10^{-2}$ is the lowest capillary number for which the CSF and SSF methods can predict the movement of the droplet accurately. For capillary numbers lower than 10^{-2} , the error in the computation of interfacial forces in the CSF and SSF methods causes the violation of the zero net force constraint on the closed interface. This error manifests itself as large spurious currents which leads to the deviation of the droplet velocity from the theoretical value.

Figure 3.9 shows the initial configuration of the droplet and velocity vector plots and their computed values for $Ca_{\text{flow}} = 10^{-4}$ at $t_d = 6$ using different methods. One can observe that for the CSF and SSF methods the droplet is not able to move due to high spurious currents caused by error accumulation in front of the droplet. The related indicator function and pressure field are shown in Figure 3.10 for the CLSF method. The pressure jump across the interface of the droplet accurately matches the analytical value of 3000 Pa.

Next, we test the same moving droplet in three dimensions with a uniform grid of resolution $R/\delta x = 16$ for the CSF, SSF and CLSF methods. Figure 3.11 shows the dimensionless average velocity of the droplet, Ca_{droplet} , as a function of dimensionless time t_d for three different velocities using the CSF, SSF and CLSF methods. Similar to the two-dimensional simulations, the CLSF formulation can model the movement of the droplet for two orders of magnitude lower capillary number ($Ca_{\text{flow}} = 10^{-4}$) compared to that of the CSF and SSF methods ($Ca_{\text{flow}} = 10^{-2}$).

Figure 3.12 shows snapshots of the velocity vector plot, the indicator function profile and computed pressure field through a centre plane at dimensionless time $t_d = 3$. In the CLSF method the predicted pressure jump across the interface is highly accurate.

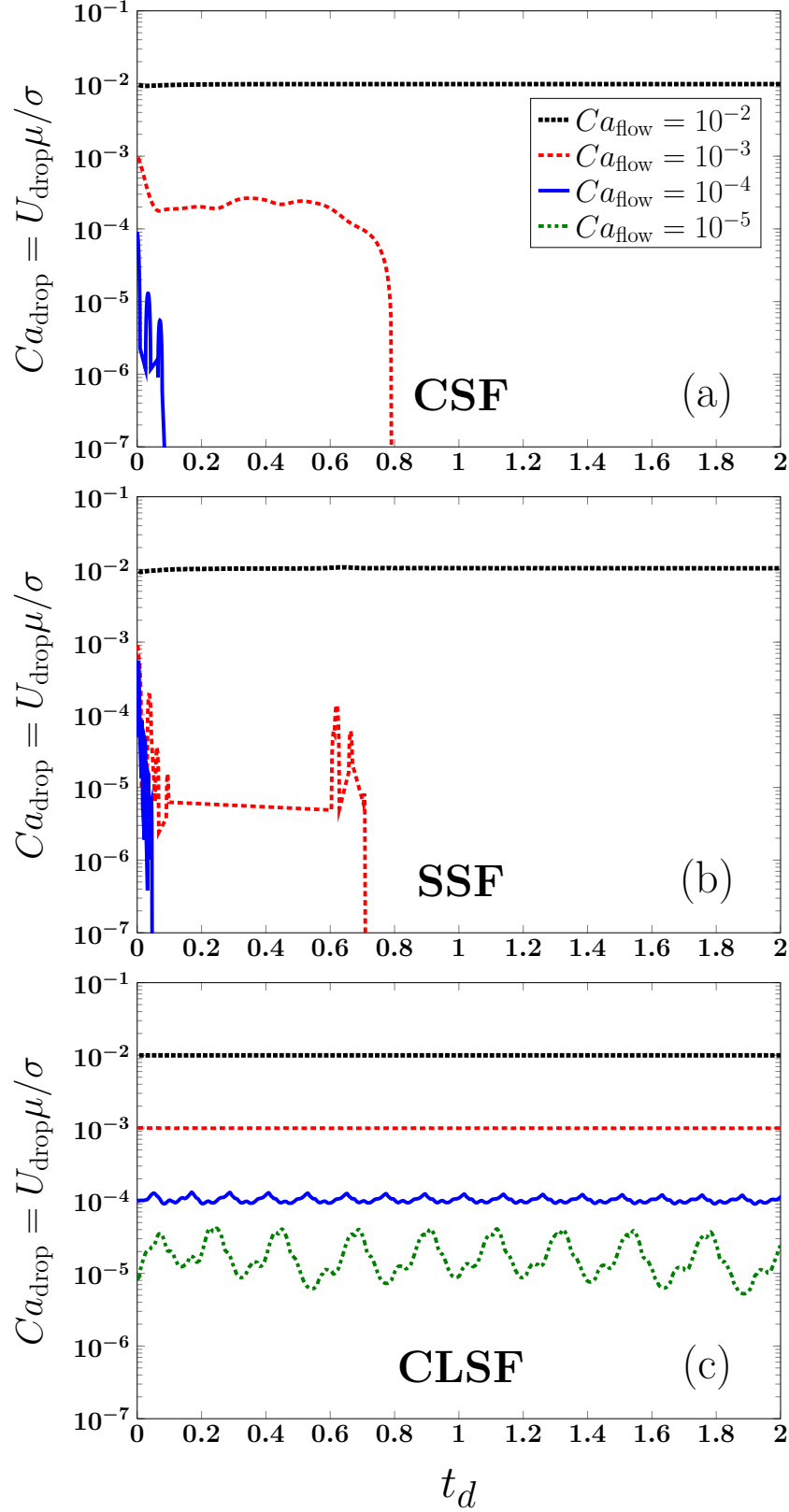


Figure 3.8. Dimensionless average droplet velocity, Ca_{droplet} , as a function of dimensionless time, t_d , Equation (3.8), for a two-dimensional droplet moving in a uniform velocity field with different values of dimensionless velocity flow, Ca_{flow} , when the interfacial force is modelled using: (a) the CSF method, (b) the SSF method, and (c) the CLSF method. The mesh is uniform and has a resolution of $R/\delta x = 16$.

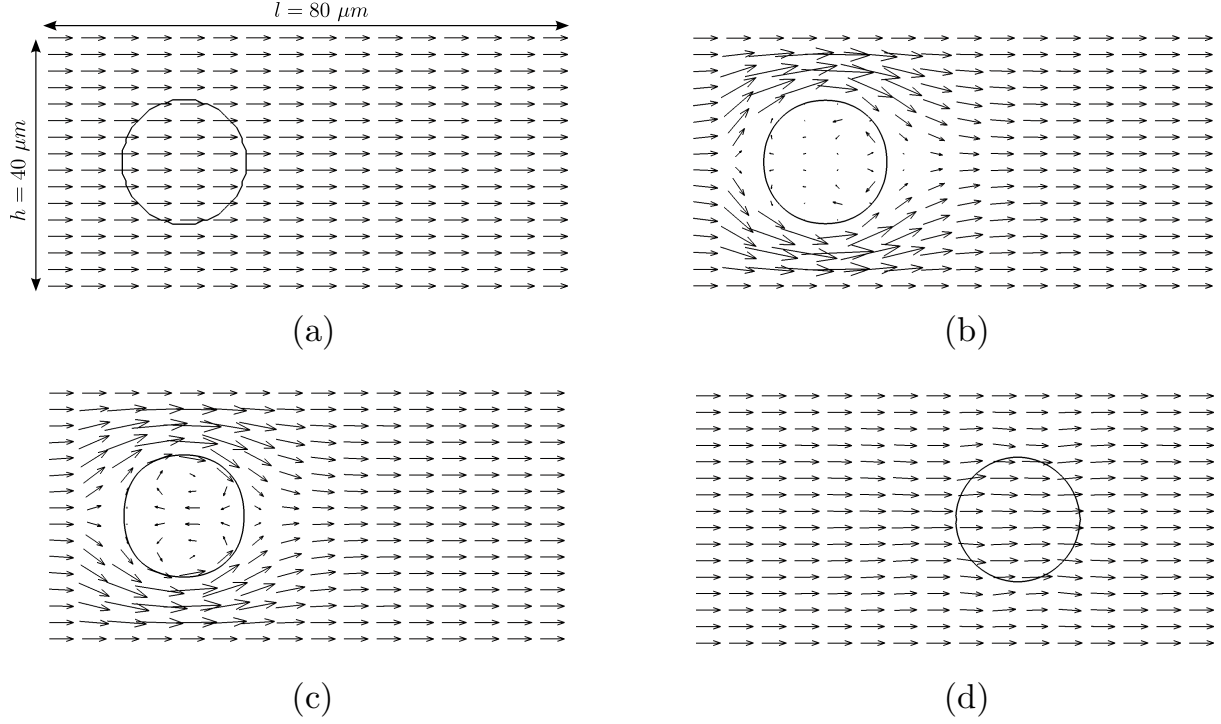


Figure 3.9. A sample visualization of a two-dimensional simulation of a droplet moving in a uniform velocity field with $U_{\text{flow}} = 0.003$ m/s equivalent to a capillary number of 10^{-4} . Shown in (a) is the initial shape and position of the droplet ($\alpha = 0.5$ contour-line). Shown in (b), (c) and (d) are velocity vector plot and position of the droplet at dimensionless time $t_d = 6$, Equation (3.8), using the CSF, SSF and CLSF methods, respectively. The mesh is uniform and has a resolution of $R/\delta x = 16$.

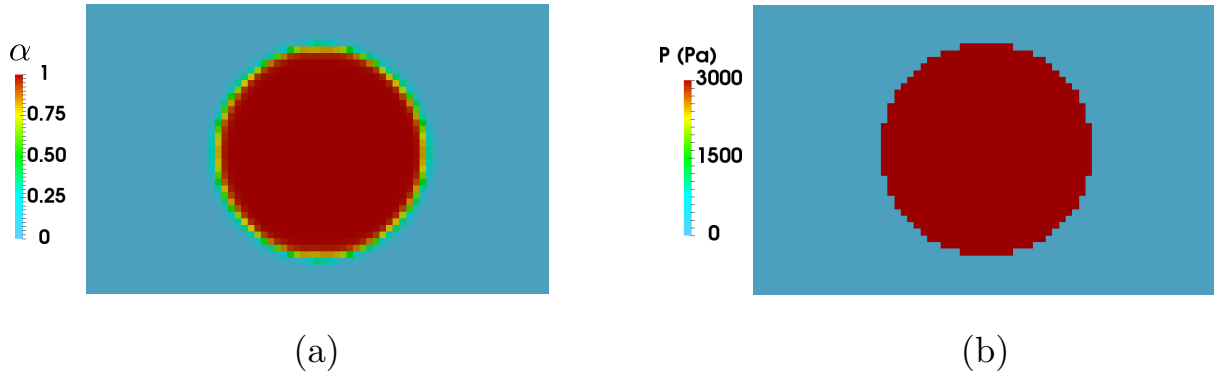


Figure 3.10. A sample visualization of: (a) indicator function, α , and (b) computed pressure field using the CLSF method at dimensionless time $t_d = 6$, Equation (3.8), for a droplet moving in a uniform velocity field with $U_{\text{flow}} = 0.003$ m/s. The mesh is uniform and has a resolution of $R/\delta x = 16$. The analytical value of the pressure jump across the interface is 3000 Pa.

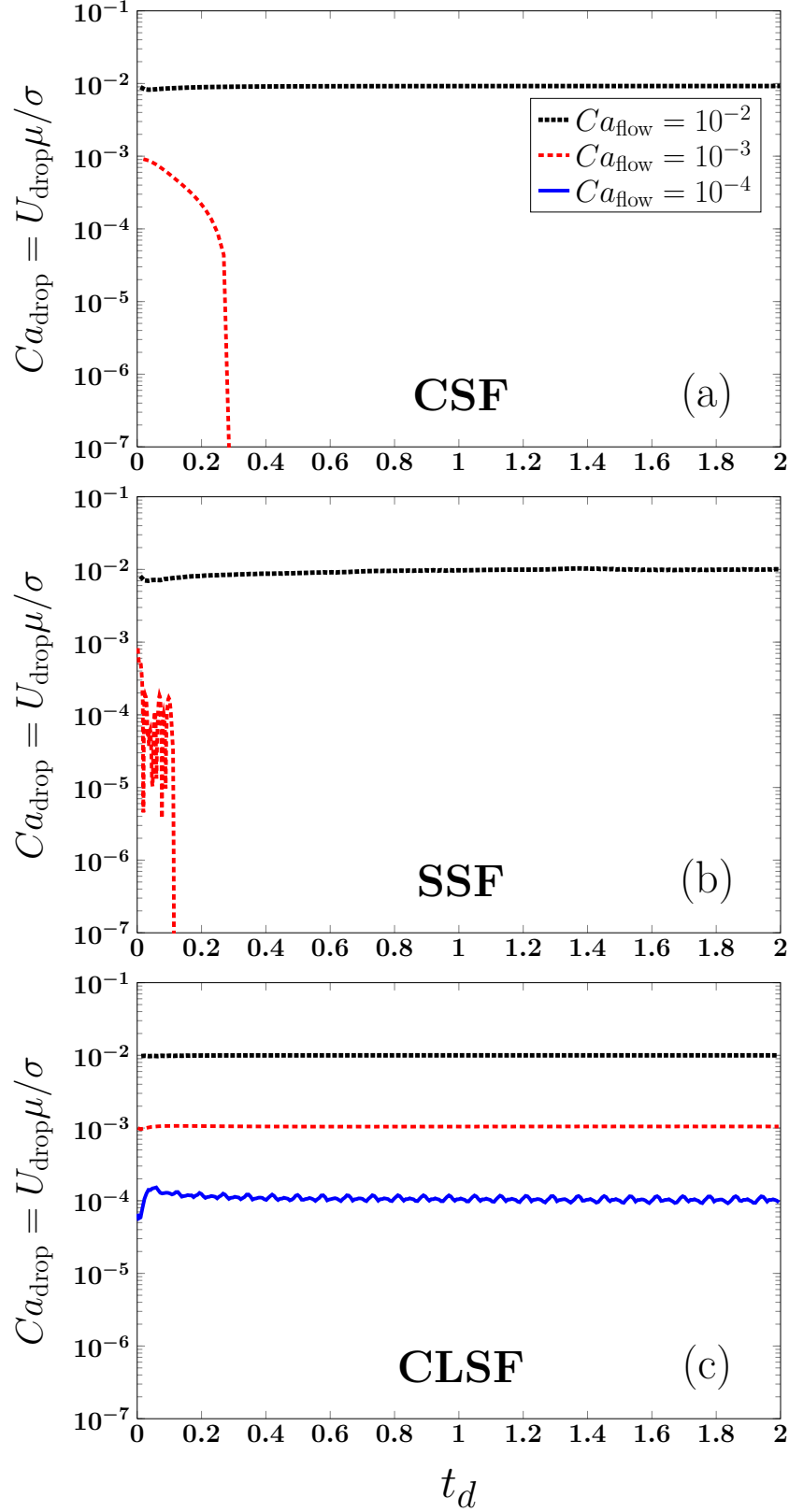


Figure 3.11. Dimensionless average droplet velocity, Ca_{droplet} , as a function of dimensionless time, t_d , Equation (3.8), for a three-dimensional droplet moving in a uniform velocity field with different values of dimensionless velocity, Ca_{flow} , when the interfacial force is modelled using: (a) the CSF method, (b) the SSF method, and (c) the CLSF method. The mesh is uniform and of resolution $R/\delta x = 16$.

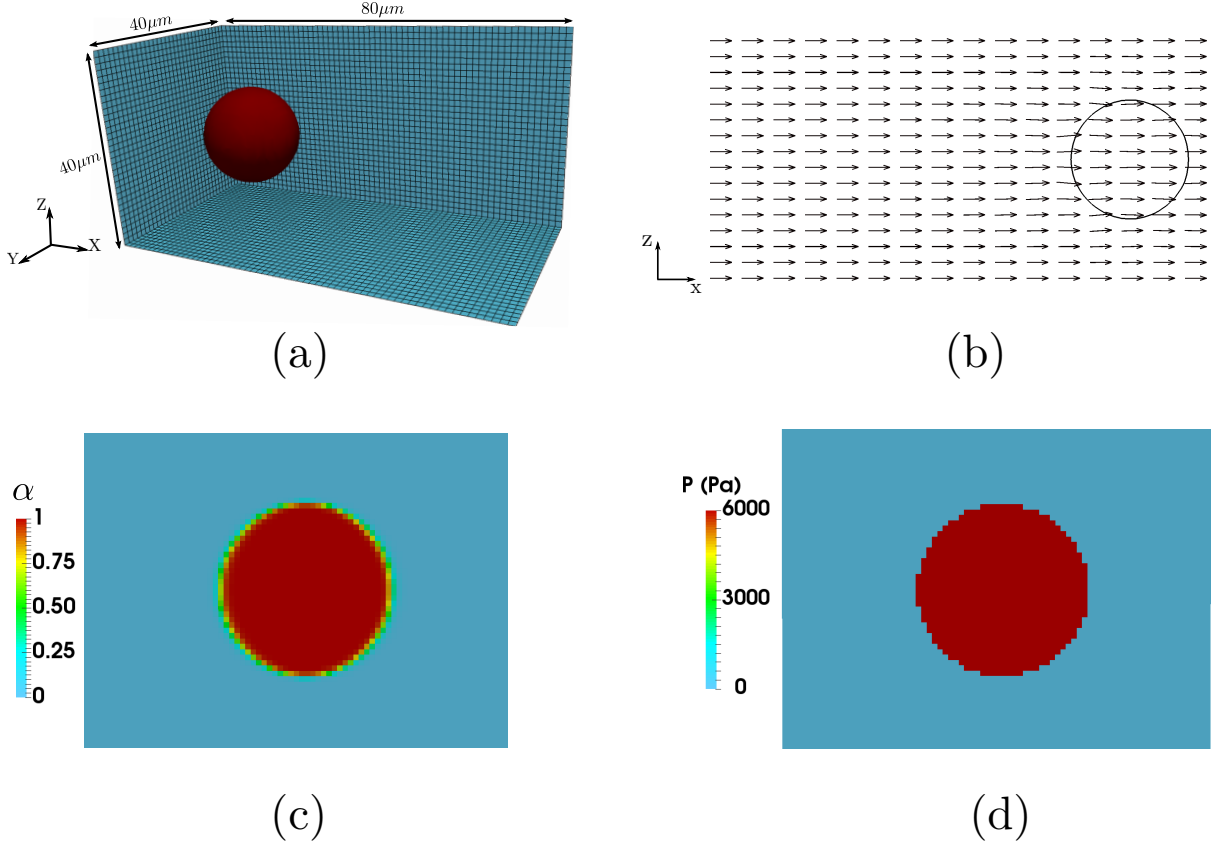


Figure 3.12. A sample visualization of a three-dimensional simulation of a moving droplet in a uniform velocity field of $U_{\text{flow}} = 0.03 \text{ m/s}$ equivalent to capillary number of 10^{-3} using the CLSF method. Shown in (a) is the initial position of the droplet ($\alpha = 0.5$). (b), (c) and (d) are snapshots of respectively, the velocity vector, the indicator function (α), and the computed pressure through a centre plane perpendicular to the flow direction at dimensionless time $t_d = 3$, Equation (3.8). The mesh has a uniform resolution of $R/\delta x = 16$.

Finally, we compute the relative error in the average velocity of the two- and three-dimensional moving droplets, $\bar{U}_{\text{droplet}}$. Figure 3.13 depicts the error in $\bar{U}_{\text{droplet}}$ over a period time of $t_d = 2$, as a function of mesh resolution, for different capillary numbers,

$$E(\bar{U}_{\text{droplet}}) = \frac{|\bar{U}_{\text{droplet}} - U_{\text{flow}}|}{U_{\text{flow}}}. \quad (3.9)$$

The solution exhibits a positive convergence for relatively high capillary numbers, $Ca_{\text{flow}} = 10^{-2}$ and $Ca_{\text{flow}} = 10^{-3}$, for both two- and three-dimensional test cases. However, the order of convergence decreases as the capillary number decreases and we need finer meshes to obtain a solution within an acceptable error range. For the two- and three-dimensional dimensional moving droplet, the lowest capillary numbers for which the solution gives a stable and fairly accurate solution (error less than 20%) are, respectively, $Ca_{\text{flow}} = 10^{-5}$ and $Ca_{\text{flow}} = 10^{-4}$.

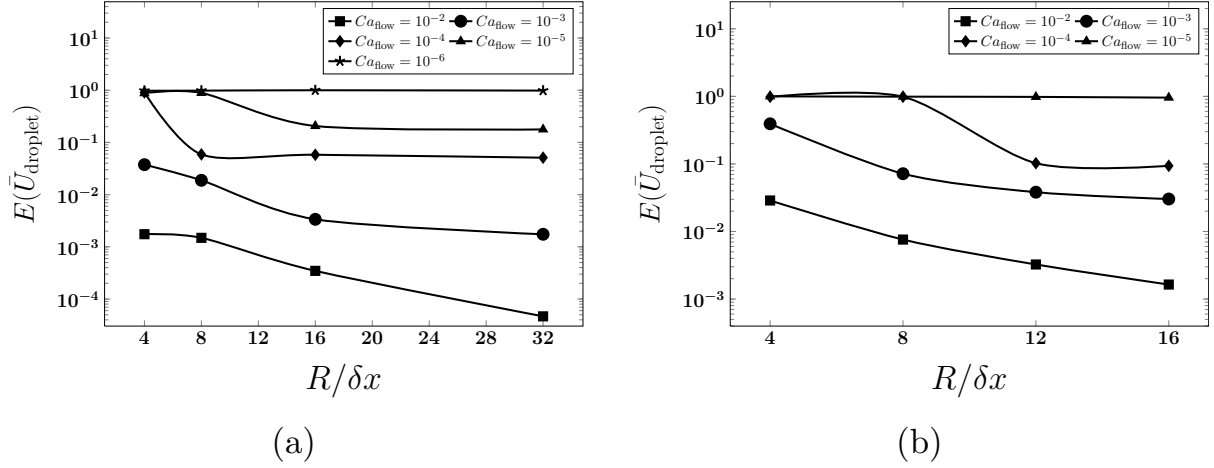


Figure 3.13. Plots of relative error in average velocity, $\bar{E}(U_{\text{droplet}})$, Equation (3.9), of (a) a two-dimensional moving droplet, and (b) a three-dimensional moving droplet, as a function of mesh resolution, $R/\delta x$, for different capillary numbers, Ca_{flow} .

3.2.2. Moving contact-line

One of the most important characteristics of immiscible two-phase flow through porous media is the presence of three-phase contact lines where the three phases (fluid–fluid–solid) are in contact. Therefore, testing the ability of our numerical method to model contact line dynamics is crucial.

Here, a two-dimensional micro-channel of width $D = 20 \mu\text{m}$, as shown in Figure 3.14, is considered to investigate the steady movement of a contact line. A no-slip boundary condition is applied at the solid walls while the velocity at the inlet is set to a uniform fixed value in the x-direction. We apply a zero-gradient boundary condition for the pressure on all the boundaries and for the velocity at the outlet. The solid boundaries are assumed to be perfectly flat and homogeneous having a fixed equilibrium contact angle of $\theta = 30^\circ$. First, we investigate the contact line dynamics when the wetting phase displaces the non-wetting phase for several steady injection velocities, U_{inj} , at the inlet, using a uniform grid of resolution $D/\delta x = 32$.

A sample visualization of the velocity vector field and the shape of the interface ($\alpha = 0.5$) at dimensionless time $t_d = 0.5$, for the case when wetting fluid is injected at an injection capillary number of $Ca_{\text{inj}} = U_{\text{inj}}\mu/\sigma = 10^{-3}$, is shown in Figure 3.14. The dimensionless time is defined based on Equation (3.8) where $U = U_{\text{inj}}$ and D is the width of the channel.

Figure 3.15a shows the dimensionless average velocity of the interface, $Ca_{\text{interface}}$, as a function of dimensionless time t_d for a range of injection capillary numbers, Ca_{inj} . The interface translates accurately and its average displacement velocity is the same as the injection velocity. This implies that the numerical method is mass conservative and the effect of spurious currents on the overall displacement of the interface is insignificant.

However, in our simulations, we observe that the contact line does not translate perfectly smoothly and experiences a periodic stick–slip motion, which introduces some small velocity

fluctuations. The error resulted from these numerical spikes is quantified by using the following L_2 error norm:

$$L_2(Ca) = L_2(Ca_{\text{interface}} - Ca_{\text{inj}}), \quad (3.10)$$

and depicted as a function of dimensionless time t_d in Figure 3.15b. The results suggest that the L_2 error norm increases as the capillary number decreases; however, the numerical errors do not introduce significant errors in the overall shape and movement of the interface.

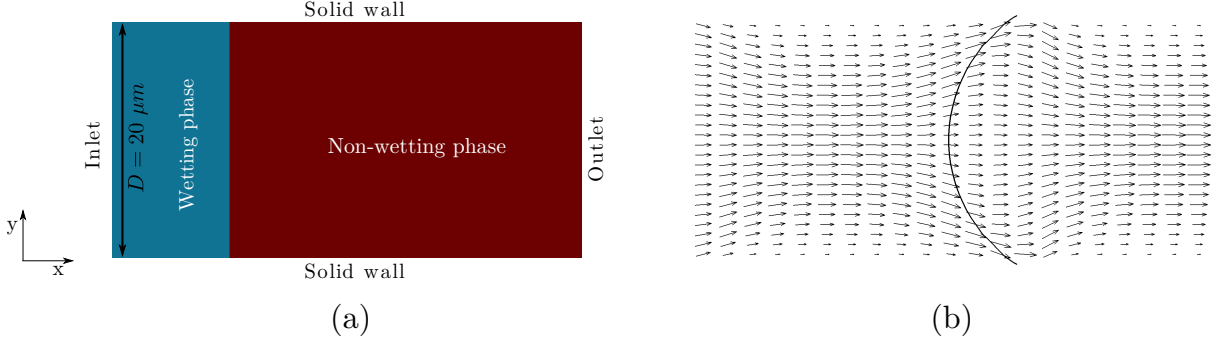


Figure 3.14. Plots of (a) initial configuration of wetting (blue) and non-wetting (red) liquids in a two-dimensional micro-channel of width $D = 20 \mu\text{m}$, and (b) a snapshot of the velocity vector field and the interface shape ($\alpha = 0.5$ contour-line) at dimensionless time $t_d = 0.5$. The interface translates steadily through the micro-channel at dimensionless injection velocity of $Ca_{\text{inj}} = 10^{-3}$. The mesh resolution is $D/\delta x = 32$. The contact angle is $\theta = 30^\circ$ for all the solid boundaries and interfacial forces are computed using the CLSF method.

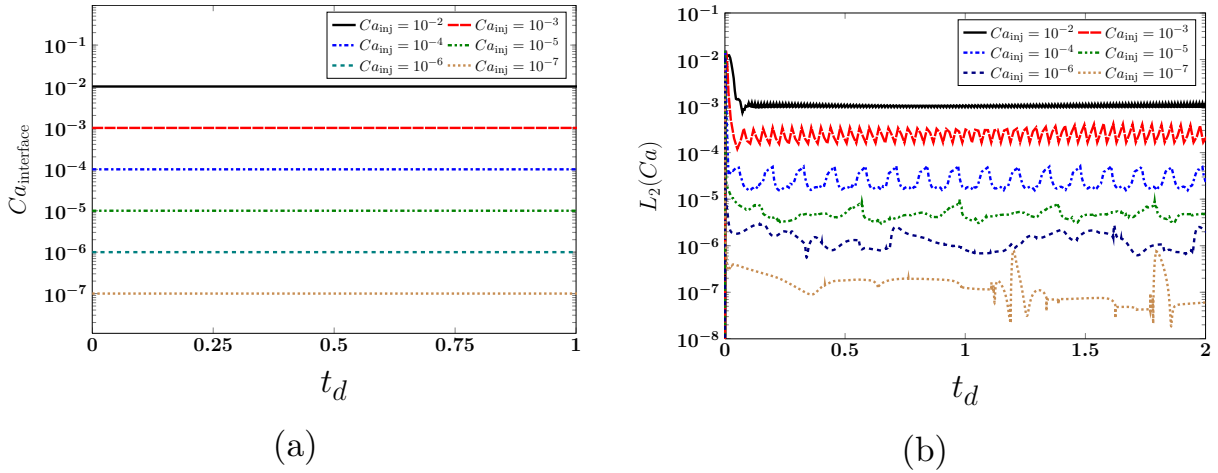


Figure 3.15. Plots of (a) the dimensionless average interface velocity, $Ca_{\text{interface}}$, and (b) $L_2(Ca)$, Equation (3.10), as a function of the dimensionless time, t_d , for steady contact line displacement in a micro-channel. The computational grid is a two-dimensional uniform mesh of resolution $D/\delta x = 32$. The contact angle is $\theta = 30^\circ$ for all the solid boundaries and the interfacial force is computed using the CLSF method.

Moreover, Figure 3.16 presents a mesh sensitivity analysis for the case with $Ca_{\text{inj}} = 10^{-3}$. It can be observed that the amplitude of the numerical spikes in the L_2 error norm decreases as

the grid is refined.

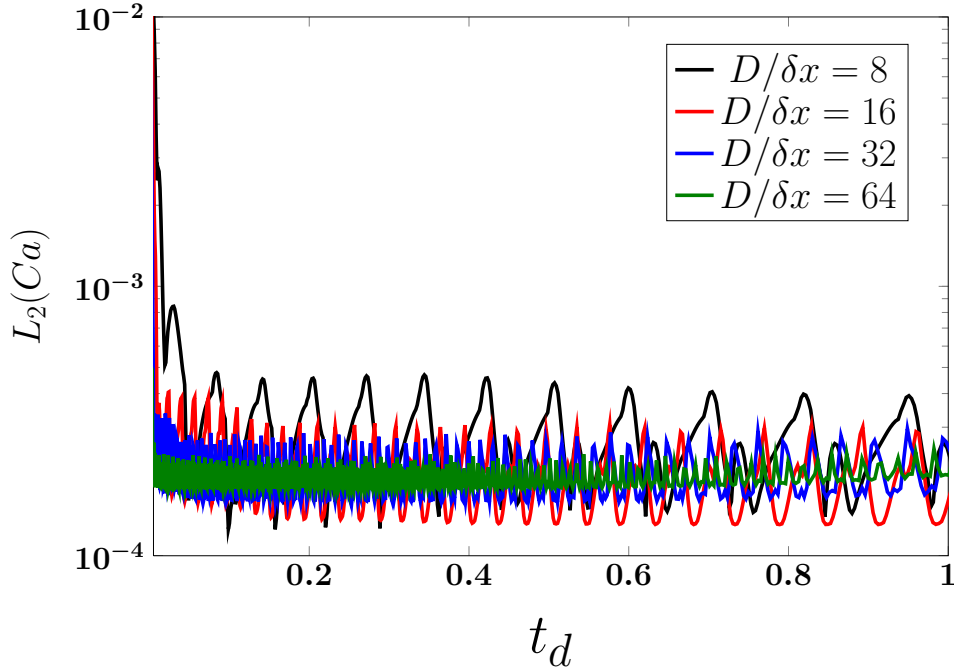


Figure 3.16. $L_2(Ca)$, Equation (3.10), as a function of the dimensionless time, t_d , for a steady contact line displacement in a micro-channel using different mesh resolutions. The contact angle is $\theta = 30^\circ$ and the interfacial force is computed using the CLSF method.

Although the assumption of perfectly smooth solid walls can be useful to simplify the study of contact line dynamics, it should not be forgotten that solid surfaces in porous rocks are usually rough. Therefore, the roughness of the solid surface can lead to physical stick-slip behaviour at the micro-scale level. As shown in Figure 3.17, the solid boundaries of the micro-channel are roughened using a triangular wave pattern characterized by roughness amplitude $A = 225$ nm and period $P = 2$ μm . The flow domain is discretized using the mesh generator from OpenFOAM (OpenFOAM, 2016) that uses a uniform initial mesh and snaps the boundary points to the solid wall, here the triangular wave roughness, so that all the solid boundary faces align with the solid wall. We also ensure that each edge of boundary faces connect to only one internal face.

Figure 3.18 compares the L_2 error norm, Equation(3.10), for the smooth and rough-wall micro-channels with $Ca_{\text{inj}} = 10^{-3}$. It is evident that the physical spikes have an amplitude of about two order of magnitudes higher than the numerical spikes in this test case.

Finally, we model the displacement of a meniscus through a three-dimensional square micro-channel, as shown in Figure 3.19. We set the equilibrium contact angle to $\theta = 60^\circ$ and keep the other simulation parameters the same as in the two-dimensional micro-channel test case.

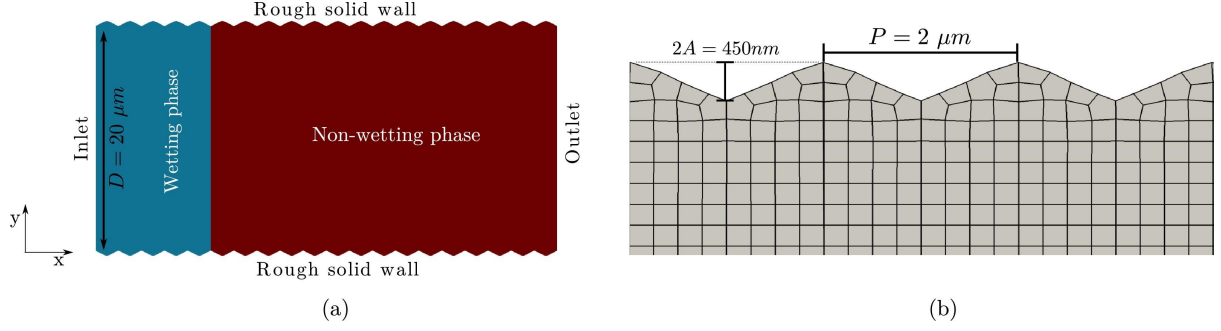


Figure 3.17. Plots of (a) initial configuration of wetting (blue) and non-wetting (red) fluids in a micro-channel of width $D = 20 \mu\text{m}$ with triangular roughness on its solid boundaries, and (b) a close-up view of the computational grid near the solid boundary. The amplitude and period of the roughness is chosen to be $A = 225 \text{ nm}$ and $P = 2 \mu\text{m}$, respectively.

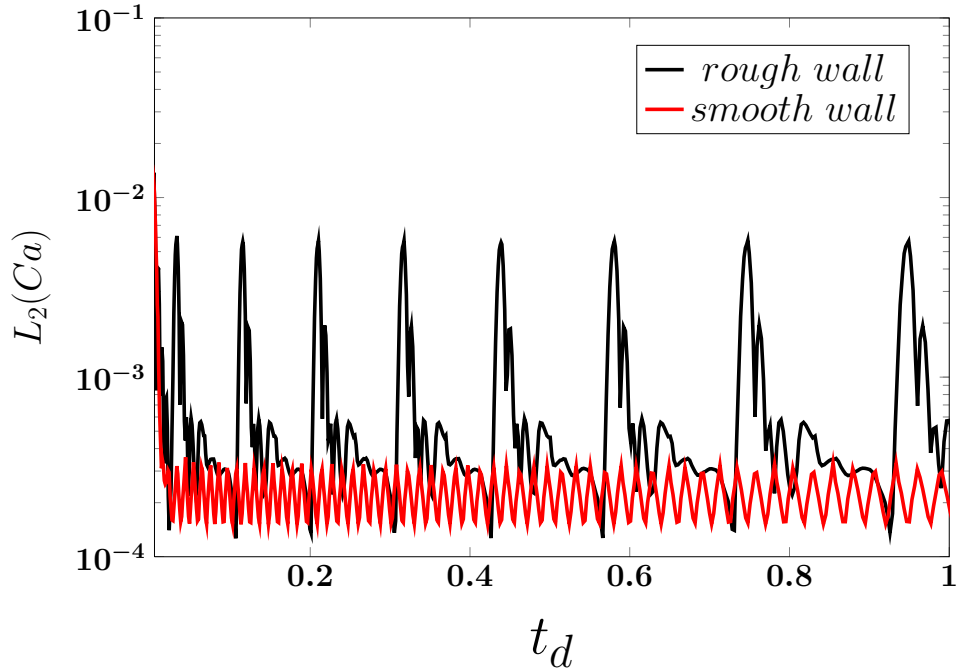


Figure 3.18. Spikes in the velocity field presented in terms of $L_2(Ca)$, Equation (3.10), as a function of the dimensionless time, t_d , for a steady contact line displacement through two-dimensional smooth and rough micro-channels on a grid of resolution $D/\delta x = 32$. The contact angle is $\theta = 30^\circ$ and the interfacial force is computed using the CLSF method.

The dimensionless average velocity of the interface, $Ca_{\text{interface}}$, and $L_2(Ca)$, Equation (3.10), as a function of dimensionless time t_d for a different range of injection capillary numbers, Ca_{inj} , are depicted in Figure 3.20. The results are similar to the two-dimensional case, and in spite of some velocity fluctuations, especially for lower capillary numbers, the interface motion is stable.

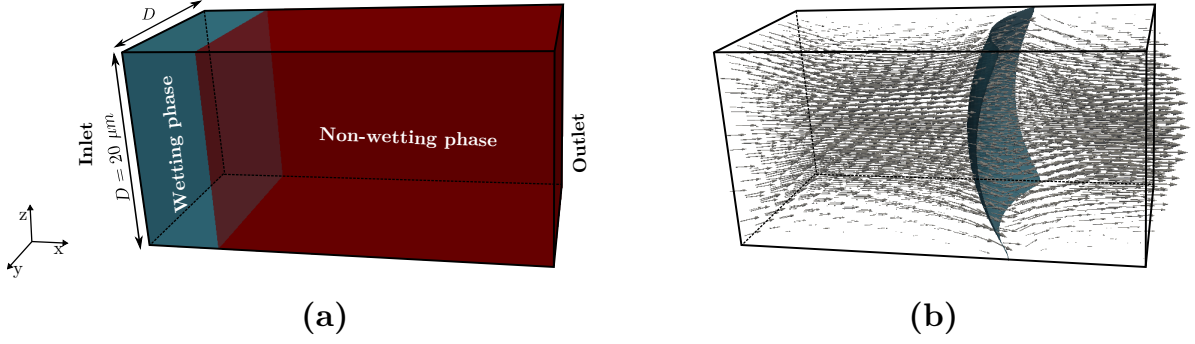


Figure 3.19. Plots of (a) initial configuration of wetting (blue) and non-wetting (red) liquids in a three-dimensional square micro-channel of width $D = 20 \mu\text{m}$, and (b) a snapshot of the velocity vector field and the interface shape ($\alpha = 0.5$ contour-line) at dimensionless time $t_d = 0.5$. The interface translates steadily through the micro-channel at dimensionless injection velocity $Ca_{\text{inj}} = 10^{-3}$. The mesh resolution is $D/\delta x = 32$. The contact angle is $\theta = 60^\circ$ for all the solid boundaries and interfacial forces are computed using the CLSF method.

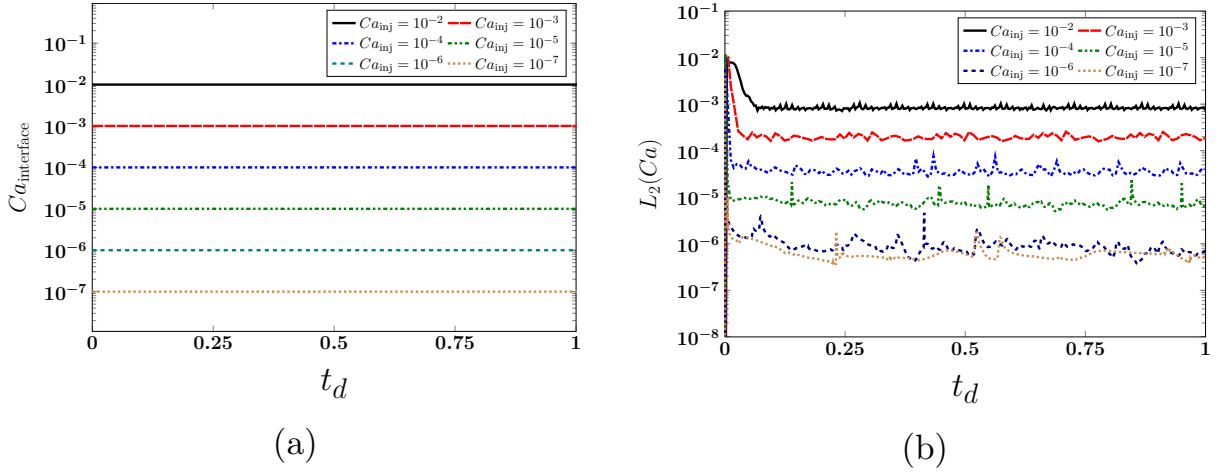


Figure 3.20. Plots of (a) the dimensionless average interface velocity, $Ca_{\text{interface}}$, and (b) $L_2(Ca)$, Equation (3.10), as a function of the dimensionless time, t_d , for steady contact line displacement through a three-dimensional square micro-channel. The computational grid is a uniform mesh of resolution $D/\delta x = 32$. The contact angle is $\theta = 60^\circ$ for all the solid boundaries and the interfacial force is computed using the CLSF method.

These results show that the CLSF method can be applied to model capillary-dominant two-phase flow in the presence of solid boundaries where the dynamics of the contact line plays an important role.

3.2.3. Corner flow

We now study two-phase flow problems typically encountered in subsurface rock geometries at the pore scale, namely flow of a wetting phase along the corners of a rock surface (Blunt and Scher, 1995). The dynamics of the corner flow of the wetting phase, especially at low capillary

numbers, plays an important role in multiphase displacement process and also in the trapping and remobilisation of the non-wetting phase (Legait, 1983; Ransohoff and Radke, 1988; Dong and Chatzis, 1995). Therefore we examine the capability of our method to model the imbibition of a wetting phase in the corners of non-circular capillary tubes.

A 60 μm square capillary tube with a length of $L = 300 \mu\text{m}$ is considered (Figure 3.21) to study the spatial convergence of the dimensionless flow resistance factor of the wetting layer, β (Ransohoff and Radke, 1988),

$$\beta = -\frac{R_l^2}{\bar{u}_x \mu} \frac{\partial p}{\partial x}, \quad (3.11)$$

where μ and $\bar{u}_x$ are the viscosity and axial average flow velocity of the wetting phase, respectively, $\partial p/\partial x$ is the pressure gradient in the wetting phase along the axial direction, and R_l is the radius of the interface curvature in the corner, calculated based on Equation (3.7), with $\gamma = \pi/4$ and $\theta = \pi/6$ as discussed in Section 3.1.2.

The initial liquid-liquid interface is a circular arc of radius $r_0 = 30 \mu\text{m}$. The flow domain is discretized by a uniform Cartesian mesh of different resolutions. The no-slip boundary condition is applied at the solid walls. At the inlet and outlet boundaries, zero-gradient boundary conditions are applied for pressure and indicator function, α . Both fluids, with the same properties, viscosities of $10^{-3} \text{ Pa}\cdot\text{s}$ and densities of $1000 \text{ kg}/\text{m}^3$, are injected at the inlet boundary in x direction, using a cyclic boundary condition; the velocity profile of the outlet boundary is replicated on the inlet boundary, with an initially uniform velocity of $U_{\text{inj}} = 0.0003 \text{ m/s}$. In addition, no surface shear viscosity between the fluid phases and no gravity are considered. The interfacial tension is $\sigma = 0.03 \text{ N/m}$ and the equilibrium contact angle is $\theta = 30^\circ$.

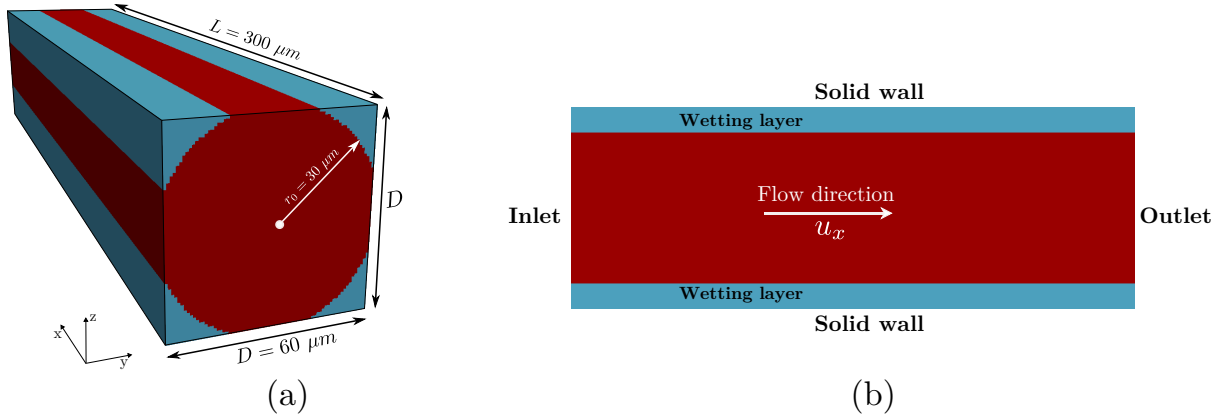


Figure 3.21. Plot of (a) initial configuration of wetting (blue) and non-wetting (red) fluids in a square capillary tube, and (b) cross-sectional view through a diagonal plane.

In the results that follow, the simulations are conducted for the whole computational domain. However, the flow resistance is calculated and analyzed for only one corner of the tube.

Figure 3.22 depicts the evolution of β as a function of time for five mesh resolutions. Through refining the mesh, the computed β converges to a value of about 52. Figure 3.22b depicts the

error in β , at time $t = 10$ ms, defined as:

$$E(\beta) = \frac{|\beta - \beta_{D/\delta x=54}|}{\beta_{D/\delta x=54}}, \quad (3.12)$$

where $\beta_{D/\delta x=54}$ is the evaluated dimensionless flow resistance on a mesh of resolution $D/\delta x = 54$. Here we observe a positive convergence behaviour for β .

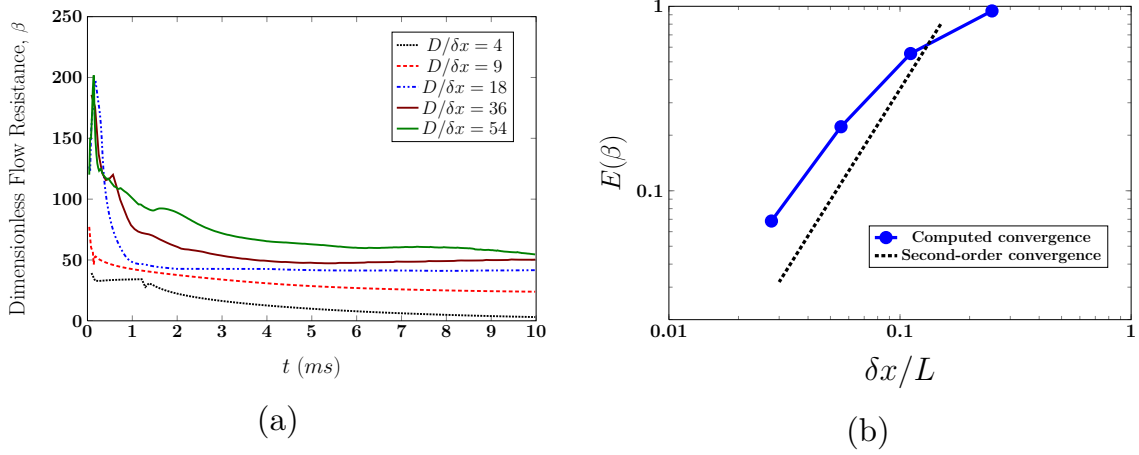


Figure 3.22. Plots of (a) the dimensionless flow resistance, β , Equation (3.11), as a function of time for different mesh resolutions, and (b) convergence of the error in β , $E(\beta)$, Equation (3.12), as a function of mesh resolution.

The computed dimensionless flow resistance in this test case, $\beta = 52$, is significantly lower than the value reported in Ransohoff and Radke (1988) for the same geometry, $\beta = 290.7$. The main reason is that the dimensionless flow resistance in Ransohoff and Radke (1988) is calculated for a gas–liquid system in which gas is assumed to be an inviscid non-wetting phase. Therefore, the stress exerted by the non-wetting phase on the wetting phase is ignored. In our example, the co-current flow of the non-wetting phase boosts the flow of the wetting phase, leading to a much lower flow resistance.

We simulate wetting layer flow on a mesh of resolution $D/\delta x = 18$ for a case where the non-wetting phase is a gas with viscosity $\mu = 10^{-5}$ Pa·s and density $\rho = 1$ kg/m³. Figure 3.23 compares the computed dimensionless resistance factor for the gas-occupied and liquid-occupied pores as a function of time. Clearly, through reducing the stress exerted by the non-wetting phase on the wetting phase in the gas-occupied system, β is increased to approximately 250, which is closer to $\beta = 290.7$ found by Ransohoff and Radke (1988). This subject is investigated in more details in Chapter 4, where we follow the approach of Ransohoff and Radke (1988) to compute the conductance of wetting layers, taking into account the viscosities of both fluids.

These results confirm that the numerical method can be used to model corner flow in non-circular capillary tubes to quantify their flow resistivity coefficients. However, the dynamics of corner flow can also be affected by fluid properties, here the viscosity of the non-wetting phase.

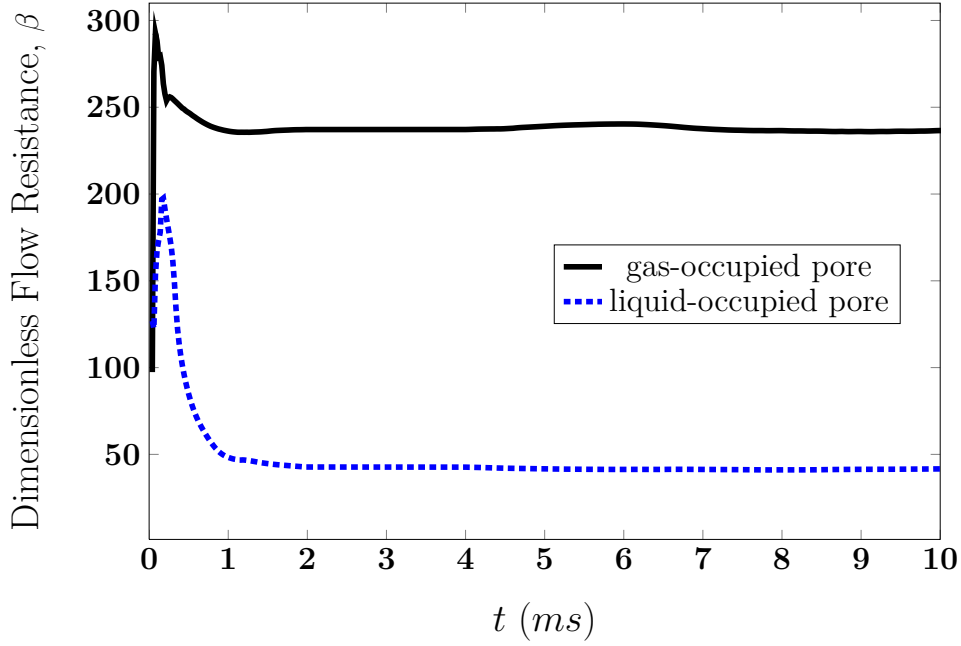


Figure 3.23. Dimensionless flow resistance, β , as a function of time for a gas-occupied pore and a liquid-occupied pore for a mesh of resolution $D/\delta x = 18$.

3.3. Closure

The stability and accuracy of the implemented scheme is validated on several two- and three-dimensional test cases, which indicate the capability of the method to model two-phase flow processes at the micro-scale.

The process of equilibration of a static droplet in two and three dimensions is simulated to demonstrate the reduction of spurious currents. The accuracy of the numerical method when liquid and solid phases come into contact is validated by modelling a wetting layer resting in the corner of a two-dimensional pore geometry with different corner and equilibrium contact angles. The ability of the model to respect zero net capillary force on closed interfaces is investigated by simulating a micro-scale moving droplet in a uniform velocity field in two and three dimensions. The dynamics of three-phase contact lines is examined by modelling the steady movement of a contact line through two- and three-dimensional micro-channels. Finally, the convergence behaviour of the method with spatial refinement is tested for corner flow of a wetting layer in a square capillary tube. Here it is demonstrated that co-current flow can lead to a greatly enhanced flow conductance when the non-wetting phase has a finite viscosity, as compared to the case where the non-wetting phase is an inviscid gas, caused by momentum transfer across the fluid-fluid interface.

Through the validation process, it is demonstrated that the explicit representation of the interface used to compute interfacial forces can efficiently eliminate the problem of spurious currents and lead to an accurate estimation of capillary pressure even for low grid resolutions.

This can be very important to model multiphase flows directly on micro-CT images of porous media for which simulations with a very fine grid resolution are prohibitively expensive using currently available computational resources.

4. Viscous coupling

4.1. Introduction

The macro-scale modelling of the processes which involve immiscible two-phase flow requires the specification of macroscopic momentum equations for each of the two fluids. These equations can be conventionally approximated as the extension of Darcy’s law to two-phase flow with relative permeabilities for each phase (Blunt, 2017). However, this traditional approach often does not take into account the viscous coupling of the fluids due to the momentum transfer across the fluid-fluid interface (Rose, 2000). The assumption of uncoupled flows of the fluids can lead to inaccurate results for those two-phase flow regimes in which the drag between fluid phases can be significant (Avraam and Payatakes, 1995a, 1999).

Several experimental and theoretical studies have reported the significance and effects of viscous coupling in two-phase flows. Whitaker (1986) employed a method of volume averaging to analyze immiscible two-phase flow. He developed a form of coupled Darcy-like equations containing additional terms that represent the influence of viscous drag exerted between fluid phases. Kalaydjian (1990) studied spontaneous counter-current flow of a non-wetting fluid ganglion by a wetting fluid in a square capillary tube. He proposed a new form of the two-phase Darcy equation in which a matrix of relative permeabilities, with equal off-diagonal terms representing the contribution of the viscous coupling, relates flow rates to pressure gradients. Avraam and Payatakes (1995b) employed a parameter estimation approach to obtain all four terms of the relative permeability matrix based upon a statistical analysis of experimental data, obtained from a set of steady-state co-current two-phase flows in a micro-model. They disputed the validity of Onsager-Casimir reciprocal relation and found that the off-diagonal coupling coefficients are not necessarily equal. Ehrlich (1993) used semi-analytical equations to study the effect of viscous coupling on relative permeabilities in two-phase flow through an idealized model of a porous medium consisting of a bundle of regular polygonal capillary tubes, suggesting that the rheology of the interface can affect the magnitude of viscous coupling.

In addition to empirical and theoretical studies, numerical simulations have been recently used to uncover mechanisms that control and describe viscous coupling effects in two-phase flow at the pore level. Various pore-scale modelling approaches, such as pore-network models (Fatt, 1956; Blunt and King, 1991), lattice Boltzmann methods (Pan et al., 2004; Shan and Chen, 1993), mesh-free Lagrangian particle methods (Tartakovsky and Meakin, 2006) and Eulerian grid-based methods (Meakin and Tartakovsky, 2009), have been employed.

Li et al. (2005) used a two-phase lattice Boltzmann model for two-phase flow through a homogeneous sphere-pack and systematically studied viscous coupling effects over a broad range of conditions, suggesting fluid-fluid interfacial area as a key parameter which can affect relative permeabilities. Dehghanpour et al. (2011) employed a high-resolution finite-element numerical method to investigate viscous coupling for sandwiched layers in angular capillaries in three-phase flow. Xie et al. (2017) proposed an improved pore-network model to accommodate viscous coupling effects and examined its efficiency through computing relative permeabilities for some

mixed- and water-wet rock samples and provided comparisons with experimental results.

Among pore-scale modelling methods, pore-network models have grown in popularity due to their computational efficiency, which enables them to study large realistic rock samples (Bryant and Blunt, 1992; Bakke and Øren, 1997; Blunt, 2001; Øren and Bakke, 2003; Van Dijke et al., 2004). However, as discussed in Chapter 1, these models rely upon a simplified representation of the pore space geometry and empirical models for hydraulic conductance and capillary entry pressure in pore/throat elements. The hydraulic conductance for each phase is a key parameter in pore-network models to relate the flow rate of a phase to pressure gradient.

Several studies have been performed to quantify and establish correlations for hydraulic conductances by relating them to pore geometry, contact angle and interface rheology. Ransohoff and Radke (1988) employed a finite-element method to model the flow of a wetting phase along corners of predominantly gas-occupied noncircular capillaries, as mentioned in the previous chapter. They quantified the relationship between the average velocity of the wetting phase in a corner, $\bar{u}$, and the pressure gradient within the phase, ∇p , as the dimensionless flow resistance, β ; see Equation (3.11). They reported the computed dimensionless flow resistance for different pore geometries, contact angles and interfacial shear viscosities.

Zhou et al. (1997) established approximate analytical solutions to relate the dimensionless flow resistance, β , to pore and interface geometry for oil flow along sandwiched layers and water flow along corners of predominantly gas-occupied noncircular capillaries. Al-Futaisi and Patzek (2003) employed a high-resolution finite-element method in conjunction with a projection-pursuit regression approach to determine analytical correlations for three-phase hydraulic conductances in angular capillaries. However, none of these models took into account the existence of viscous coupling between the flowing fluids and simply assumed that conductances were independent of viscosity ratio, i.e. uncoupled flow of the fluids.

This assumption may adversely affect the accuracy of pore-network models when used to predict macroscopic flow properties such as relative permeabilities. Therefore, it is important to establish reliable hydraulic conductance correlations that respect the existence of viscous coupling between the two fluids and incorporate them into pore-network models. To do so, one can perform direct numerical simulations on various two-phase fluid configurations in single micro-scale capillaries to calculate generalized mobilities of each fluid, stabilized by capillary forces. Then, this information can be exploited to find mathematical expressions which can be incorporated into two-phase pore-network models in the form of hydraulic conductivities.

In this chapter, we employ our new numerical method to examine the role of momentum transfer across the fluid-fluid interface in two-phase flow. In Section 4.2, we validate the accuracy of the numerical method to capture this momentum transfer. In Section 4.3, we perform two-phase direct numerical simulations on square, triangular and star-shaped pore geometries with uniform and non-uniform wettability conditions. The simulation results are then used to investigate viscous coupling effects as a function of the viscosity ratio, the wetting phase saturation and the wettability. We demonstrate that viscous coupling effects can be significant

for certain pore geometries such as oil layers sandwiched between water in the corner of mixed wettability capillaries. In Section 4.4, we present simple parametric models to estimate general mobility terms as a function of geometric properties and viscosity ratio. These models are validated by comparison with the mobilities computed using direct numerical simulation. Finally, in Section 4.5, we simulate an imbibition process through a three-dimensional nonuniform capillary tube to demonstrate the capability of our numerical model to simulate layer flow in more complex geometries.

4.2. Viscous coupling validation

Here, we validate the accuracy of the numerical model to compute the momentum transfer across the interface due to viscous coupling. Representing the interface as a discontinuity in fluid properties makes it possible to capture the viscous coupling implicitly rather than imposing kinematic and dynamic boundary conditions at prescribed interfaces.

We simulate immiscible co-current two-phase flow through a three-dimensional square tube where a non-wetting phase, fluid 2, flows in the centre of the tube while the wetting-phase, fluid 1, moves along the corners of the capillary (see Figure 4.1). Simulations are performed for three viscosity ratios with different mesh resolutions. Computed velocity fields are then compared against the semi-analytical solution given by Ehrlich (1993). The details of this semi-analytical solution are presented in Appendix A.

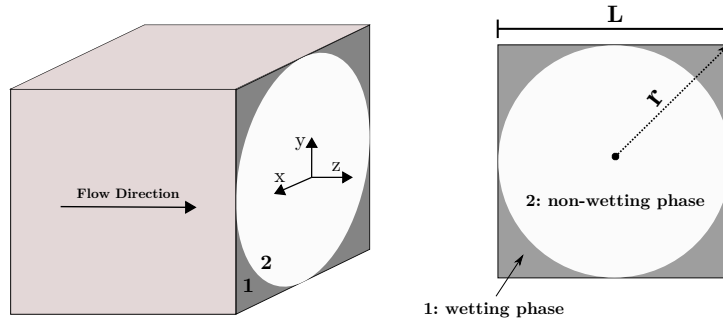


Figure 4.1. Schematic illustration of steady-state co-current two-phase flow in a square capillary tube and cross-sectional configuration of the wetting phase, fluid 1, and the non-wetting phase, fluid 2.

The flow domain is a cubic square of side $L = 20 \mu m$, predominantly filled with fluid 2 while fluid 1 resides in the corners. The volumetric saturation of the wetting fluid is $s_1 = 0.2146$. The computational mesh is uniform Cartesian, equal grid spacing $\delta x = \delta y = \delta z = h$, with mesh resolutions of $L/h = 12, 24, 48$, and 72 . We apply no-slip boundary conditions on the solid walls with a constant contact angle of zero measured through the wetting phase. Periodic boundary conditions are applied in the flow direction along the z -axis. The dynamic viscosity ratios, $M = \mu_1/\mu_2$, are chosen to be 0.1 ($\mu_1 = 0.1\mu_2 = 10^{-3}$ Pa.s), 1 ($\mu_1 = \mu_2 = 10^{-3}$ Pa.s), and 10 ($\mu_1 = 10\mu_2 = 10^{-2}$ Pa.s); the density ratio is 1 with $\rho_1 = \rho_2 = 1000$ kg/m³. The

interfacial tension is $\sigma = 0.03$ N/m and no interfacial shear viscosity at the fluid-fluid interface is considered. Constant body forces, $\xi_1 = \xi_2 = 10$ Pa/m, are imposed, along the z -axis, for both fluids to reach a steady-state flow through the tube.

Figure 4.2 compares the steady-state profiles of simulated axial velocity against the semi-analytical solution, along the diagonal of the square capillary tube, r , for various mesh resolutions and viscosity ratios.

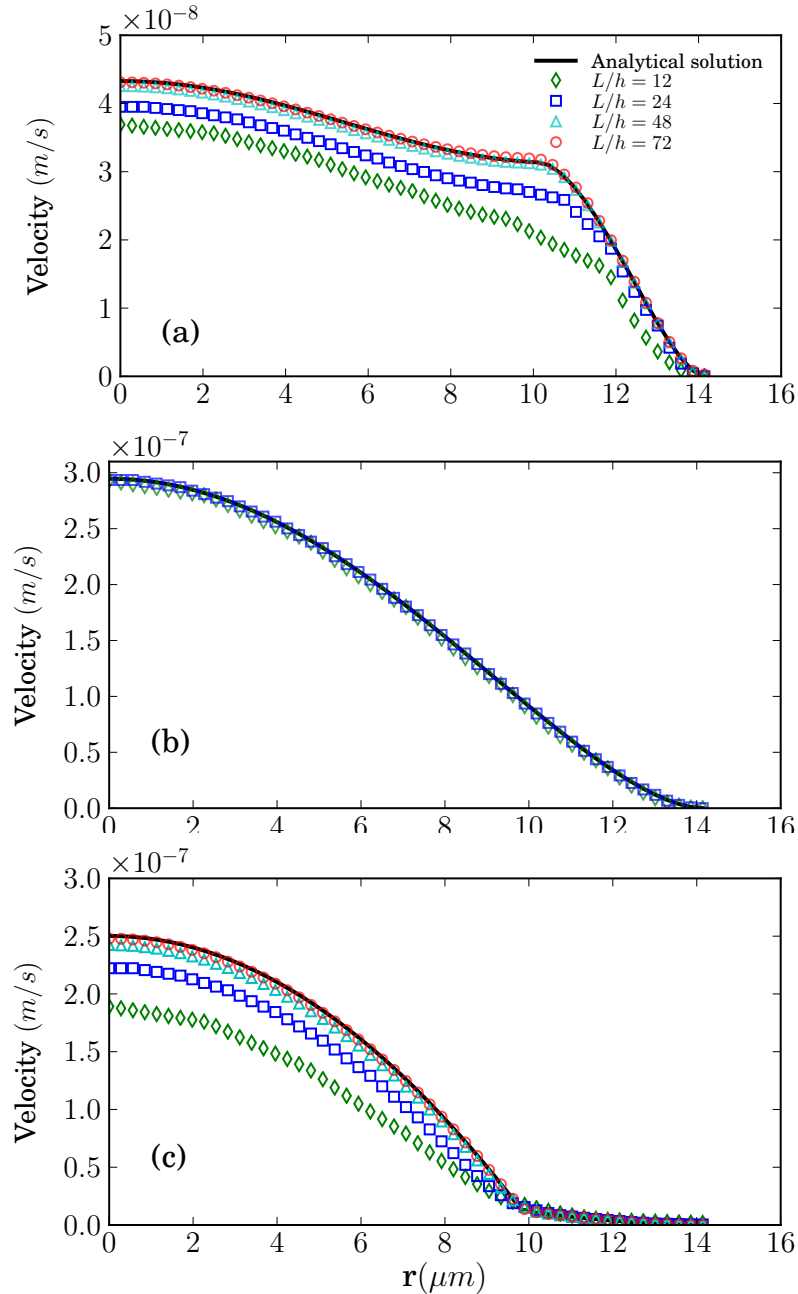


Figure 4.2. Axial velocity profiles for co-current two-phase flow along the diagonal of a square capillary tube as a function of mesh resolution in comparison to the semi-analytical solution for viscosity ratios, $M = \mu_1/\mu_2$: (a) $M = 0.1$, (b) $M = 1$, and (c) $M = 10$.

For $M = 1$, there is a good agreement between the numerical and the theoretical solutions even for a mesh resolution as low as $L/h = 12$. However, for $M = 0.1$ and $M = 10$, to obtain a velocity field in agreement with the semi-analytical solution, we require higher mesh resolutions to resolve the discontinuity of the fluid properties at the fluid-fluid interface accurately.

For a better comparison, we define the normalized error of the velocity field in a cross-section perpendicular to the flow, the $x - y$ cross-section, by

$$E(u_z) = \frac{\sum |u_z - u_z^*|}{\sum u_z^*}, \quad (4.1)$$

where u_z and u_z^* are, respectively, the numerical and semi-analytical values of velocity normal to the $x - y$ cross-section, and the summation is performed over all the faces of the cross-section.

Figure 4.3 plots the error versus mesh resolution for different viscosity ratios. According to this plot, the numerical method exhibits a second-order convergence rate when $M = 1$. However, for the viscosity ratios other than 1, $M = 0.1$ and $M = 10$, the convergence rate decreases. Therefore, to perform accurate simulations for varying viscosity ratios, the mesh resolution is chosen to be $L/h = 72$ for the rest of this study.

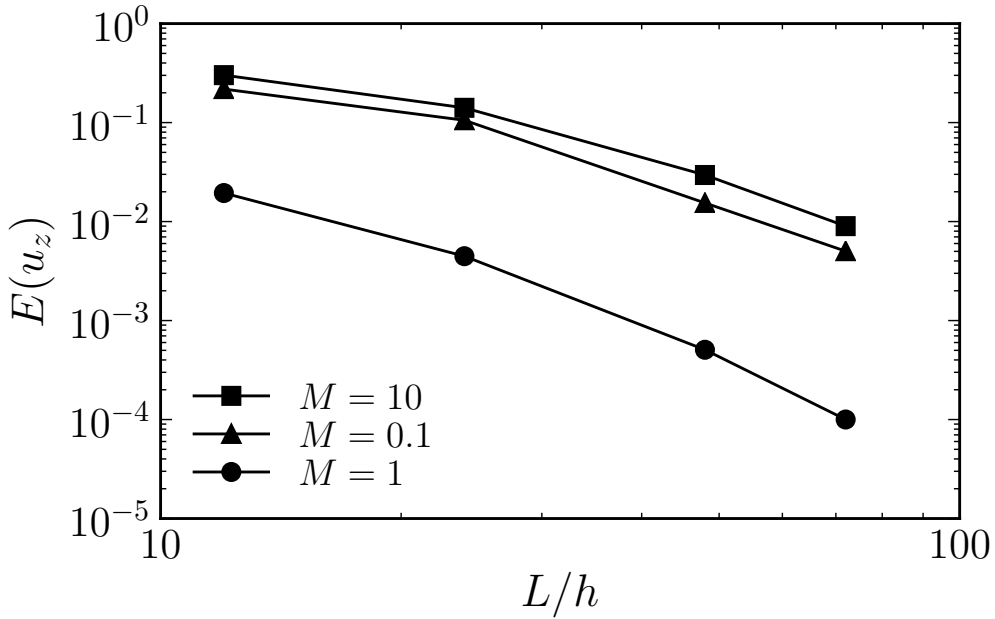


Figure 4.3. The normalized error of the computed velocity profile, $E(u_z)$, Equation (4.1), versus mesh resolution for two-phase flow with different viscosity ratios, M , in a square capillary tube.

4.3. Geometry configurations and coupled flow modelling

In this section, we first describe pore geometries and related fluid configurations for which viscous coupling effects are investigated. Then, the impact of different interface boundary

conditions on the computed hydraulic conductance for these fluid configurations is discussed. Finally, we present our approach to model the coupled flow of two phases by defining a generalized matrix of mobilities similar to the generalized Darcy equation.

Three pore geometries: square, equilateral triangular and star-shaped capillary tubes, with the same inscribed radius of $b = 10 \mu m$, and different wall lengths, l_w , are considered (see Figure 4.4). For each geometry, we set up two fluid configurations: (a) corner flow through pores with uniform wettability as schematically depicted in Figure 4.4a-c, and (b) sandwiched layer flow through pores with non-uniform wettability as shown in Figure 4.4d-f; with the grey region representing fluid 1 (water), and the white region representing fluid 2 (oil). In all cases, flow is perpendicular to the cross-section and driven by a uniform body force.

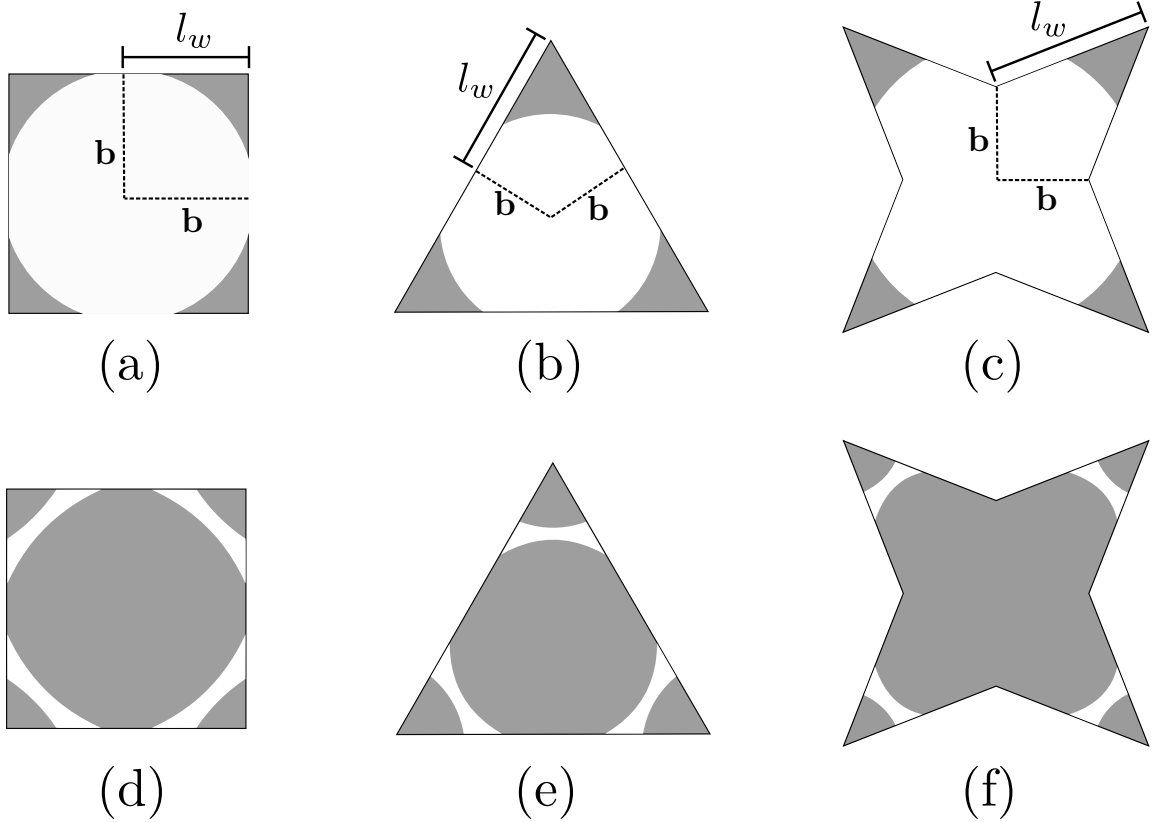


Figure 4.4. Schematic illustrations of fluid configurations for square, equilateral triangular and star-shape pore geometries with (a)-(c) uniform wettability, and (d)-(f) non-uniform wettability conditions. For uniform wettability conditions, fluid flow occurs in the corner (grey) and centre (white) of the capillaries, while for non-uniform wettability conditions, in addition to corner and centre flow (grey), we can also have fluid flow in a stabilized intermediate layer (white) sandwiched between the corner and centre of the capillaries. The geometries have different wall lengths, l_w , while the inscribed radius, b , is the same for all geometries and equal to $10 \mu m$.

Figure 4.5 depicts the parameters that control the geometry of corner and sandwiched layers in the crevices of the non-circular capillary tubes. For the pores with uniform wettability, in each corner, there is one fluid-fluid interface, Γ_{12} , separating the corner flow of fluid 1 from the centre

flow of fluid 2. The geometry of the two fluids can be defined by the corner half-angle (γ), the contact angle (θ_{12}) and the meniscus-apex distance (b_1). For the mixed-wet corners, the shape of sandwiched layers, however, depends on two fluid-fluid interfaces, Γ_{12} and Γ_{23} , which separate the creeping flow of fluid 2 in the intermediate layer from the flow of fluid 1 in the corner and the centre, regions 1 and 3. Therefore, in addition to γ , θ_{12} , and b_1 , we also need the meniscus-apex distance and contact angle associated to the Γ_{23} interface, b_2 and θ_{23} , respectively, to define the geometry of the layer (Al-Futaisi and Patzek, 2003). The meniscus-apex distances can be expressed as

$$\begin{aligned} b_1 &= r_{12} \frac{\cos(\theta_{12} + \gamma)}{\sin(\gamma)}, \\ b_2 &= r_{23} \frac{\cos(\theta_{23} + \gamma)}{\sin(\gamma)}, \end{aligned} \tag{4.2}$$

where r_{12} and r_{23} are, respectively, the radii of curvature of Γ_{12} and Γ_{23} . The contact angle θ_{23} is a free parameter in our simulations, while the contact angle θ_{12} is a hinging value to make the interfacial curvature on both sides of the layer equal, $r_{12} = r_{23}$; see Figure 4.5b.

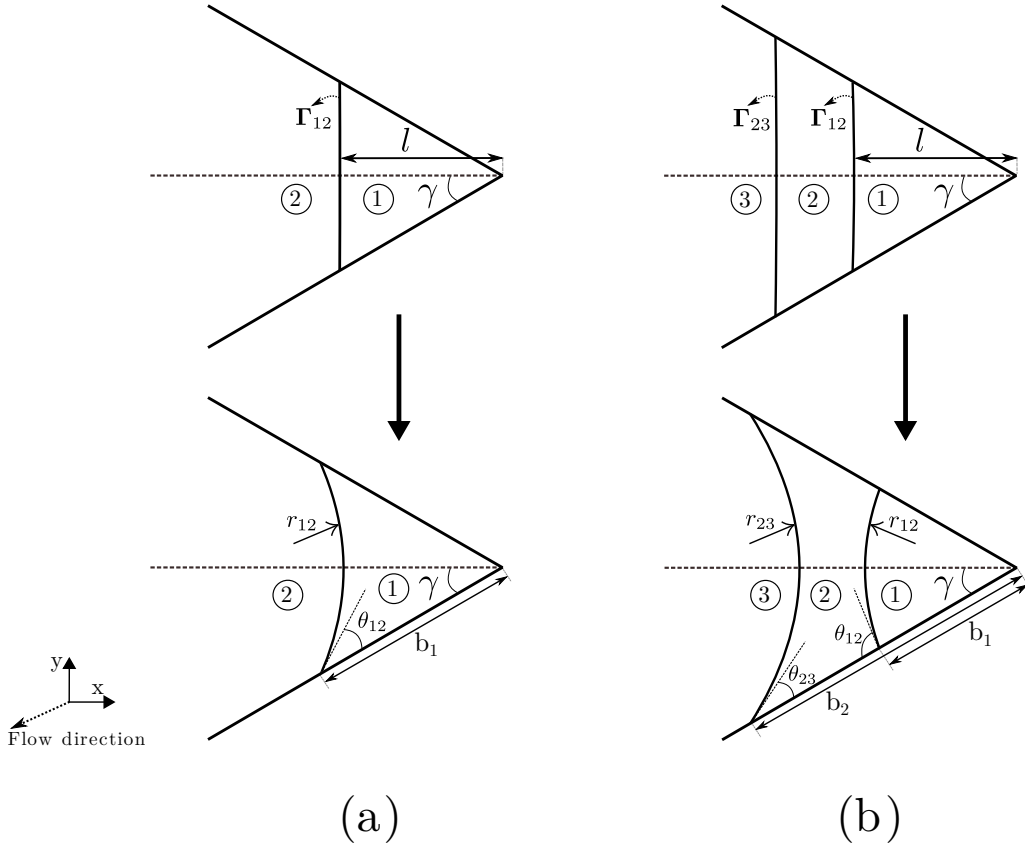


Figure 4.5. Schematic illustrations of initial and stabilized form of fluid-fluid interfaces and corresponding geometric parameters for capillaries with (a) uniform wettability conditions, and (b) non-uniform wettability conditions. The curvatures on each side of the sandwiched layer for non-uniform wettability conditions are equal, $r_{12} = r_{23}$.

For each simulation, first, interfaces are initialized as straight lines in each corner, while the parameter l , the distance between Γ_{12} centre and the vertex of the corner, is used to control the saturation of fluids in the corner (see Figure 4.5). The interfaces are then numerically stabilized for the imposed corner half-angle and contact angle.

We employ the inscribed radius, b , as the characteristic length to scale spatial coordinates, and the viscosity and pressure gradient of fluid 2 (μ_2 and ξ_2) to scale the velocity of fluids in each flow region (Al-Futaisi and Patzek, 2003; Dehghanpour et al., 2011). The scaling leads to the following dimensionless relations:

$$\begin{aligned}\tilde{b}_1 &= \frac{b_1}{b}, & \tilde{b}_2 &= \frac{b_2}{b}, \\ \tilde{l}_w &= \frac{l_w}{b}, & \tilde{A}_i &= \frac{A_i}{b^2}, \\ \tilde{\mu}_i &= \frac{\mu_i}{\mu_2}, & \tilde{\xi}_i &= \frac{\xi_i}{\xi_2}, \\ \tilde{u}_i &= \frac{u_i \mu_2}{\xi_2 b^2},\end{aligned}\tag{4.3}$$

where the subscript i denotes the flow regions in the domain, Figure 4.5, A_i is the area open to flow, and u_i and ξ_i are the velocity field and pressure gradient in each region. The dimensionless volumetric flow rate passing through region i , $\tilde{\Omega}_i$, is obtained as

$$\tilde{q}_i = \int_{\tilde{\Omega}_i} \tilde{u}_i d\tilde{A}_i.\tag{4.4}$$

The flow coupling can be influenced by the type of imposed boundary conditions on fluid-fluid interfaces (Γ_{12} , Γ_{23}). Three different boundary conditions can be considered (Al-Futaisi and Patzek, 2003):

1. No-flow boundary condition: the interface is treated as a solid boundary and the velocity of each fluid at the interface is forced to be zero.
2. Free-slip boundary condition: the interface is treated as a perfectly lubricated boundary where fluids can slip freely on top of each other.
3. Continuity boundary condition: there is continuity of velocity and shear stress along the interface and fluids exchange momentum at the interface.

In this work, we employ the direct numerical simulation technique to simulate coupled two-phase flow through capillary tubes. In the numerical method, since the interface is treated as a discontinuity in fluid properties, we do not need to explicitly impose boundary conditions on the interfaces. Velocity and stress continuity conditions are implicitly captured, i.e. we have the continuity boundary condition along the interface.

We first obtain volumetric fluxes for different flow regions in the capillary tube. Then, the following algebraic equation system is formed based on the generalized Darcy's equation (Kalay-

djian, 1990; Avraam and Payatakes, 1995b; Rose, 2000) and solved to compute the flow conductance matrix, $[\tilde{\lambda}_{ij}]$:

$$[\tilde{q}] = -[\tilde{\lambda}_{ij}][\tilde{\xi}], \quad (4.5)$$

where $[\tilde{q}]$ and $[\tilde{\xi}]$ are the column vectors of the dimensionless volumetric flux and dimensionless pressure gradient for each phase, respectively, and $[\tilde{\lambda}_{ij}]$ is the square matrix of generalized dimensionless mobilities with the off-diagonal terms representing the viscous coupling exerted between fluid phases (Kalaydjian, 1990). The matrix of mobilities is 2 by 2 for uniform wettability configurations,

$$[\tilde{\lambda}_{ij}] = \begin{bmatrix} \tilde{\lambda}_{11} & \tilde{\lambda}_{12} \\ \tilde{\lambda}_{21} & \tilde{\lambda}_{22} \end{bmatrix}, \quad (4.6)$$

and 3 by 3 for non-uniform wettability configurations,

$$[\tilde{\lambda}_{ij}] = \begin{bmatrix} \tilde{\lambda}_{11} & \tilde{\lambda}_{12} & \tilde{\lambda}_{13} \\ \tilde{\lambda}_{21} & \tilde{\lambda}_{22} & \tilde{\lambda}_{23} \\ \tilde{\lambda}_{31} & \tilde{\lambda}_{32} & \tilde{\lambda}_{33} \end{bmatrix}. \quad (4.7)$$

The coefficients of the matrix depend on the contact angle, θ , the corner half-angle, γ , the saturation, s , and the viscosity ratio, $\tilde{\mu}$, of the fluids flowing through the capillary. For each fluid configuration and viscosity ratio, to quantify the coefficients, we apply a non-zero pressure gradient to one flow region (centre, layer or corner) and zero pressure gradient to other flow region(s) and solve Equation (4.5) based on the resultant volumetric flux vector. This is repeated for all flow regions in the cross-section, two simulations for uniform wettability configurations and three simulations for non-uniform wettability configurations, to obtain all diagonal and off-diagonal terms of the matrix. From our numerical simulations, we observe that the matrix is symmetrical ($\tilde{\lambda}_{12} = \tilde{\lambda}_{21}$, $\tilde{\lambda}_{23} = \tilde{\lambda}_{32}$ and $\tilde{\lambda}_{13} = \tilde{\lambda}_{31}$) which is consistent with Onsager's reciprocity equations (Onsager, 1931).

To show the dependence of the velocity profile and consequently flow conductivity on viscosity ratio and interface boundary condition, we model two-phase flow through an equilateral triangular capillary tube with sandwiched layers. Figure 4.6 shows the initialized and equilibrium configuration of the oil layers for a saturation at the value of $s_2 = 0.2$. The viscosity of the sandwiched oil layers is kept constant and equal to $\mu_2 = 10^{-3}$, while the viscosity of water flowing in the corners and centre, μ_1 , is changed to have viscosity ratios, $\tilde{\mu}_1 = \mu_1/\mu_2$, ranging from 10^{-4} to 10^4 . A uniform pressure gradient (body force) of $\xi_1 = \xi_2 = \xi_3 = 100$ Pa/m is applied perpendicular to the cross-section of the capillary tube. The contact angle is chosen to be $\theta_{23} = 30^\circ$, the interfacial tension is $\sigma = 0.03$ N/m, and the continuity of velocity and shear stress is assumed at the interface with zero interfacial shear viscosity.

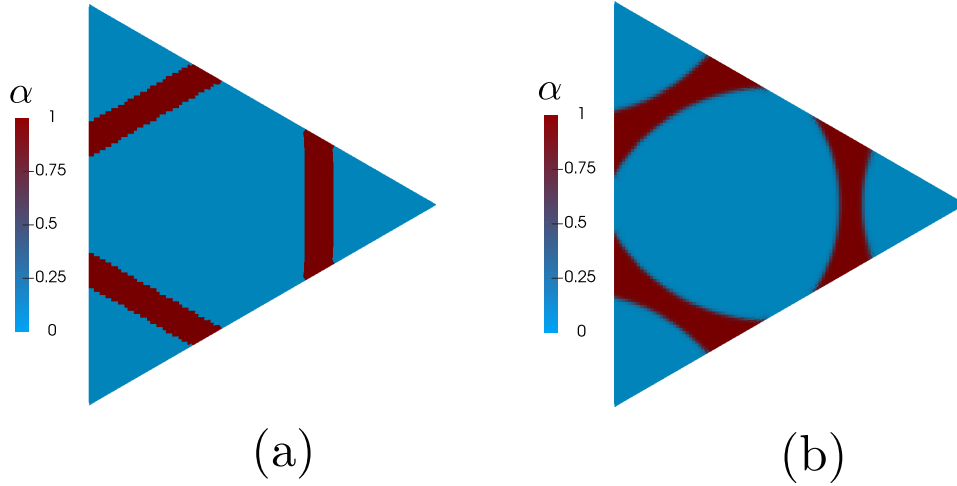


Figure 4.6. Visualizations of (a) the initialized, and (b) equilibrium configuration of sandwiched oil layers, $\alpha = 1$, in the corners of an equilateral triangular capillary with $\gamma = \theta_{23} = 30^\circ$, and $s_2 = 0.2$.

Figure 4.7 compares the steady-state velocity profiles for five sample viscosity ratios. It can be observed that the influence of the viscosity ratio on the value and profile of velocity can be quite significant. When $\tilde{\mu}_1 = 1$, the resultant velocity profile is equivalent to the single-phase flow solution for the domain. As the viscosity ratio deviates from one ($\tilde{\mu}_1 = 0.1$ and $\tilde{\mu}_1 = 10$), the flow coupling between the centre and corner regions decreases. Our simulations show that for very low or high viscosity ratios such as $\tilde{\mu}_1 = 0.001$ and $\tilde{\mu}_1 = 1000$, the flow regions become effectively decoupled from each other. When $\tilde{\mu}_1 = 1000$ the fluid-fluid interface behaves as a solid wall for the sandwiched oil layers, whereas it acts as perfectly lubricated for the water flowing in the centre and corners. The reverse pattern can be observed when $\tilde{\mu}_1 = 0.001$.

Figure 4.8 depicts the computed dimensionless total hydraulic conductance,

$$\tilde{\lambda}_i = -\tilde{q}_i/\tilde{\xi}_i, \quad (4.8)$$

for one of the oil layers, $i = 2$, as a function of viscosity ratio, and compares the results for different interface boundary conditions (free-slip, no-flow, and continuity). It is clear that no-flow and free-slip boundary conditions result in an uncoupled flow of fluids, independent of the viscosity ratio. On the other hand, the computed hydraulic conductance with the continuity boundary condition exhibits a strong dependency on the viscosity ratio. For very high viscosity ratios ($\tilde{\mu}_1 \geq 10^3$) the continuity boundary condition behaves similar to the no-flow one, due to the fact that the water phase in the centre and corners of the capillary has relatively high viscosity values and acts as a solid phase with respect to the oil layers. For very low viscosity ratios ($\tilde{\mu}_1 \leq 10^{-2}$) the conductance reaches a maximum at a value higher than the free-slip limit.

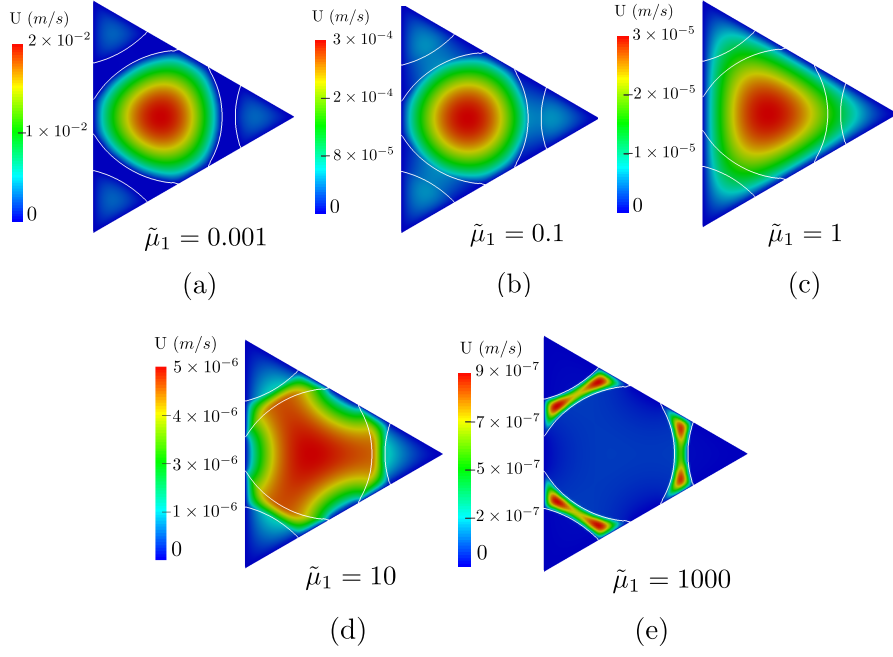


Figure 4.7. Steady-state velocity distribution across flowing fluids with different viscosity ratios in an equilateral triangular capillary with $\gamma = \theta_{23} = 30^\circ$, and $s_2 = 0.2$.

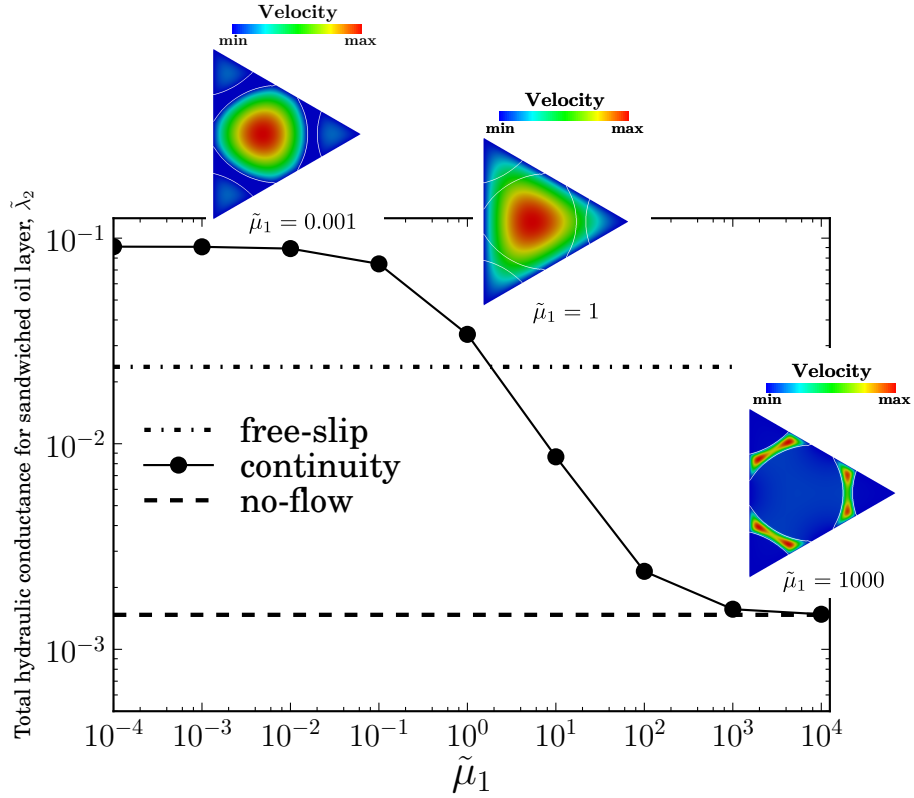


Figure 4.8. Dimensionless total hydraulic conductance of a sandwiched oil layer, $\tilde{\lambda}_2$, as a function of viscosity ratio, for different interface boundary conditions. The capillary tube is an equilateral triangle with $\gamma = \theta_{23} = 30^\circ$ and $s_2 = 0.2$.

Exceeding the no-slip limit is a clear indication of the importance of viscous coupling when the water phase drags the intermediate layer along and contributes to its conductance. Therefore, it is important to investigate the viscous coupling effect on the computed transport properties by considering continuity of velocity and shear stress along the interface.

To quantify the contribution of momentum transfer due to viscous coupling, we evaluate the hydraulic conductance matrix, Equation (4.7), for different viscosity ratios. Figure 4.9 compares the portion of the total hydraulic conductance resulting from the pressure gradient within the sandwiched oil layer, $\tilde{\lambda}_{22}$, to the portions due to the drag force from the adjacent water phase flowing in the centre, $\tilde{\lambda}_{23}$, and corner, $\tilde{\lambda}_{21}$. It can be observed that for viscosity ratios less than 0.1, the values of $\tilde{\lambda}_{23}$ become higher than $\tilde{\lambda}_{22}$, which indicates the importance of the momentum transfer across the interface between the centre and the oil layer, and also justifies the exceeding of the total conductance, $\tilde{\lambda}_2 = \tilde{\lambda}_{21} + \tilde{\lambda}_{22} + \tilde{\lambda}_{23}$, from the free-slip limit.

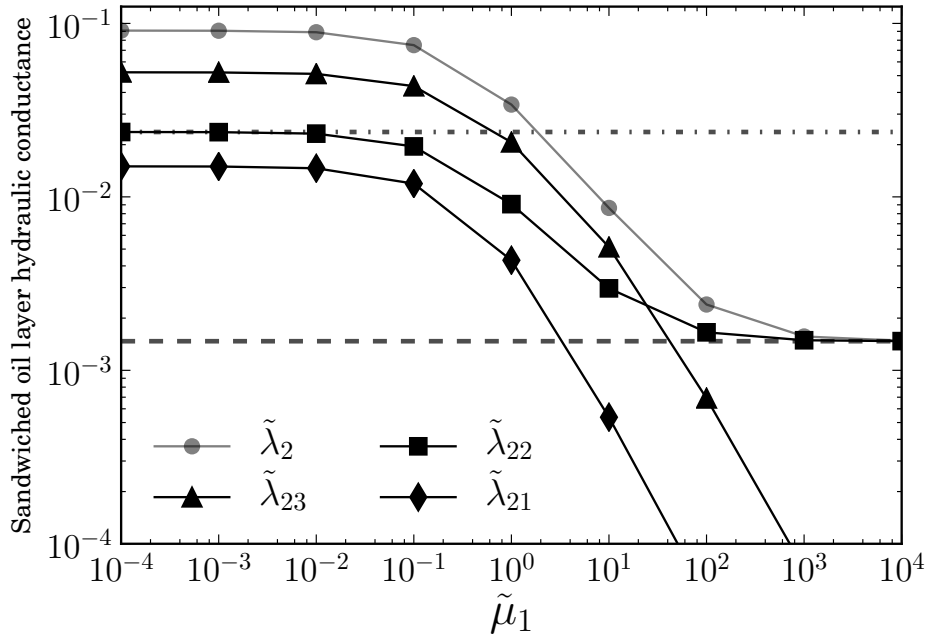


Figure 4.9. Comparison of contributing components to the total conductance of a sandwiched oil layer, $\tilde{\lambda}_2$, in a triangular capillary tube with $\gamma = \theta_{23} = 30^\circ$ and $s_2 = 0.2$: the conductance resulting from the pressure gradient within the oil phase in layer, $\tilde{\lambda}_{22}$, and the conductance due to the drag force exerted from the adjacent water phase in the centre $\tilde{\lambda}_{23}$, and corner $\tilde{\lambda}_{21}$.

To further investigate this, we model two-phase flow through a square capillary tube with uniform wettability, Figure 4.4 a. The dimensionless flow resistance, β , Equation (3.11), for the wetting liquid along one of the corners is computed for different contact angles and viscosity ratios. The results are compared with the study of Ransohoff and Radke (1988) when the comparison is possible, i.e. wetting phase flow in sharp corners while the interfacial shear viscosity, μ_s , is either zero (equivalent to the free-slip boundary condition) or infinite (equivalent to the no-flow boundary condition).

First, we consider a flow arrangement in which the wetting phase, fluid 1, flow in corners is driven by a constant non-zero pressure gradient while the pressure gradient within the central non-wetting phase, fluid 2, is zero. This means that the stress exerted by the non-wetting phase, due to its flow in the centre, on the interface is zero, which is in accordance with the assumption of having an inviscid central phase in Ransohoff and Radke (1988). We keep the viscosity of the wetting phase constant, $\mu_1 = 10^{-3}$ Pa.s, and decrease or increase the viscosity of the non-wetting phase in the centre, μ_2 , to set different viscosity ratios, $\tilde{\mu}_1 = \mu_1/\mu_2$. Figure 4.10 shows the computed dimensionless flow resistance as a function of contact angle for a large range of viscosity ratios.

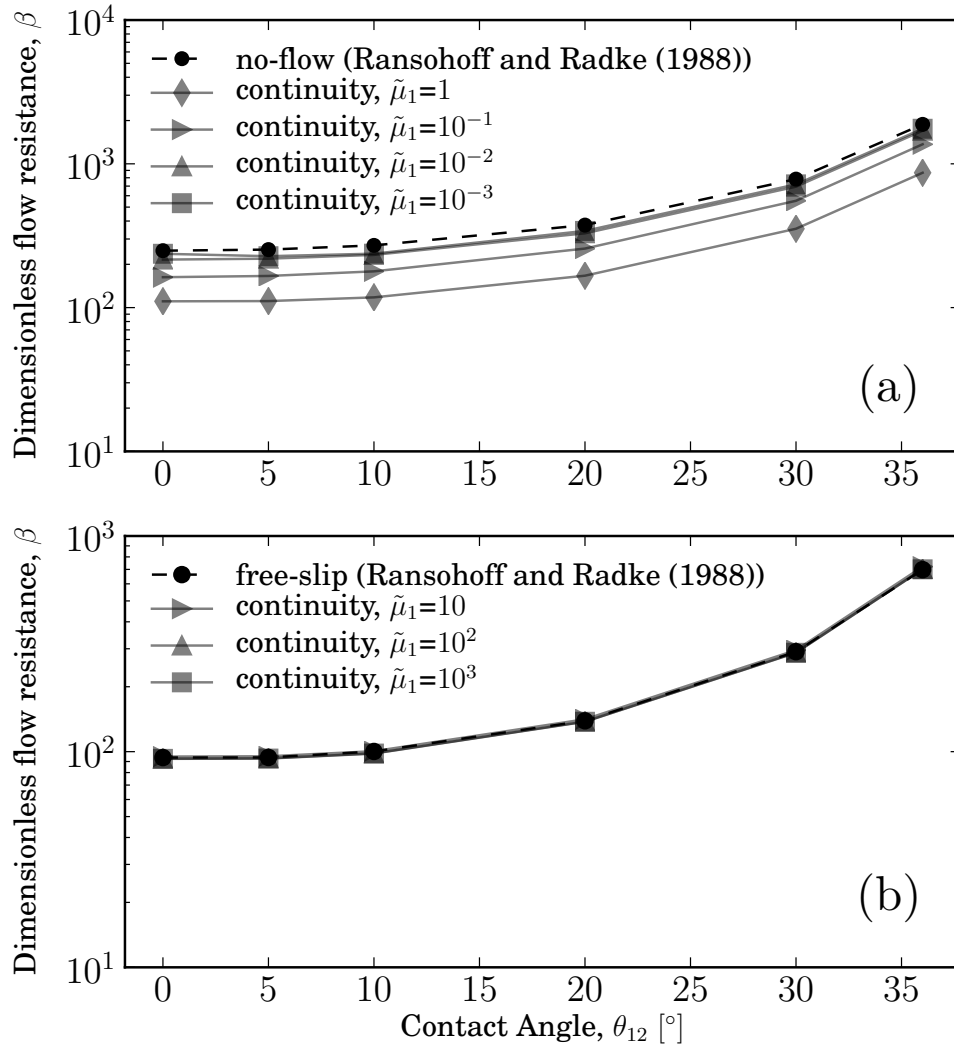


Figure 4.10. Comparisons of the dimensionless resistance, β , Equation (3.11), for wetting phase flow along the sharp corners of a square capillary tube, as a function of contact angle, θ_{12} . The wetting phase in corners, fluid 1, is driven by a constant nonzero pressure gradient, while the pressure gradient within the non-wetting phase in the centre, fluid 2, is zero: (a) $\tilde{\mu}_1 = \mu_1/\mu_2 \leq 1$, (b) $\tilde{\mu}_1 = \mu_1/\mu_2 > 1$.

For $\tilde{\mu}_1 = 1$ and $\tilde{\mu}_1 = 0.1$ the dimensionless resistances are overestimated by assuming a

no-flow boundary condition (Ransohoff and Radke, 1988) and this assumption can be a good approximation only when the viscosity of the central phase is very high compared to the wetting phase in the corners, $\tilde{\mu}_1 \leq 10^{-2}$. On the other hand, the free-slip boundary condition can be a very good approximation for viscosity ratios more than one, as shown in Figure 4.10(b). This is expected due to the fact that the non-wetting phase in the centre is relatively less viscous and since the pressure gradient within this phase is zero the drag force exerted on the interface is insignificant.

Finally, we perform a similar analysis for the case that both fluids are driven using an identical non-zero pressure gradient in a co-current flow; The computed dimensionless flow resistance as a function of contact angle and viscosity ratio is depicted in Figure 4.11.

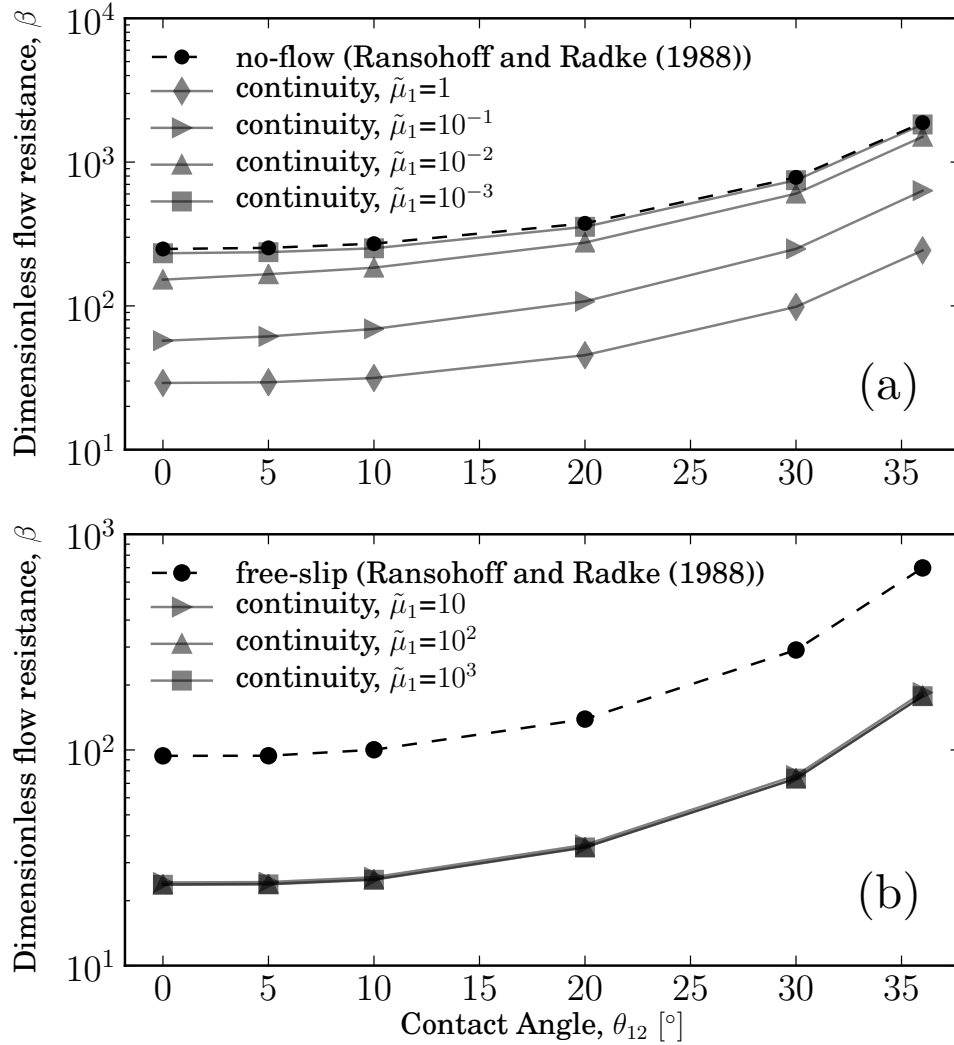


Figure 4.11. Comparisons of the dimensionless resistance, β , Equation (3.11), for wetting phase flow along the sharp corners of a square capillary tube, as a function of contact angle, θ_{12} . The wetting phase in corners, fluid 1, and the non-wetting phase, fluid 2, in the centre are driven by a constant nonzero pressure gradient, i.e. co-current flow: (a) $\tilde{\mu}_1 = \mu_1/\mu_2 \leq 1$, (b) $\tilde{\mu}_1 = \mu_1/\mu_2 > 1$.

Figure 4.11a demonstrates that the solution behaviour for $\tilde{\mu}_1 \leq 1$ is quite similar to the previous case, Figure 4.10a. However, as shown in Figure 4.11b, for $\tilde{\mu}_1 > 1$, the numerical results of Ransohoff and Radke (1988), with a free-slip boundary at the interface, significantly overestimates the dimensionless resistances. This can be explained by the fact that the non-wetting phase with a low viscosity can move at a relatively high velocity, which results in a significant drag force on the interface that enhances the flow conductance of the wetting phase in the corners.

These results highlight the importance of momentum transfer across the interface, especially for mid-range viscosity ratios, $10^{-2} \leq \tilde{\mu}_1 \leq 10^2$, where treating the coupled two-phase flow problem as independent flows of fluids separated by no-flow or free-slip interfacial boundaries can introduce significant errors in the computation of hydraulic conductance. In the next section, we propose and validate some simple relations to estimate hydraulic conductances which take into account the viscous coupling effects due to momentum exchange at the interface.

4.4. Scaling models and validation

In this section, we provide heuristic models to relate the generalized mobilities ($\tilde{\lambda}_{ij}$) to the geometrical parameters ($\gamma, \theta_{12}, \theta_{23}$) and viscosity ratio ($\tilde{\mu}$). These generalized mobilities are then compared with the corresponding numerical solutions and the average of relative absolute errors are reported. Dehghanpour et al. (2011) also developed an empirical model to estimate the generalized mobilities for wetting layers (water) and intermediate layers (oil) in three-phase flow through angular capillaries, assuming the central fluid (gas) is decoupled and does not exchange momentum with the oil and water. We follow a similar argument to develop expressions to estimate the generalized mobilities in two-phase flow for (a) uniform wettability where oil in the centre exchanges momentum with water in the corners of a capillary, and (b) non-uniform wettability conditions where there is flow coupling between oil in the sandwiched layers and water in the centre and corners of a capillary.

4.4.1. Conventional (diagonal) terms

For laminar fully-developed pressure-driven single-phase flow through a straight duct with a constant cross-section, the volumetric flow rate, $\tilde{q}$, can be related to the fluid pressure drop, $\tilde{\xi}$, as follows (Dehghanpour et al., 2011):

$$\tilde{q} = \tilde{\lambda} \tilde{\xi}, \quad (4.9)$$

where

$$\tilde{\lambda} = \frac{c}{\tilde{\mu}} \frac{(\tilde{A})^3}{(\tilde{p}_w)^2}. \quad (4.10)$$

Here c is a proportionality constant which depends only on the duct shape, $\tilde{A}$ is the open area to flow, and $\tilde{p}_w$ is the wetted perimeter defined as the length along which the fluid is in contact with solid walls where the velocity is zero. Since the diagonal terms of the matrix of mobilities rep-

resent the uncoupled pressure-driven flow of each fluid under its own pressure gradient through a duct-shaped passage, in analogy with Equation (4.10), the following parametric equation is employed to estimate the diagonal mobilities:

$$\tilde{\lambda}_{ii} = \frac{c_i (\tilde{A}_i)^{a_i+2}}{\tilde{\mu}_i (\tilde{p}_{w,i})^{2a_i}}, \quad i = 1, 2, 3 \quad (4.11)$$

where the subscript i denotes the flow region, and c_i and a_i are constant parameters for the flow region i .

In two-phase flow, the wetted perimeter of the flow region i , $\tilde{p}_{w,i}$, in addition to the fluid–solid boundary, can include the fluid–fluid interface, depending on the viscosity ratio of the adjacent fluids (Dehghanpour et al., 2011). For the case that the adjacent phase viscosity becomes much higher than the viscosity of the phase in region i , the interface acts as a no-flow boundary for region i and $\tilde{p}_{w,i}$ should include the length of the interface. On the other hand, when the viscosity of the adjacent phase is much lower than the viscosity of the phase in region i , the adjacent phase is inviscid compared to the phase in region i and $\tilde{p}_{w,i}$ does not include the length of the interface. Therefore, we use the following expressions to relate the wetted perimeter to viscosity ratio for (a) the uniform wettability condition (Dehghanpour et al., 2011),

$$\begin{aligned} \text{corner: } \tilde{p}_{w,1} &= 2\tilde{b}_1 + \tilde{l}_{12}f(\tilde{\mu}_1), \\ \text{centre: } \tilde{p}_{w,2} &= 2(\tilde{l}_w - \tilde{b}_1) + \tilde{l}_{12}f\left(\frac{1}{\tilde{\mu}_1}\right), \end{aligned} \quad (4.12)$$

and (b) the non-uniform wettability condition,

$$\begin{aligned} \text{corner: } \tilde{p}_{w,1} &= 2\tilde{b}_1 + \tilde{l}_{12}f(\tilde{\mu}_1), \\ \text{layer: } \tilde{p}_{w,2} &= 2(\tilde{b}_2 - \tilde{b}_1) + \tilde{l}_{12}f\left(\frac{1}{\tilde{\mu}_1}\right) + \tilde{l}_{23}f\left(\frac{1}{\tilde{\mu}_1}\right), \\ \text{centre: } \tilde{p}_{w,3} &= 2(\tilde{l}_w - \tilde{b}_2) + \tilde{l}_{23}f(\tilde{\mu}_1). \end{aligned} \quad (4.13)$$

Here $\tilde{l}_{12}$ and $\tilde{l}_{23}$ are, respectively, the dimensionless length of interface Γ_{12} and Γ_{23} , scaled by the inscribed radius, b , and the function f is defined using the following decay function:

$$f(x) = \frac{1}{1 + nx^n}, \quad (4.14)$$

where the value of $n = 2$ is chosen to fit the simulation data.

The values reported in Table 4.1 for parameters in Equation (4.11) are found to fit our simulations best for uniform and non-uniform wettability conditions.

To validate the scaling model we have simulated two-phase flow through square ($\gamma = 45^\circ$), triangular ($\gamma = 30^\circ$), and star-shaped ($\gamma = 22.5^\circ$) pore geometries, see Figure 4.4, for different contact angles ($\theta_{12} = 30^\circ, 45^\circ$ and 60°) and volume saturations (s_2). For each case, the coefficients of the matrix of dimensionless mobilities are computed as described in Section 4.3.

Table 4.1.

Fitted values for the parameters of Equation (4.11), used to estimate the diagonal terms in the general mobility matrix for uniform and non-uniform wettability configurations.

	uniform wettability		non-uniform wettability		
	$\tilde{\lambda}_{11}$ (corner)	$\tilde{\lambda}_{22}$ (centre)	$\tilde{\lambda}_{11}$ (corner)	$\tilde{\lambda}_{22}$ (layer)	$\tilde{\lambda}_{33}$ (centre)
c_i	1/7	1/6	1/7	1/3	1/5
a_i	0.45	0.2	0.45	0.75	0.4

Figure 4.12 compares the predicted values of the diagonal terms, $\tilde{\lambda}_{11}$, $\tilde{\lambda}_{22}$, and $\tilde{\lambda}_{33}$, using the proposed scaling model, Equation 4.11, with the numerically simulated values for uniform and non-uniform wettability cases. The proposed correlation agrees well with the simulated values over four orders of magnitude in conductance.

To quantify the error, we define the mean absolute relative error as follows:

$$\bar{E}(\tilde{\lambda}_{ii}) = \sum_{\mathbf{N}} \left(\frac{|\tilde{\lambda}_{ii}^{\text{num}} - \tilde{\lambda}_{ii}^{\text{scale}}|}{\tilde{\lambda}_{ii}^{\text{num}}} \right) / N, \quad i = 1, 2, 3 \quad (4.15)$$

where $\tilde{\lambda}_{ii}^{\text{num}}$ and $\tilde{\lambda}_{ii}^{\text{scale}}$ are the values of the dimensionless mobility computed using numerical simulation and the scaling model, respectively, and $N = 144$ is the total number of fluid configurations which have been simulated. The error values are reported in Table 4.2.

Table 4.2.

The mean relative errors, Equation (4.15), in the predicted diagonal terms using Equation (4.11).

	uniform wettability		non-uniform wettability		
	$\tilde{\lambda}_{11}$ (corner)	$\tilde{\lambda}_{22}$ (centre)	$\tilde{\lambda}_{11}$ (corner)	$\tilde{\lambda}_{22}$ (layer)	$\tilde{\lambda}_{33}$ (centre)
$\bar{E}(\tilde{\lambda}_{ii})$	13%	14%	12%	17%	13%

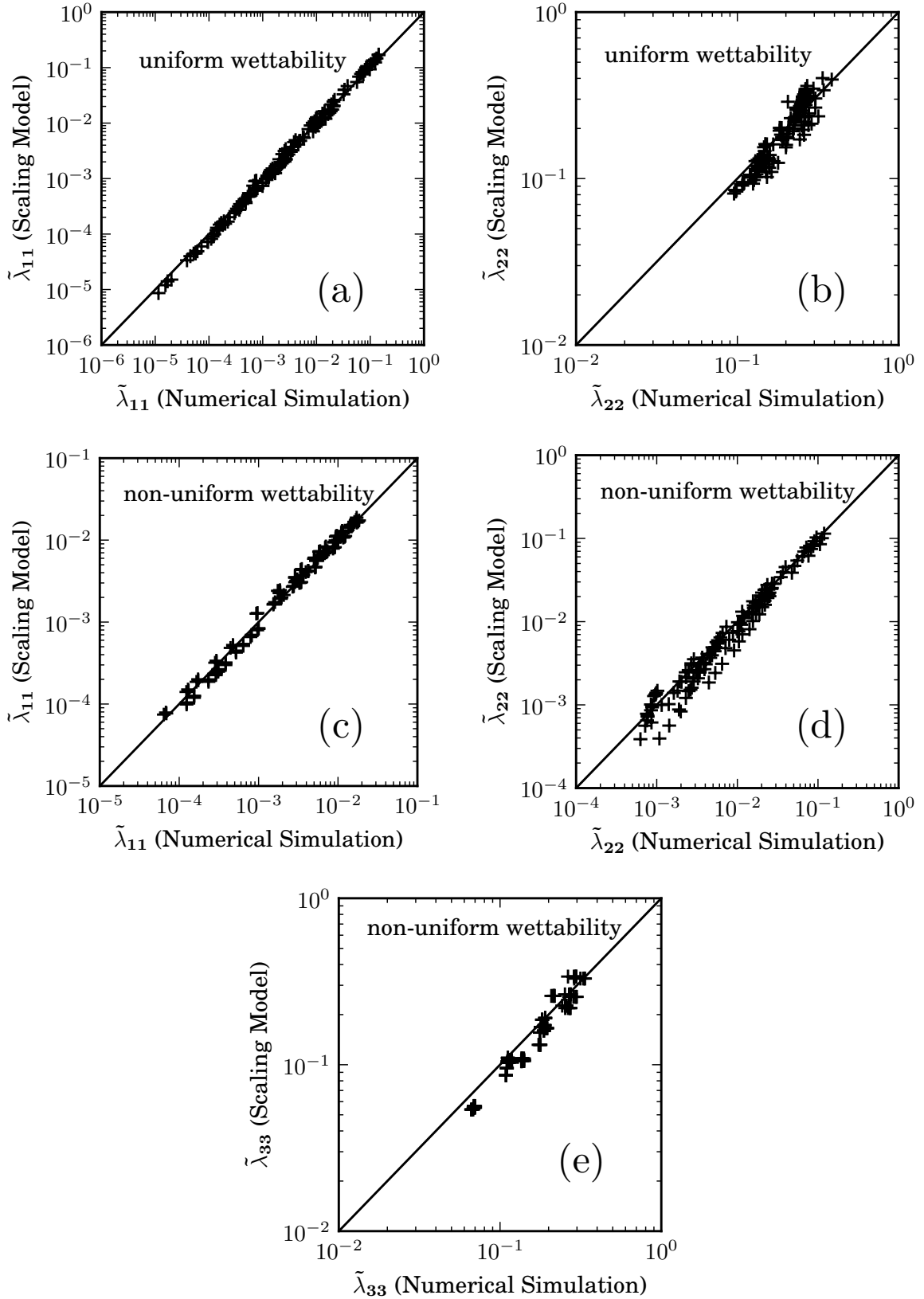


Figure 4.12. Comparison of the predicted values of the scaling model, Equation (4.11), with the simulated values of the diagonal terms. (a)-(b) The diagonal mobilities for corner and centre flow in capillaries with uniform wettability, $\tilde{\lambda}_{11}$ and $\tilde{\lambda}_{22}$, respectively. (c)-(e) The diagonal mobilities for corner, sandwiched layer, and centre flow in capillaries with nonuniform wettability, $\tilde{\lambda}_{11}$, $\tilde{\lambda}_{22}$, and $\tilde{\lambda}_{33}$, respectively.

4.4.2. Coupling (off-diagonal) terms

The off-diagonal terms of the matrix of mobilities represent the coupled drag-driven flow of each fluid in a flow region resulting from the pressure gradient in the other adjacent flow regions. The simplest type of flow in fluid mechanics similar to this drag-driven flow in a capillary tube, is Couette flow in which we have a laminar flow in the space between two parallel plates due to a shear stress, τ_s , exerted to one of the plates while the other is fixed (Dehghanpour et al., 2011). The volumetric flow rate in Couette flow can be related to the shear stress, open area to flow and wetted perimeter in the following dimensionless form (Wendl, 1999):

$$\tilde{q} = \frac{1}{\tilde{\mu}} \frac{(\tilde{A})^2}{\tilde{p}_w} \tilde{\tau}_s. \quad (4.16)$$

In the case of two-phase flow through a capillary, by analogy with Equation (4.16), the volumetric flow rate of the fluid in region i due to the drag force resulting from the pressure gradient in the adjacent flow region j , can be estimated as

$$\tilde{q}_i = \frac{c_{ij}}{\tilde{\mu}_i} \frac{(\tilde{A}_i)^2}{\tilde{p}_{w,i}} \tilde{\tau}_{ij}, \quad i \neq j, \quad (4.17)$$

where c_{ij} is a constant parameter, and the shear stress exerted on the fluid–fluid interface, $\tilde{\tau}_{ij}$, can be expressed as a function of flow geometry, viscosity ratio and pressure gradient as follows (Dehghanpour et al., 2011):

$$\tilde{\tau}_{ij} = g(\tilde{\mu}_1) \frac{\tilde{A}_j}{\tilde{p}_{w,j}} \tilde{\xi}_j, \quad i \neq j. \quad (4.18)$$

Here the function $g(\tilde{\mu}_j)$ is used to relate $\tilde{\tau}_{ij}$ to the viscosity ratio and is estimated by finding the best fit for simulated values of the coupling term as a function of the viscosity ratio.

By substituting Equation (4.18) in Equation (4.17) and comparing with $\tilde{q}_i = \tilde{\lambda}_{ij} \tilde{\xi}_j$, the following parametric equation can be written for the coupling terms:

$$\tilde{\lambda}_{ij} = c_{ij} \frac{g(\tilde{\mu}_1)}{\tilde{\mu}_i} \frac{(\tilde{A}_i)^{a_{ij}+1.5}}{(\tilde{p}_{w,i})^{2a_{ij}}} \frac{(\tilde{A}_j)^{d_{ij}+0.5}}{(\tilde{p}_{w,j})^{2d_{ij}}}, \quad i = 1, 2, \quad j = i + 1, \quad (4.19)$$

where a_{ij} and d_{ij} are constant parameters.

The scaling model for $\tilde{\lambda}_{13}$, however, is computed slightly differently from the one for $\tilde{\lambda}_{12}$ and $\tilde{\lambda}_{23}$, due to the fact that flow regions 1 and 3 are filled with the same fluid separated by an intermediate layer in region 2. Since the shear stress gets transmitted via an intermediate layer, the geometrical parameters of the layer ($\tilde{A}_2$ and $\tilde{p}_{w,2}$) as well as the viscosity ratio can affect $\tilde{\lambda}_{13}$. Therefore, the function g in Equation (4.18) is expressed as a function of both viscosity ratio and relative thickness of the intermediate layer. In addition, Equation (4.19) is modified

to include the momentum dissipation through the wetted perimeter of the intermediate layer:

$$\tilde{\lambda}_{13} = c_{13} \frac{g(\tilde{\mu}_1, \tilde{A}_r)}{\tilde{\mu}_1} \frac{(\tilde{A}_3)^{a_{13}+1.5}}{(\tilde{p}_{w,2} + \tilde{p}_{w,3})^{2a_{13}}} \frac{(\tilde{A}_1)^{d_{13}+0.5}}{(\tilde{p}_{w,1})^{2d_{13}}}, \quad (4.20)$$

where $\tilde{p}_{w,1} = 2\tilde{b}_1$, $\tilde{p}_{w,2} = 2(\tilde{b}_2 - \tilde{b}_1)$, $\tilde{p}_{w,3} = 2(\tilde{l}_w - \tilde{b}_2)$, and the function $g(\tilde{\mu}_1, \tilde{A}_r)$ is used to relate the shear stress, $\tilde{\tau}_{13}$, to both viscosity ratio and relative thickness of the intermediate layer, $\tilde{A}_r$, defined as

$$\tilde{A}_r = \left(\frac{\tilde{A}_2}{\tilde{A}_1 + \tilde{A}_3} \right)^{0.5}. \quad (4.21)$$

The relative thickness $\tilde{A}_r$ controls the momentum dissipation in the intermediate layer. Larger values of $\tilde{A}_r$ means more momentum dissipation through the intermediate layer and consequently, less momentum exchange and viscous coupling between fluids in regions 1 and 3. Therefore the function g should have an inverse relation to $\tilde{A}_r$. Moreover, if $\tilde{\mu}_1 \ll 1$ or $\tilde{\mu}_1 \gg 1$, i.e. the intermediate layer acts as a solid barrier or an inviscid phase, g approaches to zero to decouple the flows in region 1 and 3, $\tilde{\lambda}_{13} = 0$.

Table 4.3 reports the constant parameters (a_{ij} , c_{ij} and d_{ij}) and function g , used in Equations (4.19) and (4.20), which are found based on the best fit to the values of $\tilde{\lambda}_{ij}$ computed from our numerical simulations for all geometries.

Table 4.3.

Fitted values for the parameters of Equations. (4.19) and (4.20) to estimate coupling terms in the general mobility matrix for uniform and nonuniform wettability configurations.

	uniform wettability	non-uniform wettability		
	$\tilde{\lambda}_{12}$ (centre-corner)	$\tilde{\lambda}_{12}$ (corner-layer)	$\tilde{\lambda}_{23}$ (layer-centre)	$\tilde{\lambda}_{13}$ (centre-corner)
c_{ij}	0.25	0.5	0.4	0.8
a_{ij}	0.5	0.5	0.3	1.1
d_{ij}	γ	γ	1	γ
g	$\frac{2}{2+5\tilde{\mu}_1}$	$\frac{5}{5+4/\tilde{\mu}_1}$	$\frac{1.2}{5+7/\tilde{\mu}_1}$	$\frac{6(1/\tilde{\mu}_1)^2}{(0.4\tilde{A}_r+2/\tilde{\mu}_1)^{2.5}}$

Figure 4.13 compares the predicted values for the coupling terms, $\tilde{\lambda}_{12} = \tilde{\lambda}_{21}$, $\tilde{\lambda}_{23} = \tilde{\lambda}_{32}$, and $\tilde{\lambda}_{13} = \tilde{\lambda}_{31}$, based on the proposed scaling model, Equations 4.19 and 4.20, with the numerical results, for both uniform and non-uniform wettability cases. One can observe that the scaling model can estimate the coupling mobilities with a good accuracy.

The mean relative errors, Equation (4.15), for the coupling terms are given in Table 4.4.

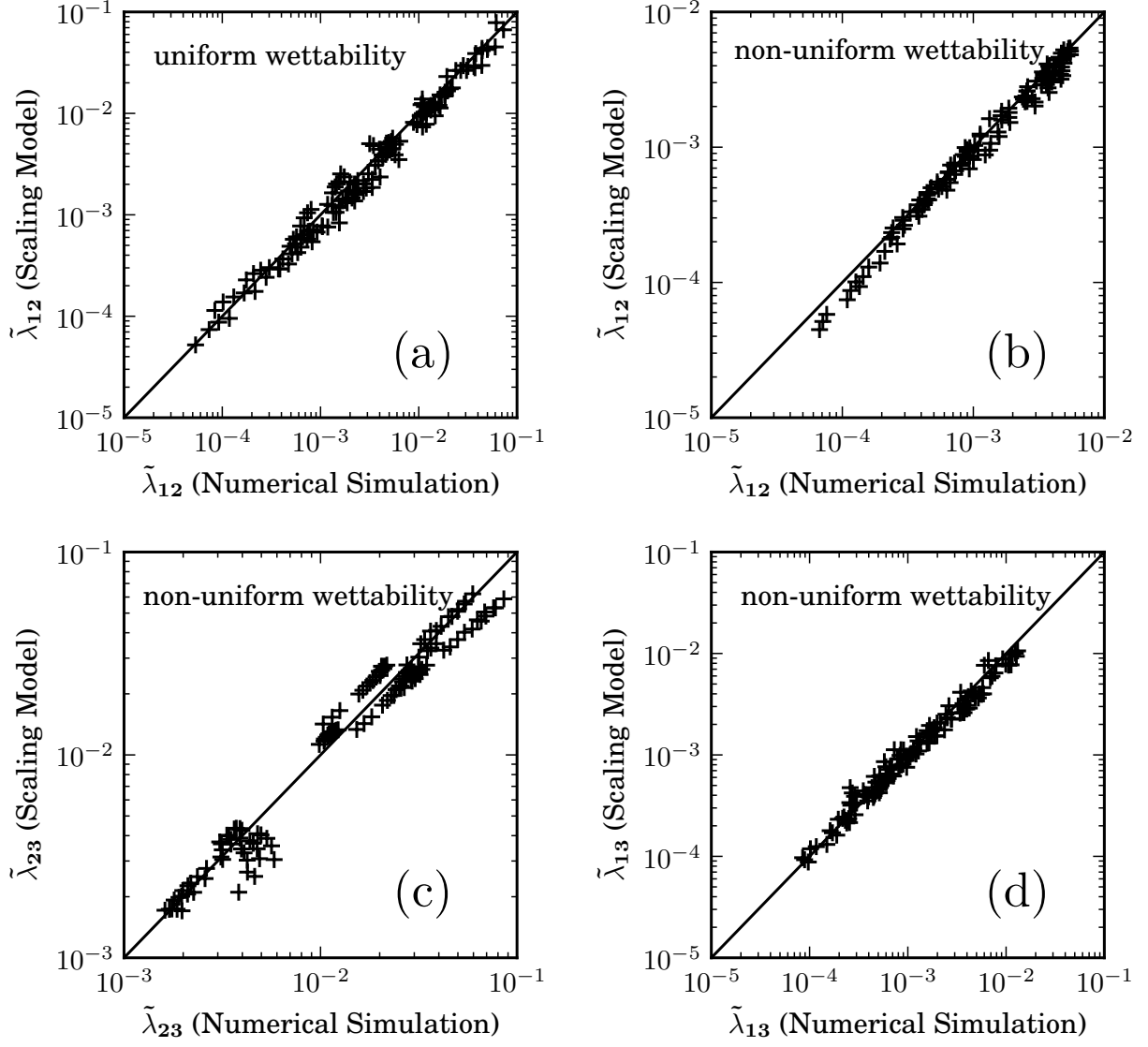


Figure 4.13. Comparison of the predicted values of the scaling model, Equations (4.19) and (4.20), with the simulated values of the coupling terms: (a) the centre-corner coupled mobility term, $\tilde{\lambda}_{12}$, in capillaries with uniform wettability, and (b)-(d) the layer-corner coupled mobility term, $\tilde{\lambda}_{12}$, the layer-centre coupled mobility term, $\tilde{\lambda}_{23}$, and the centre-corner coupled mobility term, $\tilde{\lambda}_{13}$, in capillaries with nonuniform wettability.

Table 4.4.

The mean relative errors, Eq. (4.15), in predicted coupling terms using Equations (4.19) and (4.20).

	uniform wettability	non-uniform wettability	
	$\tilde{\lambda}_{12}$ (centre-corner)	$\tilde{\lambda}_{12}$ (corner-layer)	$\tilde{\lambda}_{23}$ (layer-centre)
			$\tilde{\lambda}_{13}$ (centre-corner)
$\bar{E}(\tilde{\lambda}_{ij})$	19%	11%	16%
			15%

4.5. Three-dimensional geometries with nonuniform cross-sections

The scaling models presented in Section 4.4 are obtained based on two-phase flow simulations through capillary tubes with uniform cross-sections. However, our numerical model is able to model two-phase flow through three-dimensional geometries such as capillary tubes with nonuniform cross-sections. Even though layer flow in three-dimensional geometries with contractions and expansions can be more complex compared to the one in geometries with uniform cross-sections, the same work-flow can be applied to study viscous coupling in single tubes with nonuniform cross-sections. In this section, we only present a two-phase flow simulation through a three-dimensional star-shaped geometry with a nonuniform cross-section without dealing with the viscous coupling analyses.

As shown in Figure 4.14, we consider a three-dimensional star-shaped geometry where two pores with inscribed radii of $R_p = 30 \mu m$ are connected through a throat with an inscribed radius of $R_t = 12 \mu m$. Total length of the pore is $l = 320 \mu m$; the pores are of the same size with the length of $l_p = 130 \mu m$ connected via a throat with the length of $l_t = 30 \mu m$. The geometry has a corner angle of 45° . The mesh resolution is $R_t/\delta x = 20$. The unstructured mesh is created using SnappyHexMesh, a mesh generator from OpenFOAM (OpenFOAM, 2016) that uses a uniform initial mesh and snaps the boundary points to the solid wall, so that all the solid boundary faces align with the solid wall.

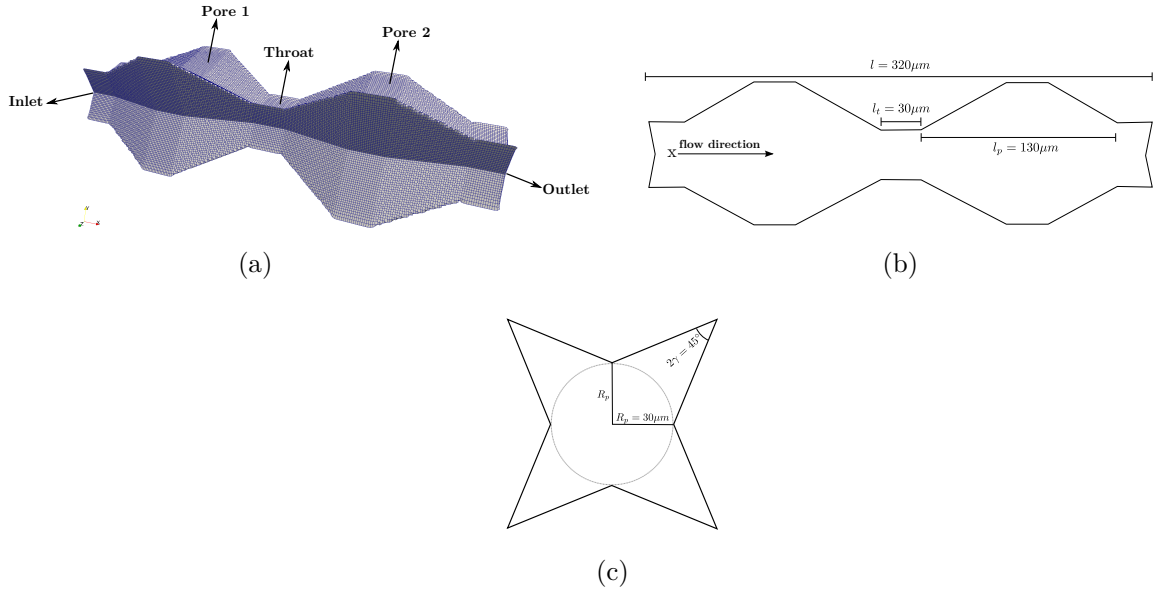


Figure 4.14. (a) A visualization of a three-dimensional star-shaped pore-throat system used to simulate a snap-off process, (b) the wetting fluid is injected in the x -direction, the length of the pore is $l = 320 \mu m$, the pores are of the same size with the length of $l_p = 130 \mu m$ connected via a throat with the length of $l_t = 30 \mu m$, and (c) the cross-sectional view of the flow domain, the corner angle is $\gamma = 45^\circ$, the radius of the pore is $R_p = 30 \mu m$, and the expansion ratio is $R_p/R_t = 2.5$.

We perform a dynamic two-phase flow simulation where the wetting phase, fluid 1, displaces the non-wetting phase, fluid 2. A no-slip boundary condition is applied on the tube walls with a constant contact angle of 30° . The boundary conditions used at the inlet are zero-gradient for pressure and fixed value for the indicator function and velocity. The boundary conditions at the outlet are fixed value for pressure and zero-gradient for the indicator function and velocity. The fluid viscosities and densities are equal in both fluids, $\mu = 10^{-3}$ Pa·s and $\rho = 1000$ kg/m³, and the interfacial tension is constant and taken to be $\sigma = 0.03$ N/m. Figure 4.15(a) shows a visualization of the initial profile of the fluids. A small portion of the geometry near the inlet, 15% of the total length, l , is filled with the injection fluid, wetting phase, while the rest of the tube is occupied with the nonwetting phase. The wetting phase is injected at the inlet with a constant velocity equal to 0.1 mm/s.

Figure 4.15 shows the snapshots of the saturation profile of the fluids at different times. The wetting phase encroaches the corners of the star-shaped geometry and after the breakthrough, $t = 0.02$ s, the wetting phase layers start growing. The layers in the throat may become unstable and snap-off happens, which leads to the trapping of the non-wetting phase in the first pore.

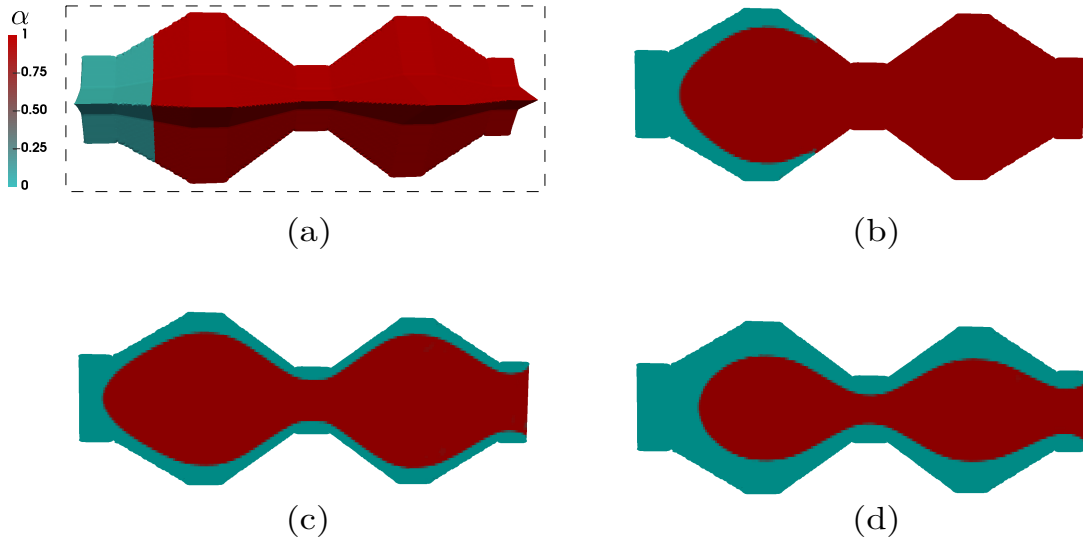


Figure 4.15. A visualization of the saturation profiles of the wetting phase (blue) and the nonwetting phase (red) at different time steps for an imbibition process in the three-dimensional nonuniform star-shaped geometry: (a) initial profile at $t = 0$ s, (b) $t = 0.0045$ ms, (c) $t = 0.02$ s, and (d) $t = 0.2$ s.

This test case simply demonstrates that two-phase flow in complex geometries can lead to more complicated layer configurations that may not even be stable. Computing conductivities for wetting layers with nonuniform cross-sectional area and analyzing the viscous coupling effects between fluid phases can be the subject of the future work. For example, [Raeini et al. \(2018\)](#) employed the numerical method developed in this study to perform two-phase direct numerical simulations on different three-dimensional pore geometries with nonuniform cross-

sections. They computed wetting layer conductivities for different fluid configurations, before and after the snap-off event, and used the values to validate their pore network model.

4.6. Closure

This chapter is dedicated to the study of viscous coupling effects in two-phase flow through non-circular capillary tubes with uniform and non-uniform wettability conditions. The results indicate that momentum transfer across the interface due to viscous coupling can significantly affect the hydraulic conductance of fluid layers that form in corners of a capillary. It is demonstrated that for clean interfaces where the interfacial shear viscosity is zero, the amount of flow in corners and sandwiched layers using free-slip and no-flow boundary conditions, for a specific range of viscosity ratios, can deviate significantly than that computed from the physically correct continuity boundary condition.

Two-phase direct numerical simulation results have been used in conjunction with basic arguments from fluid mechanics to present simple hydraulic conductance relations that take into account the viscous coupling effects. These relations have been validated against numerical results for a wide range of geometric parameters and viscosity ratios which can then be incorporated into pore-to-Darcy-scale flow models, for example two-phase pore-network models, to study the effects of viscous coupling on macroscopic flow properties such as relative permeabilities.

5. Conclusions and future work

5.1. Conclusions

This thesis introduces a finite-volume based volume-of-fluid approach to accurately model two-phase flow at the micro-scale where capillary forces are dominant. We propose a numerical scheme within a finite-volume volume-of-fluid framework, for immiscible two-phase flow at relatively low capillary numbers, $Ca = 10^{-4}$ to 10^{-5} . We adapt interFoam (Deshpande et al., 2012), a volume-of-fluid based solver, in OpenFOAM (OpenFOAM, 2016), an open-source C++ library for solving continuum mechanics problems with an emphasis on computational fluid dynamics (CFD) (Jasak, 1996; Jasak et al., 2007), as the basis for implementing our numerical method.

Through this study the following contributions have been made to improve the numerical solution procedure:

- Implementation of a new simple and robust face-based reconstruction algorithm to define the fluid–fluid interface as a sharp iso-line/surface, based on the underlying volume fractions of the fluids.
- Implementation of a novel interfacial force model, so-called contour-level surface force (CLSF) model, which effectively suppresses the spurious currents.

These contributions improve the stability and accuracy of the numerical algorithm. The interfacial force model is implemented in a well-balanced and conservative way, which makes the improved numerical algorithm suitable for studying two-phase flow problems for low capillary numbers. The stability and accuracy of the implemented scheme is validated on several two- and three-dimensional test cases, which indicate the capability of the method to model two-phase flow processes at the micro-scale.

The following contributions have been made in terms of pore-scale studies:

- Investigation of the role and importance of momentum transfer across the fluid–fluid interface in two-phase flow.
- Formulation and validation of simple hydraulic conductance relations that take into account viscous coupling effects across the fluid–fluid interface. These scale models can be incorporated into pore-to-Darcy-scale flow models such as pore-network models to study the effects of viscous coupling on macroscopic flow properties such as relative permeabilities.

In the following the main conclusions are summarized:

- In Chapter 2, we introduced a novel, accurate and robust numerical technique for computing interfacial forces at low capillary numbers. This method is based on the evaluation of line integrals over closed boundaries of reconstructed interfacial surface elements. The interfacial forces are computed using a sharp surface force model that can efficiently eliminate the problem of spurious currents. The explicit representation of the interface used

to compute interfacial forces leads to an accurate estimation of capillary pressure even for low grid resolutions. This can be very important to model multiphase flows directly on micro-CT images of porous media for which simulations with a very fine grid resolution are prohibitively expensive using currently available computational resources.

The main advantages of this method are: (1) It employs a sharp indicator function to mark mixed-faces cut by the fluid-fluid interface. The interfacial force is considered only on the mixed-faces that leads to a well-balanced method that can predict the sharp profile of the pressure jump across the interface accurately, (2) It does not require the estimation of interface curvature as the gradient of normal interface unit vectors. This simplifies the computation procedure by not requiring the numerical estimation of a gradient operator, (3) It computes the interfacial forces only on reconstructed interface elements in a fully conserved fashion. Transferring the computed forces to corresponded mixed-faces is accompanied by a regularization (smoothing) procedure to preserve the force conservation to a great extent, (4) A second-order least-squares method is used to numerically estimate the gradient of the indicator function in the process of interface reconstruction. This leads to a more localized estimation of the gradient operator that is crucial to pinpoint the location of the interface accurately, (5) The interface reconstruction phase is quite simple and applicable to both two- and three-dimensional meshes without any additional effort.

- In Chapter 3, we validated the numerical method using several static and dynamic test cases. We showed that the new interfacial force formulation, the CLSF model, correctly predicts the pressure inside a stationary droplet in two and three dimensions, as given by Young-Laplace equation. The method remarkably reduces non-physical velocities referred to as spurious currents, which is a direct consequence of discrepancy between pressure gradient and computed interfacial force. Passing this test case verifies that the method is able to compute the interfacial force reasonably accurate in a well-balanced fashion. Comparing the performance of this model to SSF and CSF models, shows that employing a sharp indicator function to concentrate the computed interfacial force in a narrower band, can reduce or eliminate spurious currents in the static droplet test case.

Modelling the translation of a two- or three-dimensional droplet in a uniform velocity field can be quite challenging for two main reasons: (1) the indicator function gets disturbed constantly, therefore the numerical model should be able to balance the forces as quickly as possible, and (2) errors in computation of the interfacial force can accumulate with time and violate the conservation of interfacial force on the closed surface of the droplet. The violation of the force conservation often manifests itself as high spurious currents which either get the droplet pinned or make it to move with a non-physical velocity. We showed that the CLSF method is able to simulate a two-dimensional moving droplet in a uniform velocity field with the capillary number as low as 10^{-5} . This means three orders of magnitude improvement in comparison to the CSF and SSF models. For a three-dimensional test case the method can also predict the droplet motion even if the capillary

number goes down to 10^{-4} , while the lowest capillary number for which the CSF and SSF models can simulate the test case is 10^{-2} . Rigorous sensitivity analyses are performed on the moving droplet test case to investigate the performance and accuracy of the numerical model with different mesh resolutions and capillary numbers.

We examined the ability of the method to model contact-line statics and dynamics where the fluid-fluid interface comes into contact with a solid surface. Results from several two- and three-dimensional numerical experiments with different contact angles demonstrated the efficiency and accuracy of the CLSF model in simulating static and moving contact-lines in presence of a solid boundary.

In our test cases, we also showed, for instance, how the consideration of co-current flow of two viscous fluids leads to a much lower flow resistance in layers than computed previously assuming that the centre of the pore space was gas-filled. This opened up the opportunity for future work where we used high-resolution pore-scale simulations to quantify flow conductance for input into larger scale flow models as discussed in Chapter 4.

- In Chapter 4, we investigated viscous coupling effects, due to momentum transfer across the fluid-fluid interface, in immiscible two-phase flow through single non-circular micron-size capillary tubes, with respect to the corner angle, the contact angle, the wetting saturation, the viscosity ratio and the wettability condition. We validated the numerical method by verifying the velocity profile for co-current flow of two immiscible fluids with different viscosity ratios through a square capillary tube. We demonstrated that the momentum transfer between the two fluid phases can significantly affect the flow conductance of sandwiched layers in the corners of a capillary. We showed that applying no-flow or free-slip boundary conditions may lead to under- or over-estimation of the layer flow conductance compared to the physically correct continuity boundary condition.

By analogy with simple flow models such as Poiseuille flow and Couette flow, we put forward new parametric scaling models to estimate the flow conductivities for fluids in centre and corner of capillaries with uniform wettability as well as layers sandwiched between centre and corner of capillaries with non-uniform wettability. We validated scaling models by comparing the predicted values based on these models to those obtained from direct numerical simulations for different fluid configurations and viscosity ratios. These scaling models can be incorporated into two-phase network models to estimate the effects of flow coupling on macroscopic flow properties such as relative permeability.

5.2. Future work

The suggested improvements and extensions are as follows:

- In this work, the implementation of the interfacial force is explicit in time, and therefore small time steps have to be taken to satisfy the numerical capillary time step constraint,

Equation (3.1). Implementing the interfacial force implicitly or semi-implicitly in time can remove or relax this restriction and allow for larger time steps in our simulations. This can greatly improve the computational efficiency of the method. An example of a semi-implicit implementation of the CSF method within a finite element framework can be found in Hysing (2006). Raessi et al. (2009) later presented an implementation of Hysing (2006) in a finite volume context and showed that the time step can be increased by a factor of 5 without compromising the stability and accuracy of the method. One can follow a similar procedure to implement the CLSF method semi-implicitly in time and then examine the performance of the method on the presented test cases in Chapter 3.

- In this work, the mathematical paradox of a contact-line moving along a solid surface with no-slip boundary condition is implicitly resolved by translating the contact-line using face-centred velocities in the vicinity of the solid boundary. However the implicit slip introduced by this approach, as discussed in Afkhami et al. (2009), is a function of grid spacing and the solution does not converge with mesh refinement. Therefore, implementing other boundary conditions such as the Navier condition or the mesh-dependent dynamic contact angle boundary condition introduced in Afkhami et al. (2009), and investigating the impact of these boundary conditions on the contact-line dynamics would be useful.
- In this work, the wettability condition is modelled through imposing a constant static contact angle and modifying the interface normal vectors at the solid boundary in accordance with the contact angle. Implementing dynamic contact angle models that honour contact angle hysteresis and velocity of the moving contact-line can be of great importance when simulating immiscible two-phase flow including imbibition and drainage of wetting and non-wetting phases; see Fang et al. (2008) for an example of implementing contact angle hysteresis in a three-dimensional volume-of-fluid framework at the micro-scale.
- In this work, the interfacial tension coefficient, σ , is assumed to be uniform and constant all over the fluid-fluid interface. The interfacial tension, however, can be a function of temperature and concentration, and its gradient on the interface leads to a tangential driving force acting on the interface. Therefore, another worthy addition would be the implementation of a variable interfacial force model in the context of the CLSF method. This would enable us to apply the method to simulate immiscible two-phase flow including surfactant flooding; see Seric et al. (2018) for an example of implementing a variable interfacial force model within a volume-of-fluid framework.
- We made use of the numerical method to investigate viscous coupling effects in two-phase flow through capillary tubes with uniform cross section, i.e. contraction ratio is equal to 1, and suggested parametric scaling models to estimate flow conductivities for different phases. For these cases, however, the thickness of corner and sandwiched layers is uniform along the tubes, which is not the case for two-phase flow in geological porous media.

Therefore, one can follow a similar procedure for capillary tubes with non-uniform cross-sectional areas and include the contraction ratio as another free parameter in the related analyses and scaling models.

- A comprehensive study is required to investigate the performance and accuracy of the numerical method to model two-phase direct numerical simulations on micro-CT pore-space images of porous media. Being able to perform two-phase flow directly on these images can be quite useful to explore dynamic pore-scale mechanisms, which control macroscopic properties and dictate the structure of the phase distribution and residual saturation within porous media. It would be helpful to benchmark and validate our work through direct pore-by-pore comparisons with experiments where pore-scale imaging is performed during a displacement. We single out the experimental work by Singh et al. (2017) as an example of a three-dimensional dynamic visualization study of pore-scale processes during immiscible two-phase flow in geological porous media. They employed fast synchrotron micro-CT to image real-time displacement processes and obtain time-dependent information on ganglia and disconnected non-wetting phase clusters. They analyzed the information to describe the dynamics of snap-off and pore-filling processes in detail. The numerical method presented in this thesis can be used to simulate similar pore-scale displacements in local pore-space geometries with limited numbers of pores and throats, which are cropped from the full size image. The fluids can be initialized and equilibrated through the computational domain based on visualized information obtained from experiments. By applying appropriate boundary conditions, one can simulate the imbibition displacement process for pore-space geometries and fluid configurations presented in their work to check whether the numerical simulations predict similar results, namely local capillary pressures and snap-off events, to the experiments. These numerical simulations can be quite useful to resolve the situations where experimental results do not follow well-known classic rules, e.g. snap-off in a throat with a smaller aspect ratio (the ratio of pore radius to throat radius) while there are other throats with larger aspect ratios connected to the pore. In addition, possible sources of discrepancy between experiments and numerical simulations can be investigated to improve the numerical method.
- Moreover, these numerical simulations can also be exploited to obtain up-scaled relationships to determine flow and displacement capillary pressure for input into pore network models, similar to the approach described in Chapter 4. These network models provide a much more computationally efficient framework for the simulation of flows on full size images. Again, the pore-by-pore prediction of the displacement sequence and local occupancy of the phases using network models with up-scaled properties derived from direct simulation can be compared with imaging experiments. This type of analysis can then be extended to study a variety of rocks types and different wettability conditions, providing a useful tool for the prediction and characterization of multiphase flow in porous media.

Bibliography

- Afkhami, S., Buongiorno, J., Guion, A., Popinet, S., Scardovelli, R., and Zaleski, S. (2017). Transition in a numerical model of contact line dynamics and forced dewetting. *arXiv preprint*.
- Afkhami, S. and Bussmann, M. (2008). Height functions for applying contact angles to 2D VOF simulations. *International Journal for Numerical Methods in Fluids*, 57(4):453–472.
- Afkhami, S. and Bussmann, M. (2009). Height functions for applying contact angles to 3D VOF simulations. *International Journal for Numerical Methods in Fluids*, 61(8):827–847.
- Afkhami, S., Zaleski, S., and Bussmann, M. (2009). A mesh-dependent model for applying dynamic contact angles to VOF simulations. *Journal of Computational Physics*, 228(15):5370–5389.
- Ahrenholz, B., Tölke, J., Lehmann, P., Peters, A., Kaestner, A., Krafczyk, M., and Durner, W. (2008). Prediction of capillary hysteresis in a porous material using lattice-Boltzmann methods and comparison to experimental data and a morphological pore network model. *Advances in Water Resources*, 31(9):1151–1173.
- Al-Futaisi, A. and Patzek, T. W. (2003). Three-phase hydraulic conductances in angular capillaries. *SPE Journal*, 8(03):252–261.
- Alpak, F. O., Riviere, B., and Frank, F. (2016). A phase-field method for the direct simulation of two-phase flows in pore-scale media using a non-equilibrium wetting boundary condition. *Computational Geosciences*, 20(5):881–908.
- Anderson, D. M., McFadden, G. B., and Wheeler, A. A. (1998). Diffuse-interface methods in fluid mechanics. *Annual Review of Fluid Mechanics*, 30(1):139–165.
- Avraam, D. G. and Payatakes, A. C. (1995a). Flow regimes and relative permeabilities during steady-state two-phase flow in porous media. *Journal of Fluid Mechanics*, 293:207–236.
- Avraam, D. G. and Payatakes, A. C. (1995b). Generalized relative permeability coefficients during steady-state two-phase flow in porous media, and correlation with the flow mechanisms. In *Multiphase Flow in Porous Media*, pages 135–168. Springer.
- Avraam, D. G. and Payatakes, A. C. (1999). Flow mechanisms, relative permeabilities, and coupling effects in steady-state two-phase flow through porous media. The case of strong wettability. *Industrial and Engineering Chemistry Research*, 38(3):778–786.
- Bakke, S. and Øren, P. E. (1997). 3-D pore-scale modelling of sandstones and flow simulations in the pore networks. *SPE Journal*, 2(2):136–149.

- Balhoff, M. T. and Wheeler, M. F. (2009). A predictive pore-scale model for non-Darcy flow in porous media. *SPE Journal*, 14(4):579–587.
- Blunt, M. J. (2001). Flow in porous mediapore-network models and multiphase flow. *Current Opinion in Colloid and Interface Science*, 6(3):197–207.
- Blunt, M. J. (2017). *Multiphase flow in permeable media: a pore-scale perspective*. Cambridge University Press.
- Blunt, M. J., Bijeljic, B., Dong, H., Gharbi, O., Iglauer, S., Mostaghimi, P., Paluszny, A., and Pentland, C. (2013). Pore-scale imaging and modelling. *Advances in Water Resources*, 51:197–216.
- Blunt, M. J. and King, P. (1991). Relative permeabilities from two-and three-dimensional pore-scale network modelling. *Transport in Porous Media*, 6(4):407–433.
- Blunt, M. J. and Scher, H. (1995). Pore-level modeling of wetting. *Physical Review E*, 52(6):6387.
- Brackbill, J. U., Kothe, D. B., and Zemach, C. (1992). A continuum method for modeling surface tension. *Journal of Computational Physics*, (100):335–354.
- Bryant, S. and Blunt, M. J. (1992). Prediction of relative permeability in simple porous media. *Physical Review A*, 46(4):2004–2011.
- Chen, H., Chen, S., and Matthaeus, W. H. (1992). Recovery of the Navier-Stokes equations using a lattice-gas Boltzmann method. *Physical Review A*, 45(8):R5339.
- Chen, S. and Doolen, G. D. (1998). Lattice Boltzmann Method. *Annual Review of Fluid Mechanics*, 30:329–364.
- Cox, R. G. (1986). The dynamics of the spreading of liquids on a solid surface. Part 1. Viscous flow. *Journal of Fluid Mechanics*, 168:169–194.
- Dehghanpour, H., Aminzadeh, B., and DiCarlo, D. A. (2011). Hydraulic conductance and viscous coupling of three-phase layers in angular capillaries. *Physical Review E*, 83(6):66320.
- Deshpande, S., Anumolu, L., and Trujillo, M. F. (2012). Evaluating the performance of the two-phase flow solver interFoam. *Computational Science and Discovery*, 5(1):014016.
- Dong, H. and Blunt, M. J. (2009). Pore-network extraction from micro-computerized-tomography images. *Physical Review E*, 80:036307.
- Dong, M. and Chatzis, I. (1995). The imbibition and flow of a wetting liquid along the corners of a square capillary tube. *Journal of Colloid and Interface Science*, 172(2):278–288.
- Dussan, E. B. (1979). On the spreading of liquids on solid surfaces: static and dynamic contact lines. *Annual Review of Fluid Mechanics*, 11(1):371–400.

- Ehrlich, R. (1993). Viscous coupling in two-phase flow in porous media and its effect on relative permeabilities. *Transport in Porous Media*, 11(3):201–218.
- Eral, H. B., Oh, J. M., and Others (2013). Contact angle hysteresis: a review of fundamentals and applications. *Colloid and Polymer Science*, 291(2):247–260.
- Fang, C., Hidrovo, C., Wang, F.-m., Eaton, J., and Goodson, K. (2008). 3-D numerical simulation of contact angle hysteresis for microscale two phase flow. *International Journal of Multiphase Flow*, 34(7):690–705.
- Fatt, I. (1956). The network model of porous media. *Petroleum Transactions, AIME*, 207:144–181.
- Ferrari, A. and Lunati, I. (2013). Direct numerical simulations of interface dynamics to link capillary pressure and total surface energy. *Advances in Water Resources*, 57:19–31.
- Ferziger, J. H. and Peric, M. (2012). *Computational methods for fluid dynamics*. Springer Science & Business Media.
- Francois, M. M., Cummins, S. J., Dendy, E. D., Kothe, D. B., Sicilian, J. M., and Williams, M. W. (2006). A balanced-force algorithm for continuous and sharp interfacial surface tension models within a volume tracking framework. *Journal of Computational Physics*, 213:141–173.
- Fyfe, D. E., Oran, E. S., and Fritts, M. J. (1988). Surface tension and viscosity with Lagrangian hydrodynamics on a triangular mesh. *Journal of Computational Physics*, 76(2):349–384.
- Gao, L. and McCarthy, T. J. (2006). Contact angle hysteresis explained. *Langmuir*, 22(14):6234–6237.
- Glimm, J., Grove, J. W., Li, X. L., and Zhao, N. (1999). Simple front tracking. *Contemporary Mathematics*, 238(2):133–149.
- Glimm, J., McBryan, O. A., Menikoff, R., and Sharp, D. H. (1986). Front tracking applied to Rayleigh-Taylor instability. *SIAM Journal on Scientific and Statistical Computing*, 7(1):230–251.
- Gueyffier, D., Li, J., Nadim, A., Scardovelli, R., and Zaleski, S. (1999). Volume-of-Fluid interface tracking with smoothed surface stress methods for three-dimensional flows. *Journal of Computational Physics*, 152:423–456.
- Gupta, L. and Wasan, D. T. (1974). Surface shear viscosity and related properties of adsorbed surfactant films. *Industrial and Engineering Chemistry Fundamentals*, 13(1):26–33.
- Harlow, F. H. and Welch, J. E. (1965). Numerical calculation of time-dependent viscous incompressible flow of fluid with free surface. *The Physics of Fluids*, 8:2182–2189.

- He, W., Yi, J. S., and Van Nguyen, T. (2000). Two-phase flow model of the cathode of PEM fuel cells using interdigitated flow fields. *AIChE Journal*, 46(10):2053–2064.
- Hirt, C. and Nichols, B. (1981). Volume of fluid (VOF) method for the dynamics of free boundaries. *Journal of Computational Physics*, 39(1):201–225.
- Hysing, S. (2006). A new implicit surface tension implementation for interfacial flows. *International Journal for Numerical Methods in Fluids*, 51(6):659–672.
- Issa, R. I. (1986). Solution of the implicitly discretised fluid flow equations by operator-splitting. *Journal of Computational Physics*, 62(1):40–65.
- Jacqmin, D. (1999). Calculation of two-phase NavierStokes flows using phase-field modeling. *Journal of Computational Physics*, 155(1):96–127.
- Jacqmin, D. (2000). Contact-line dynamics of a diffuse fluid interface. *Journal of Fluid Mechanics*, 402:57–88.
- Jamet, D., Torres, D., and Brackbill, J. U. (2002). On the theory and computation of surface tension: the elimination of parasitic currents through energy conservation in the second-gradient method. *Journal of Computational Physics*, 182:262–276.
- Jasak, H. (1996). Error analysis and estimation for the finite volume method with applications to fluid flows. *PhD thesis, Imperial College London*.
- Jasak, H., Jemcov, A., Tukovic, Z., and Others (2007). OpenFOAM: A C++ library for complex physics simulations. In *International workshop on coupled methods in numerical dynamics*, pages 1–20. IUC Dubrovnik, Croatia.
- Kalaydjian, F. (1990). Origin and quantification of coupling between relative permeabilities for two-phase flows in porous media. *Transport in Porous Media*, 5(3):215–229.
- Ketcham, R. A. and Carlson, W. D. (2001). Acquisition, optimization and interpretation of X-ray computed tomographic imagery: applications to the geosciences. *Computers and Geosciences*, 27(4):381–400.
- Lafaurie, B., Nardone, C., Scardovelli, R., Zaleski, S., and Zanetti, G. (1994). Modelling merging and fragmentation in multiphase flows with SURFER. *Journal of Computational Physics*, 113(1):134–147.
- Lake, L. W. (1989). *Enhanced oil recovery*. Prentice Hall.
- Legait, B. (1983). Laminar flow of two phases through a capillary tube with variable square cross-section. *Journal of Colloid and Interface Science*, 96(1):28–38.
- Legendre, D. and Maglio, M. (2015). Comparison between numerical models for the simulation of moving contact lines. *Computers and Fluids*, 113:2–13.

- Li, H., Pan, C., and Miller, C. T. (2005). Pore-scale investigation of viscous coupling effects for two-phase flow in porous media. *Physical Review E*, 72(2):26705.
- Lindquist, W. B., Lee, S.-M., Coker, D. A., Jones, K. W., and Spanne, P. (1996). Medial axis analysis of void structure in three-dimensional tomographic images of porous media. *Journal of Geophysical Research: Solid Earth*, 101(B4):8297–8310.
- Liu, M. B. and Liu, G. R. (2010). Smoothed particle hydrodynamics (SPH): an overview and recent developments. *Archives of Computational Methods in Engineering*, 17(1):25–76.
- Liu, Y. and Yu, X. (2016). A coupled phase-field and volume-of-fluid method for accurate representation of limiting water wave deformation. *Journal of Computational Physics*, 321:459–475.
- Lopez, X., Valvatne, P. H., and Blunt, M. J. (2003). Predictive network modeling of single-phase non-Newtonian flow in porous media. *Journal of Colloid and Interface Science*, 264(1):256–265.
- Marini, L. (2006). *Geological sequestration of carbon dioxide: thermodynamics, kinetics, and reaction path modeling*. Elsevier.
- McKee, S., Tomé, M. F., Ferreira, V. G., Cuminato, J., Castelo, A., Sousa, F. S., and Mangiacchi, N. (2008). The MAC method. *Computers and Fluids*, 37(8):907–930.
- Meakin, P. and Tartakovsky, A. (2009). Modeling and simulation of pore-scale multiphase fluid flow and reactive transport in fractured and porous media. *Reviews of Geophysics*, 47:RG3002.
- Mercer, J. W. and Cohen, R. M. (1990). A review of immiscible fluids in the subsurface: properties, models, characterization and remediation. *Journal of Contaminant Hydrology*, 6(2):107–163.
- Monaghan, J. J. (1994). Simulating free surface flows with SPH. *Journal of Computational Physics*, 110(2):399–406.
- Mulligan, C. N., Yong, R. N., and Gibbs, B. F. (2001). Surfactant-enhanced remediation of contaminated soil: a review. *Engineering Geology*, 60(1):371–380.
- Onsager, L. (1931). Reciprocal relations in irreversible processes. I. *Physical Review*, 37(4):405.
- OpenFOAM (2016). The open source CFD toolbox. URL <http://www.openfoam.com>.
- Øren, P. E. and Bakke, S. (2003). Reconstruction of Berea sandstone and pore-scale modelling of wettability effects. *Journal of Petroleum Science and Engineering*, 39(3-4):177–199.
- Osher, S. and Fedkiw, R. P. (2001). Level set methods: an overview and some recent results. *Journal of Computational Physics*, 169(2):463–502.

- Osher, S. and Sethian, J. A. (1988). Fronts propagating with curvature dependent speed: algorithms based on Hamilton-Jacobi formulations. *Journal of Computational Physics*, 79:12–49.
- Pan, C., Hilpert, M., and Miller, C. T. (2004). Lattice-Boltzmann simulation of two-phase flow in porous media. *Water Resources Research*, 40(1):W01501.
- Piri, M. and Blunt, M. (2005a). Three-dimensional mixed-wet random pore-scale network modeling of two- and three-phase flow in porous media. II. Results. *Physical Review E*, 71(2):1–11.
- Piri, M. and Blunt, M. J. (2005b). Three-dimensional mixed-wet random pore-scale network modeling of two- And three-phase flow in porous media. I. Model description. *Physical Review E*, 71(2):1–30.
- Popinet, S. (2018). Numerical models of surface tension. *Annual Review of Fluid Mechanics*, 50:49–75.
- Popinet, S. and Zaleski, S. (1999). A front-tracking algorithm for accurate representation of surface tension. *International Journal for Numerical Methods in Fluids*, 30(6):775–793.
- Raeini, A. Q., Bijeljic, B., and Blunt, M. J. (2015). Modelling capillary trapping using finite-volume simulation of two-phase flow directly on micro-CT images. *Advances in Water Resources*, 83:102–110.
- Raeini, A. Q., Bijeljic, B., and Blunt, M. J. (2017). Generalized network modeling: Network extraction as a coarse-scale discretization of the void space of porous media. *Physical Review E*, 96(1):13312.
- Raeini, A. Q., Bijeljic, B., and Blunt, M. J. (2018). Generalized network modeling of capillary-dominated two-phase flow. *Physical Review E*, 97(2):23308.
- Raeini, A. Q., Blunt, M. J., and Bijeljic, B. (2012). Modelling two-phase flow in porous media at the pore scale using the volume-of-fluid method. *Journal of Computational Physics*, 231(17):5653–5668.
- Raeini, A. Q., Blunt, M. J., and Bijeljic, B. (2014). Direct simulations of two-phase flow on micro-CT images of porous media and upscaling of pore-scale forces. *Advances in Water Resources*, 74:116–126.
- Raessi, M., Bussmann, M., and Mostaghimi, J. (2009). A semi-implicit finite volume implementation of the CSF method for treating surface tension in interfacial flows. *International journal for numerical methods in fluids*, 59(10):1093–1110.
- Ramstad, T., Øren, P.-E., Bakke, S., and Others (2010). Simulation of two-phase flow in reservoir rocks using a lattice Boltzmann method. *SPE Journal*, 15(04):917–927.

- Ransohoff, T. C. and Radke, C. J. (1988). Laminar flow of a wetting liquid along the corners of a predominantly gas-occupied noncircular pore. *Journal of Colloid and Interface Science*, 121(2):392–401.
- Raoof, A., Nick, H. M., Hassanizadeh, S. M., and Spiers, C. J. (2013). PoreFlow: a complex pore-network model for simulation of reactive transport in variably saturated porous media. *Computers and Geosciences*, 61:160–174.
- Renardy, M., Renardy, Y., and Li, J. (2001). Numerical simulation of moving contact line problems using a volume-of-fluid method. *Journal of Computational Physics*, 171(1):243–263.
- Renardy, Y. and Renardy, M. (2002). PROST: a parabolic reconstruction of surface tension for the volume-of-fluid method. *Journal of Computational Physics*, 183:400–421.
- Rose, W. (2000). Myths about later-day extensions of Darcy’s law. *Journal of Petroleum Science and Engineering*, 26(1):187–198.
- Rusche, H. (2002). Computational fluid dynamics of dispersed two-phase flows at high phase fractions. *PhD thesis, Imperial College London*.
- Ryskin, G. and Leal, L. G. (1984). Numerical solution of free-boundary problems in fluid mechanics. Part 2. Buoyancy-driven motion of a gas bubble through a quiescent liquid. *Journal of Fluid Mechanics*, 148:19–35.
- Scardovelli, R. and Zaleski, S. (1999). Direct numerical simulation of free-surface and interfacial flow. *Annual Review of Fluid Mechanics*, 31(1):567–603.
- Seric, I., Afkhami, S., and Kondic, L. (2018). Direct numerical simulation of variable surface tension flows using a Volume-of-Fluid method. *Journal of Computational Physics*, 352:615–636.
- Shan, X. (2006). Analysis and reduction of the spurious current in a class of multiphase lattice Boltzmann models. *Physical Review E*, 73:047701.
- Shan, X. and Chen, H. (1993). Lattice Boltzmann model for simulating flows with multi phases and components. *Physical Review E*, 47(3):1815–1819.
- Silin, D. and Patzek, T. (2006). Pore space morphology analysis using maximal inscribed spheres. *Physica A: Statistical Mechanics and its Applications*, 371(2):336–360.
- Singh, K. and Blunt, M. J. (2018). High resolution X-ray micro-tomography datasets for in-situ effective contact angle analysis in carbonate rocks. URL <http://www.digitalrockportal.org/projects/125>.

- Singh, K., Menke, H., Andrew, M., Lin, Q., Rau, C., Blunt, M. J., and Bijeljic, B. (2017). Dynamics of snap-off and pore-filling events during two-phase fluid flow in permeable media. *Scientific Reports*, 7(1):5192.
- Spelt, P. D. M. (2005). A level-set approach for simulations of flows with multiple moving contact lines with hysteresis. *Journal of Computational Physics*, 207(2):389–404.
- Srinivasan, S. (2006). *Fuel cells: from fundamentals to applications*. Springer Science & Business media.
- Sussman, M., Smereka, P., and Osher, S. (1994). A level set approach for computing solutions to incompressible two-phase flow. *Journal of Computational Physics*, 114(1):146–159.
- Tanguy, S., Ménard, T., and Berlemont, A. (2007). A level set method for vaporizing two-phase flows. *Journal of Computational Physics*, 221(2):837–853.
- Tartakovsky, A. and Meakin, P. (2005). Modeling of surface tension and contact angles with smoothed particle hydrodynamics. *Physical Review E*, 72:026301.
- Tartakovsky, A. M. and Meakin, P. (2006). Pore scale modeling of immiscible and miscible fluid flows using smoothed particle hydrodynamics. *Advances in Water Resources*, 29(10):1464–1478.
- Tartakovsky, A. M., Trask, N., Pan, K., Jones, B., Pan, W., and Williams, J. R. (2016). Smoothed particle hydrodynamics and its applications for multiphase flow and reactive transport in porous media. *Computational Geosciences*, 20(4):807–834.
- Thompson, K. E., Willson, C. S., White, C. D., Nyman, S., Bhattacharya, J., and Reed, A. H. (2008). Application of a new grain-based reconstruction algorithm to microtomography images for quantitative characterization and flow modeling. *SPE Journal*, 13(2):164–176.
- Tørå, G., Øren, P.-E., and Hansen, A. (2012). A dynamic network model for two-phase flow in porous media. *Transport in Porous Media*, 92(1):145–164.
- Tryggvason, G., Bunner, B., Esmaeeli, A., Juric, D., Al-Rawahi, N., Tauber, W., Han, J., Nas, S., and Jan, Y.-J. (2001). A front-tracking method for the computations of multiphase flow. *Journal of Computational Physics*, 169:708–759.
- Tryggvason, G., Scardovelli, R., and Zaleski, S. (2011). *Direct numerical simulations of gas-liquid multiphase flows*. Cambridge University Press.
- Unverdi, S. O. and Tryggvason, G. (1992). A front-tracking method for viscous, incompressible, multi-fluid flows. *Journal of Computational Physics*, 100(1):25–37.
- Valvatne, P. H. and Blunt, M. J. (2004). Predictive pore-scale modeling of two-phase flow in mixed wet media. *Water Resources Research*, 40(7):W07406.

- Van Dijke, M. I. J., Sorbie, K. S., Sohrabi, M., Tehrani, D., and Danesh, A. (2004). Three-phase flow in WAG processes in mixed-wet porous media: pore-scale network simulations and comparison with micromodel experiments. *SPE Journal*, 9(1):57–66.
- Weller, H. G., Tabor, G., Jasak, H., and Fureby, C. (1998). A tensorial approach to computational continuum mechanics using object-oriented techniques. *Computers in Physics*, 12(6):620.
- Wendl, M. C. (1999). General solution for the Couette flow profile. *Physical Review E*, 60(5):6192.
- Whitaker, S. (1986). Flow in porous media II: the governing equations for immiscible, two-phase flow. *Transport in Porous Media*, 1(2):105–125.
- Wildenschild, D. and Sheppard, A. P. (2013). X-ray imaging and analysis techniques for quantifying pore-scale structure and processes in subsurface porous medium systems. *Advances in Water Resources*, 51:217–246.
- Xie, C., Raeini, A. Q., Wang, Y., Blunt, M. J., and Wang, M. (2017). An improved pore-network model including viscous coupling effects using direct simulation by the lattice Boltzmann method. *Advances in Water Resources*, 100:26–34.
- Young, T. (1805). III. An essay on the cohesion of fluids. *Philosophical Transactions of the Royal Society of London*, 95:65–87.
- Zhou, D., Blunt, M., and Orr, F. M. (1997). Hydrocarbon drainage along corners of noncircular capillaries. *Journal of Colloid and Interface Science*, 187(1):11–21.
- Zhu, Y., Fox, P. J., and Morris, J. P. (1999). A pore-scale numerical model for flow through porous media. *International Journal for Numerical and Analytical Methods in Geomechanics*, 23(9):881–904.

A. Semi-analytical solution of the velocity profile for two-phase flow through a uniform single tube

The equations of motion for low-Reynolds-number axial flow of an incompressible Newtonian fluid through a horizontal single tube with a uniform regular s -sided polygonal cross-section, reduce to (Ehrlich, 1993)

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} + \frac{\xi}{\mu} = 0, \quad (\text{A.1})$$

where r and θ are, respectively, the radial and angular coordinates in the cylindrical coordinate system with reference to the centre of the tube, O , u is the axial velocity, μ is the fluid viscosity and ξ is the pressure gradient in the flow direction, see Figure A.1.

Ehrlich (1993) presented the following series solution for Equation (A.1)

$$u(r, \theta) = \frac{\xi}{\mu} \left(\frac{-r^2}{4} + \sum_{n=0}^{\infty} a_n r^{sn} \cos(sn\theta) \right), \quad (\text{A.2})$$

by assuming that the solution is bounded at $r = 0$ and flow is symmetric with respect to planes $\theta = i\pi/s$, where i is an integer, $i \in \mathbb{Z}$, and s is the number of the sides of the polygonal cross-section. This solution is subjected to a no-slip boundary condition at the tube wall.

For two-phase flow where the non-wetting phase, fluid 2, flows in the centre of the tube while the wetting phase, fluid 1, resides in the corners, the velocity distributions are given by the series

$$u_1(r, \theta) = \frac{\xi}{\mu_1} \left(\frac{-r^2}{4} + \sum_{n=0}^{\infty} b_n r^{sn} \cos(sn\theta) + \sum_{n=1}^{\infty} c_n r^{-sn} \cos(sn\theta) \right), \quad (\text{A.3})$$

and

$$u_2(r, \theta) = \frac{\xi}{\mu_2} \left(\frac{-r^2}{4} + \sum_{n=0}^{\infty} a_n r^{sn} \cos(sn\theta) \right). \quad (\text{A.4})$$

These solutions are subjected to three boundary conditions as follows:

1. Zero velocity at the tube wall, w ,

$$u_1(r_w, \theta) = u_2(r_w, \theta) = 0. \quad (\text{A.5})$$

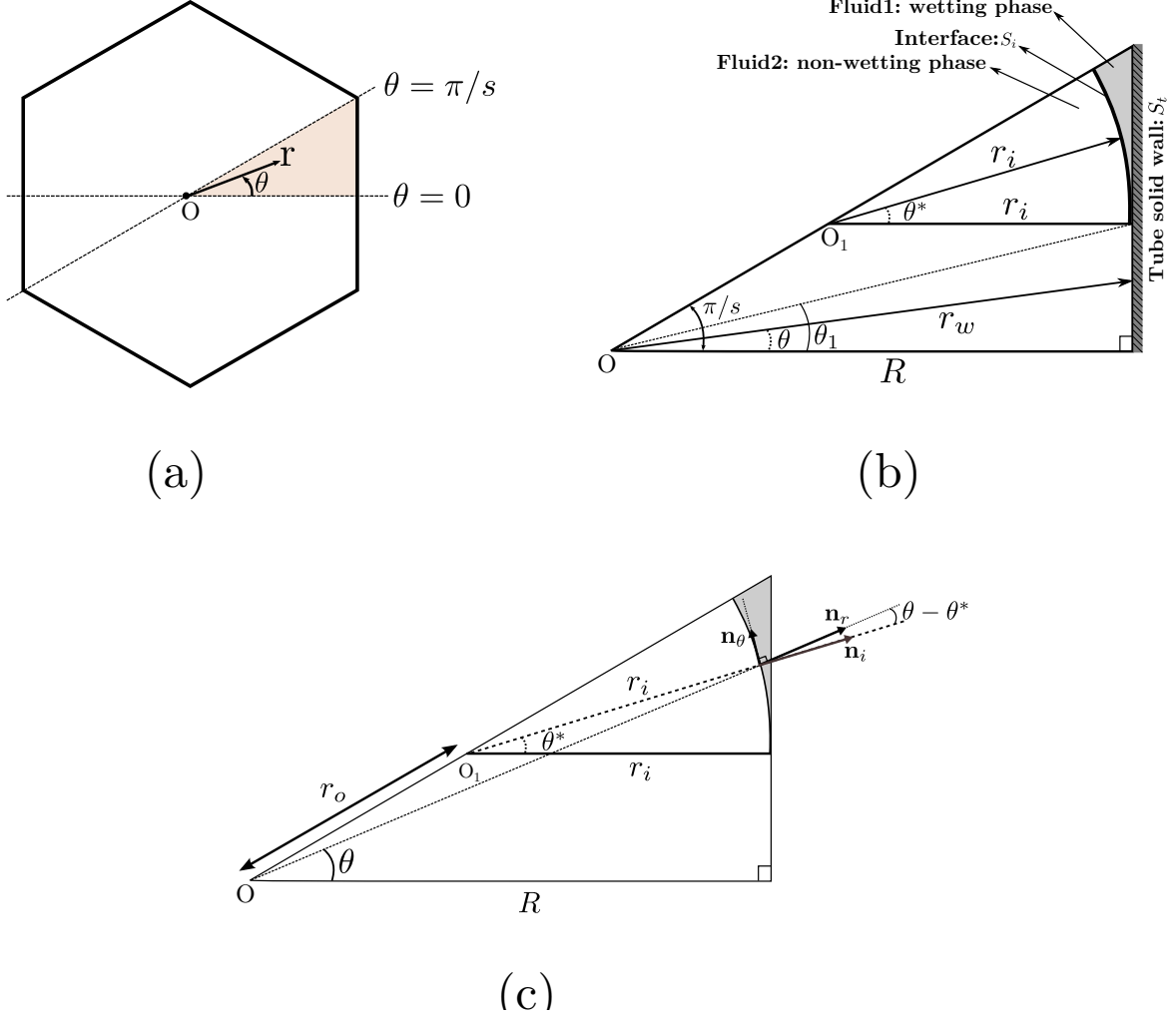


Figure A.1. Schematic of a uniform polygonal tube geometry: (a) Cross-sectional view of a polygonal uniform tube with two of its symmetry planes at $\theta = 0$ and $\theta = \pi/s$, (b) a symmetry element of the tube with the fluid-fluid interface, and (c) the unit normal at the interface and its relation to the cylindrical coordinate system. The distance between the centre of the tube O and the centre of the interface circular segment is r_o . The contact angle between the interface and the tube wall is zero, and the radius of the interface curvature is r_i .

2. Velocity continuity at the interface, i ,

$$u_2(r_i, \theta) - u_1(r_i, \theta) = 0. \quad (\text{A.6})$$

3. Tangential stress continuity at the interface (the interfacial shear viscosity is assumed to be zero),

$$\mu_2 \left(n_r \frac{\partial u_2}{\partial r} \Big|_i + \frac{n_\theta}{r_i} \frac{\partial u_2}{\partial \theta} \Big|_i \right) - \mu_1 \left(n_r \frac{\partial u_1}{\partial r} \Big|_i + \frac{n_\theta}{r_i} \frac{\partial u_1}{\partial \theta} \Big|_i \right) = 0, \quad (\text{A.7})$$

where r_w is the radial distance to a point on the tube wall with reference to the centre of the tube, O , and r_i is the radius of the interface curvature with reference to the centre

of the circular interface segment, O_1 , see Figure A.1(b). The contact angle between the interface and the tube wall is assumed to be zero. Here n_r and n_θ are the magnitude of the interfacial unit normal vector projected, respectively, onto the radial and angular directions in the cylindrical system. At each point on the interface we have

$$\begin{aligned} n_r &= \cos(\theta - \theta^*), \\ n_\theta &= \sin(\theta - \theta^*), \end{aligned} \quad (\text{A.8})$$

where,

$$\theta = \tan^{-1} \left(\frac{r_o \cos(\pi/s) + r_i \cos \theta^*}{r_o \sin(\pi/s) + r_i \sin \theta^*} \right), \quad (\text{A.9})$$

and,

$$r_i = R - r_o \cos(\pi/s) \quad (\text{A.10})$$

Here θ^* represents the angular coordinate in the cylindrical system with reference to the centre of the circular interface segment, O_1 , as shown in Figure A.1(c), r_o is the distance from the centre of the polygon to the the centre of the interface circular segment, and R is the vertical distance from O to the tube wall.

By satisfying these boundary conditions, the following integrals must approach zero (Ehrlich, 1993)

$$S_1 = \int_{S_t} u^2(r_w, \theta) dS_t, \quad (\text{A.11})$$

$$S_2 = \int_{S_i} [u_2(r_i, \theta) - u_1(r_i, \theta)]^2 dS_i, \quad (\text{A.12})$$

$$S_3 = \int_{S_i} \left[\mu_2 \left(n_r \frac{\partial u_2}{\partial r} \Big|_i + \frac{n_\theta}{r_i} \frac{\partial u_2}{\partial \theta} \Big|_i \right) - \mu_1 \left(n_r \frac{\partial u_1}{\partial r} \Big|_i + \frac{n_\theta}{r_i} \frac{\partial u_1}{\partial \theta} \Big|_i \right) \right]^2 dS_i, \quad (\text{A.13})$$

where S_t and S_i denote, respectively, the tube wall and the fluid-fluid interface surfaces. We have

$$\begin{aligned} S_t &= R \tan \theta \Rightarrow dS_t = \frac{R}{\cos^2 \theta} d\theta, \\ dS_i &= r_i d\theta^* \\ r_w &= R \sec \theta \end{aligned} \quad (\text{A.14})$$

The axial velocities, $u_1(r, \theta)$ and $u_2(r, \theta)$, can be approximated in a semi-analytical fashion. First, the series, Equations (A.3) and (A.4), are truncated to a finite number at $n = N$. Then, we find the optimal values for the $3N + 2$ undetermined coefficients ($a_{n,n=0,N}$, $b_{n,n=0,N}$, and $c_{n,n=1,N}$) by minimizing the sum of the integrals presented by Equations (A.11), (A.12) and (A.13),

$$S = S_1 + S_2 + S_3. \quad (\text{A.15})$$

From Equations (A.3) and (A.4), we have

$$\begin{aligned}
\frac{\partial u_1}{\partial r}|_i &= \frac{\xi}{\mu_1} \left(\frac{-r_i}{2} + \sum_{n=0}^N b_n(sn) r_i^{sn-1} \cos(sn\theta) + \sum_{n=1}^N c_n(-sn) r_i^{-sn-1} \cos(sn\theta) \right), \\
\frac{\partial u_1}{\partial \theta}|_i &= \frac{\xi}{\mu_1} \left(-\sum_{n=0}^N b_n(sn) r_i^{sn} \sin(sn\theta) + \sum_{n=1}^N c_n(-sn) r_i^{-sn} \sin(sn\theta) \right), \\
\frac{\partial u_2}{\partial r}|_i &= \frac{\xi}{\mu_2} \left(\frac{-r_i}{2} + \sum_{n=0}^N a_n(sn) r_i^{sn-1} \cos(sn\theta) \right), \\
\frac{\partial u_2}{\partial \theta}|_i &= \frac{\xi}{\mu_2} \left(-\sum_{n=0}^N a_n(sn) r_i^{sn} \sin(sn\theta) \right).
\end{aligned} \tag{A.16}$$

By substituting these derivatives back into Equation (A.7), we have

$$\begin{aligned}
X(r_i, \theta) &= \mu_2 \left(n_r \frac{\partial u_2}{\partial r}|_i + \frac{n_\theta}{r_i} \frac{\partial u_2}{\partial \theta}|_i \right) - \mu_1 \left(n_r \frac{\partial u_1}{\partial r}|_i + \frac{n_\theta}{r_i} \frac{\partial u_1}{\partial \theta}|_i \right) = \\
&+ \xi \left(\sum_{n=0}^N a_n(sn) r_i^{sn-1} [n_r \cos(sn\theta) - n_\theta \sin(sn\theta)] \right) \\
&+ \xi \left(\sum_{n=0}^N b_n(sn) r_i^{sn-1} [n_\theta \sin(sn\theta) - n_r \cos(sn\theta)] \right) \\
&+ \xi \left(\sum_{n=1}^N c_n(sn) r_i^{-sn-1} [n_r \cos(sn\theta) - n_\theta \sin(sn\theta)] \right)
\end{aligned} \tag{A.17}$$

For a symmetry element of the cross-section, Figure A.1(b), we have

$$\begin{aligned}
S_1 &= \int_0^{\theta_1} u_2^2(r_w, \theta) \frac{R}{\cos^2 \theta} d\theta + \int_{\theta_1}^{\pi/s} u_1^2(r_w, \theta) \frac{R}{\cos^2 \theta} d\theta, \\
S_2 &= \int_0^{\pi/s} [u_2(r_i, \theta^*) - u_1(r_i, \theta^*)]^2 R_1 d\theta^*, \\
S_3 &= \int_0^{\pi/s} X^2(r_i, \theta^*) R_1 d\theta^*,
\end{aligned} \tag{A.18}$$

here θ_1 is the angular coordinate where the fluid-fluid interface meets the tube wall.

In order to minimize $S = S_1 + S_2 + S_3$, we set the gradients of S with respect to the undetermined coefficients to zero,

$$\begin{aligned}
\frac{\partial S}{\partial a_i} &= \int_0^{\theta_1} 2u_2(r_w, \theta) \frac{\partial u_2(r_w, \theta)}{\partial a_i} \frac{R}{\cos^2 \theta} d\theta + \int_{\theta_1}^{\pi/s} 2u_1(r_w, \theta) \frac{\partial u_1(r_w, \theta)}{\partial a_i} \frac{R}{\cos^2 \theta} d\theta \\
&+ \int_0^{\pi/s} 2(u_2(r_i, \theta^*) - u_1(r_i, \theta^*)) \frac{\partial (u_2(r_i, \theta^*) - u_1(r_i, \theta^*))}{\partial a_i} R_1 d\theta^* \\
&+ \int_0^{\pi/s} 2X(r_i, \theta^*) \frac{\partial X(r_i, \theta^*)}{\partial a_i} R_1 d\theta^* = 0, \quad i = 0, 1, \dots, N
\end{aligned} \tag{A.19}$$

$$\begin{aligned}
\frac{\partial S}{\partial b_i} &= \int_0^{\theta_1} 2u_2(r_w, \theta) \frac{\partial u_2(r_w, \theta)}{\partial b_i} \frac{R}{\cos^2 \theta} d\theta + \int_{\theta_1}^{\pi/s} 2u_1(r_w, \theta) \frac{\partial u_1(r_w, \theta)}{\partial b_i} \frac{R}{\cos^2 \theta} d\theta \\
&+ \int_0^{\pi/s} 2(u_2(r_i, \theta^*) - u_1(r_i, \theta^*)) \frac{\partial (u_2(r_i, \theta^*) - u_1(r_i, \theta^*))}{\partial b_i} R_1 d\theta^* \\
&+ \int_0^{\pi/s} 2X(r_i, \theta^*) \frac{\partial X(r_i, \theta^*)}{\partial b_i} R_1 d\theta^* = 0, \quad i = 0, 1, \dots, N
\end{aligned} \tag{A.20}$$

$$\begin{aligned}
\frac{\partial S}{\partial c_i} &= \int_0^{\theta_1} 2u_2(r_w, \theta) \frac{\partial u_2(r_w, \theta)}{\partial c_i} \frac{R}{\cos^2 \theta} d\theta + \int_{\theta_1}^{\pi/s} 2u_1(r_w, \theta) \frac{\partial u_1(r_w, \theta)}{\partial c_i} \frac{R}{\cos^2 \theta} d\theta \\
&+ \int_0^{\pi/s} 2(u_2(r_i, \theta^*) - u_1(r_i, \theta^*)) \frac{\partial (u_2(r_i, \theta^*) - u_1(r_i, \theta^*))}{\partial c_i} R_1 d\theta^* \\
&+ \int_0^{\pi/s} 2X(r_i, \theta^*) \frac{\partial X(r_i, \theta^*)}{\partial c_i} R_1 d\theta^* = 0, \quad i = 1, \dots, N
\end{aligned} \tag{A.21}$$

where

$$\begin{aligned}
\frac{\partial u_1(r_w, \theta)}{\partial a_i} &= 0, \\
\frac{\partial u_2(r_w, \theta)}{\partial a_i} &= \frac{\xi}{\mu_2} r_w^{si} \cos(si\theta), \\
\frac{\partial (u_2(r_i, \theta^*) - u_1(r_i, \theta^*))}{\partial a_i} &= \frac{\xi}{\mu_2} r_i^{si} \cos(si\theta^*), \\
\frac{\partial X(r_i, \theta^*)}{\partial a_i} &= \xi ((si)r_i^{si-1} [n_r \cos(si\theta^*) - n_\theta \sin(si\theta^*)]),
\end{aligned} \tag{A.22}$$

$$\begin{aligned}
\frac{\partial u_1(r_w, \theta)}{\partial b_i} &= \frac{\xi}{\mu_1} r_w^{si} \cos(si\theta), \\
\frac{\partial u_2(r_w, \theta)}{\partial b_i} &= 0, \\
\frac{\partial (u_2(r_i, \theta^*) - u_1(r_i, \theta^*))}{\partial a_i} &= -\frac{\xi}{\mu_1} r_i^{si} \cos(si\theta^*), \\
\frac{\partial X(r_i, \theta_*)}{\partial b_i} &= \xi ((si)r_i^{si-1} [n_\theta \sin(si\theta^*) - n_r \cos(si\theta^*)])
\end{aligned} \tag{A.23}$$

$$\begin{aligned}
\frac{\partial u_1(r_w, \theta)}{\partial c_i} &= \frac{\xi}{\mu_1} r_w^{-si} \cos(si\theta), \\
\frac{\partial u_2(r_w, \theta)}{\partial c_i} &= 0, \\
\frac{\partial(u_2(r_i, \theta^*) - u_1(r_i, \theta^*))}{\partial c_i} &= -\frac{\xi}{\mu_1} r_i^{-si} \cos(si\theta^*), \\
\frac{\partial X(r_i, \theta^*)}{\partial c_i} &= \xi \left((si) r_i^{-si-1} [n_r \cos(si\theta^*) + n_\theta \sin(si\theta^*)] \right).
\end{aligned} \tag{A.24}$$

This leads to a set of $3N + 2$ linear equations solved to obtain the optimal parameter values for $a_{n,n=0,N}$, $b_{n,n=0,N}$, and $c_{n,n=1,N}$.