A NUMERICAL MODEL FOR OIL/WATER SEPARATION FROM A SOLID PARTICLE

by

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Abstract

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A computational fluid dynamics model has been developed to study an oil-coated particle immersed in a uniform aqueous flow, to determine the conditions that favour oil separation. The governing flow equations are discretized using a finite volume approach, and the oil/water interface is captured using the Volume-of-Fluid (VOF) method in a 2D spherical coordinate system. The model predicts different mechanisms for oil separation. At a Reynolds number, Re, equal to 1, and at a low capillary number, Ca \ll 1, the high interfacial tension can induce rapid contact line motion, to the extent that the oil film can advance past its equilibrium position and separate from the particle. This mechanism requires that the contact angle measured through the oil phase is large. On the other hand, as Ca approaches 1, the shear exerted by the external flow stretches the oil into a thread that will eventually rupture and separate.
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Chapter 1

Introduction

Canada has some of the largest oil reserves in the world, in the form of highly viscous bitumen found in oil sands deposits in Alberta. The proven reserves recoverable via current technology are estimated to be 170.4 billion barrels; of that, approximately 20% can be recovered using mining techniques, and 80% via in-situ recovery processes. These oil sands deposits foster economic growth by attracting investment - estimated to exceed $10 billion in 2009 - and provide many job opportunities [25].

Athabasca oil sand is a mixture of bitumen, water, clay, and quartz sand that makes up most of the material. The bitumen is much heavier and more viscous than conventional crude oil, and is effectively immobile in the deposits. The bitumen saturation ranges from 0-18% by weight (the average is 12%), water saturation from 3-6%, and mineral content from 84-86% [7]. The grade of oil sand is categorized by its bitumen content, and one common scheme is as follows: greater than 12% bitumen by weight for “rich oil sand”, 10-11% for “average”, 6-9% for “lean”, while less than 6% is not of “ore-grade” quality [58].

For deep deposits, the bitumen must be recovered using in-situ methods. Conventional in-situ methods involve drilling wells down into the oil-bearing formation. Energy is supplied through injection wells, which drives the oil up to the surface through pro-
duction wells. A brief overview of in-situ methods including fire floods, steam drive processors, and nuclear stimulation is given in [8]. For shallow deposits, the oil sands are open pit mined, and then transported to facilities where the bitumen can be recovered using methods such as hot water extraction, cold water extraction, and solvent extraction.

The focus of this thesis is a study of oil/water/solid particle separation, which is fundamental to the aforementioned ex-situ extraction processes. The analysis considers a single particle coated with a film of oil, immersed in a uniform aqueous flow, as shown in Fig. 1.1(a). It is of interest to determine whether all the oil remains attached to the particle, Fig. 1.1(b), or whether a portion of the oil separates, Fig. 1.1(c), or whether all of the oil separates from the particle, Fig. 1.1(d), as a function of particle size and oil film thickness, fluid properties, and flow conditions. The work presented here addresses the hydrodynamic effects associated with the external shear on the oil separation; while most work in the literature focuses on the effects of reducing interfacial tension [55, 69]. A highly simplified system is used as a first step to understand this complicated situation. The results of this study provide valuable insights on the operating conditions that favour oil separation, and thus may contribute to the design of improved extraction processes. The rest of this chapter presents further details of two applications of oil/water/particle separation, then surveys the relevant academic literature, presents an overview of numerical methods for solving such flows, and finally summarizes the objectives of the work presented here.

1.1 Hot Water Extraction

The hot water separation process [12] was developed to recover bitumen from the Athabasca oil sands, and is commercially used by Syncrude Canada [26] and Suncor [18]. It basically involves three stages: conditioning, separation and scavenging. In the conditioning
Figure 1.1: (a) An oil-coated particle immersed in a uniform aqueous flow; (b) an equilibrium configuration is established; (c) a portion of the oil separates; and (d) all the oil separates from the particle.
stage, the mined oil sands are mixed with hot water, steam, and chemical reagents such as NaOH in a large rotating tumbler. NaOH reacts to produce surfactants that reduce interfacial tension and modify surface electric charges to improve recovery [55]. In general the temperature of the slurry is maintained at 80 to 90°C at a pH of 8 to 8.5. Heat, shear and the reagents break down large lumps of oil sands by ablation, and break up/separate the bitumen film from individual sand particles.

The second stage is separation, where the bitumen, separated previously in the conditioning stage, is collected. Before the slurry from the conditioning tumbler enters the separation cell, it is screened for rocks and remaining large clusters of oil sand. In addition, the slurry may be further diluted and/or aerated. Once the slurry enters the separation cell, the heavy sand particles rapidly settle to the bottom, while the bitumen floats to the surface. This results in three streams: the bitumen froth at the surface that can be recovered, the sand tailings at the bottom that are disposed of, and a middling stream consisting of water, dispersed sand particles, and a small portion of suspended bitumen in the middle.

The third stage is scavenging, to salvage the remaining bitumen from the middling stream, often by conventional froth flotation processes. The remaining tasks are to concentrate the froth from both the primary separation cell and the scavenging process by centrifugation to segregate the bitumen from water and fine minerals. Then the resulting bitumen is upgraded to synthetic crude oil. Finally, the rocks, sand tailings, and sludge are disposed of.

### 1.2 Soil Washing

Another application of oil/water/particle separation is the soil washing process [2]. Soil washing is an ex-situ method that removes contaminants from soil by washing with a water-based fluid. A common contaminant is fuel oil that leaks from underground stor-
age tanks. Soil washing can also handle other contaminants such as petroleum residues, creosote, heavy metals, pesticides, semi-volatiles and volatiles. Unlike bitumen extraction processes, the end product of interest in this case is the clean sand that can be redeposited back on to a site. Soil washing in general is more effective in cleaning larger-sized sand/gravel particles; thus it is often used as a volume reduction step, which cleans and separates coarser particles, and concentrates the contaminants into finer soil particles. The result is a smaller volume of contaminated soil requiring more complicated and expensive treatments.

The first step in soil washing is to excavate the contaminated soil and screen out any oversize materials. Then the soil is mixed with water and surfactants (to lower interfacial tension), and/or other cleaning agents if needed. The soil is separated into two fractions based on particle size. The coarser particles are easier to clean by washing with water; the finer particles are more attached to the contaminants. Consequently, the washing step results in a large volume of clean coarse soil that can be redeposited on site, a small volume of contaminated fine soil that requires additional remediation treatment, and a dirty spent water stream that can be reused in the washing step or disposed of after proper treatment.

1.3 Literature Overview

A few authors have studied fundamental aspects of oil/water/particle separation, focusing on the small scale (e.g. a cluster of oil phase and solid particles). Niven et al. [42] analyzed the separation of a mixed particle n-plet - a dispersed liquid droplet attached to n monosized solid particles - via a thermodynamic approach, by numerically calculating the Gibbs free energy associated with the rupturing process. However, their analysis only considered the work of interfacial adhesion and cohesion - i.e. the work needed to separate the solid and fluid, and to split the fluid, respectively. Neither the work associated with
the distortion of fluid prior to rupture nor other forces such as electrostatic and double layer effects were included in the model. In addition, they argued, and justified in their results, that the minimum energy process is when an individual solid grain, with or without dispersed fluid attached, separates one at a time; thus they only calculated the Gibbs free energy for this case. For a singlet, if the dispersed droplet is non-wetting (i.e. if the contact angle measured through the dispersed phase is greater than 90°), the energy required to divide the droplet in half is much greater than to separate the solid grain; while for a wetting droplet, more energy is required to separate the solid grain than to split the dispersed phase. In general, the energy required increases with higher total dispersed phase volume and lower contact angle. In a subsequent paper [41], comparisons were made with the estimated energy in a fluidized bed.

More directly related to this thesis is a series of papers by Smith and van de Ven. In the first [61], they studied the behaviour of a cluster of a dispersed fluid phase and solid particles in a simple shear flow created using a Couette device, albeit for water dispersed within a continuous silicon oil phase. The study focused on trends observed in the cluster behaviour and rupture process, for different volume fractions of solid particles, interfacial tension and wetting characteristics of the solid surface. For a polystyrene/water/silicone oil system at low volume fraction (approximately 3%), the cluster deformed into an ellipsoidal shape, and mostly singlets or doublets, covered with an aqueous film, separated at the tip of the ellipsoid. At higher volume fractions (approximately 10 to 20%), the dispersed fluid phase ruptured into multiple smaller clusters. At the highest volume fraction considered (approximately 50%), individual particles to small clusters separated at the fluid surface. Next the interfacial tension was lowered by replacing water with a surfactant solution. The cluster strength decreased, fewer three-phase contacts formed, and the rupture modes were different, which was especially noticeable at high volume fraction, where the cluster disintegrated into numerous smaller clusters. Finally, when the solid was modified to be less wetting, for intermediate to high volume fractions, an
increased number of three phase contact formations was observed. The resulting clusters had lower strength and tended to rupture at lower shear rates. The particles also tended to break away with less dispersed phase fluid.

At an even smaller scale, Smith and van de Ven [59] examined the behaviour of a single solid particle partially or entirely coated by a dispersed liquid phase in a linear shear flow. The continuous medium was silicone oil, and the dispersed phase was water, pale-4-oil or Ucon oil. The partially coated solid/liquid pair deformed, whereby the liquid periodically extended and compressed and displayed contact-angle hysteresis, and rotated under the shear flow. The liquid/liquid/solid separation depended strongly on the system properties. For example, with a water drop as the dispersed phase, rupture occurred near the contact circle as the majority of the drop separated from the particle. A very different behaviour was observed as a Pale-4-oil drop, with a smaller contact angle and higher viscosity, stretched into a thread and upon rupture left behind a much higher fraction of oil still attached to the particle. Finally, for a particle fully coated by highly viscous Ucon oil, rupture only occurred for impulsively started flow at high shear rates. The impulsive start deformed the drop too far from the steady state configuration, which was considered the cause of the rupture.

Smith and van de Ven [60] also investigated an axisymmetric oil-coated particle submerged in a continuous phase fluid, acted upon only by gravity and interfacial tension. This simple configuration allowed for a theoretical analysis to predict equilibrium configurations of oil films that partially coat a solid particle. The model involved two parameters: a Bond number $\lambda = r_{sph}^2 \Delta \rho \frac{g}{\sigma}$ to reflect the ratio of gravity to surface tension ($\Delta \rho$ is the density difference between the fluids, $g$ is the gravitational acceleration, $\sigma$ is the interfacial tension, and $r_{sph}$ is the particle radius); and the oil volume $\zeta$, in their case non-dimensionalized by $r_{sph}^3$. For given $\lambda$ and $\zeta$, the model yielded plots of contact angle, $\alpha$, versus the equilibrium position of the oil drop as defined by the filling angle $\psi$, illustrated in Fig. 1.2. While the theory typically predicts two equilibrium positions
for a given contact angle, in an experiment, the contact line will likely stop at the first position it reaches. The model also yielded the maximum contact angle for which an equilibrium configuration of the oil could exist; larger values lead to separation of the oil phase. Alternatively, the model can be used to determine the maximum oil volume a particle could retain, as a function of $\alpha$ and $\lambda$: in general, the maximum volume decreases with $\alpha$ and $\lambda$. Finally, a geometric relation was provided to describe the shape of the spherical cap of oil that partially coats a solid spherical particle for a given contact angle $\alpha$, as occurs when $\lambda = 0$, refer to Fig. 1.2(a). This is an equation that can be solved for $\alpha(\psi)$ for a given $\zeta$:

$$\zeta = \frac{\pi}{3} \left\{ \left[ \frac{\sin \psi}{\sin(\alpha + \psi)} \right]^3 F(\alpha + \psi) - F(\psi) \right\}$$

where

$$F(\psi) = 2 - 3 \cos \psi + \cos^3 \psi$$

Smith and van de Ven [60] conducted experiments using silicone oil to coat a particle, with water or Pale-4-oil as the lighter continuous medium. The experimentally observed
and theoretically predicted oil profiles at equilibrium agreed well. They observed that once a contact line formed and the film started to de-wet, its velocity either decreased monotonically until it stopped at the equilibrium position, if one existed; otherwise at some point, it increased again until rupture, which for all experiments occurred near $\psi = 0^\circ$, resulting in less than 0.1% of oil remaining on the sphere.

The work presented here builds on this work of Smith and van de Ven [60], but rather than by gravity, the oil is subjected to an external aqueous flow. This is a more complicated phenomena for which no analytical theory is available, and so a computational fluid dynamics (CFD) model has been developed. The following section provides some background on CFD.

1.4 Computational Fluid Dynamics

A powerful tool to analyze fluid behaviors is Computational Fluid Dynamics (CFD). Rapid advancements in computational power and numerical methods have made CFD an alternative tool to actual experiments. A simulation can be less expensive to run than an experiment, and can allow better control of the variables. In a CFD model, the governing equations are discretized and solved at a number of grid points or control volumes. The most commonly used discretization methods include the Finite Difference, Finite Volume, and Finite Element methods. For detailed descriptions of these, refer to [21, 46]. For multiphase flows, additional complexities arise due to the existence of interfaces. Fortunately, many techniques have been developed to represent interfaces; these generally fall into two categories: interface-tracking and interface-capturing methods, that are briefly presented here.
1.4.1 Interface-Tracking Methods

In an interface-tracking method, the interface is explicitly traced with a body-fitted grid. The grid deforms so that the cell edges (in 2D) or cell faces (in 3D) always align with the moving interface, which facilitates the implementation of interface boundary conditions. Although interface-tracking methods can achieve high accuracy, they are limited to simple interfacial phenomena [40], because as the interface advances, the mesh can become increasingly distorted and a new grid must be generated. Examples of interface-tracking methods applied to free surface flows can be found in [17, 40, 66].

1.4.2 Interface-Capturing Methods

On the other hand, an interface-capturing method relies on some kind of marker function on a fixed mesh to distinguish the different fluid phases and to implicitly locate the interface. Such methods are generally used to model more complicated interfacial phenomena such as breaking and merging of droplets or waves. In addition, they are compatible with the “one-fluid” approach, in which only one set of governing equations is solved over the entire domain. Three well known interface-capturing methods are presented next.

Marker-and-Cell

The Marker-and-Cell (MAC) method introduced by Harlow and collaborators [27] was the first to successfully model free surface flows. This method keeps track of marker particles uniformly distributed in each fluid phase, where the outermost particles mark the interface. Although this method can handle complex interfacial flows, a substantial computational resource must be allocated to track the large number of particles.

Level-Set

The Level-Set method, introduced by Osher and Sethian [45], keeps track of a level-set function, $\phi$, which is initialized as a signed distance function from the interface. $\phi$
is positive in one fluid, negative in the other and zero at the interface. As the flow advances, the $\phi = 0$ contour will continue to represent the interface, but the level-set function at other locations will deviate from a distance function. To maintain accuracy, values of $\phi$ near the interface should be re-initialized as a distance function every time step. The level-set method is robust and can capture the interface normal and curvature accurately. The original method does not address mass conservation, but it can be achieved by following the approach in [73].

**Volume-of-Fluid**

The Volume-of-Fluid (VOF) method keeps track of a volume fraction, $f$, in each computational cell. $f = 1$ implies that the cell is full of one of the fluids, $f = 0$ that the cell is full of the other fluid, and $0 < f < 1$ implies the existence of an interface. There are a few versions of VOF that differ in the way the interface is reconstructed in an interface cell. The original VOF method of Hirt and Nichols [28] reconstructs an interface as line segments parallel to the coordinate axes that align better with the actual interface, which are determined from the volume fractions in the neighbouring cells. Youngs [72] improved the reconstruction method by allowing the interface to orient in any direction, not necessarily parallel to a coordinate axis; thus the line segments better resemble the interface. This approach is referred to as piecewise linear interface (PLIC) calculation. Rudman [52] tested different versions of the VOF method and concluded Youngs’ method to be the most accurate. Fig. 1.3 illustrates these two VOF reconstructions.
Figure 1.3: The two fluids (a) are stored as volume fractions of fluid 1 (b); (c) Hirt and Nichols VOF reconstruction; (d) Youngs’ PLIC reconstruction.
1.5 An Overview of the Numerical Approach

The model presented in this thesis considers a single oil-coated particle immersed in a uniform aqueous flow. The governing equations are discretized using the finite volume method and the oil/water interface is captured using the VOF technique. The equations are solved in a 2D spherical coordinate system, where the innermost $r$ grid line conforms to the solid particle surface.

1.5.1 Spherical Coordinates

Discretizing the governing equations in the spherical coordinate system is common when the model involves, for example, flow over a rigid sphere [33, 36, 51], flow over a viscous sphere [19, 31], and Couette flow between two concentric spheres [39, 56]. Nevertheless, implementing VOF in a spherical coordinate system is novel, as there is only one other implementation which has done so. To investigate the free surface flow in a rotating cone reactor, Janse et al. [29] implemented Hirt and Nichols’ VOF method in a spherical coordinate system, in which the interface line segments are only parallel/perpendicular to the $r$-axis. By contrast, this thesis utilizes the more accurate, but also more complicated, Youngs’ method, in which the interface line segments can be oriented in any direction.

The benefit of using the spherical coordinate system to model the oil/water/particle separation process is the alignment of a $r$ grid line with the solid sphere surface. This facilitates the precise imposition of the no-slip boundary condition and of the contact angle at the particle surface. And as the flow is assumed to be axisymmetric in the $\phi$ direction, the numerical analysis can be simplified to two dimensions ($r, \theta$).

The drawback of the spherical coordinate system is that it is geometrically more complex than a Cartesian coordinate system. This is especially true when calculating the fluid volume in an interfacial cell. For example, instead of two prototypical interface cells, the spherical system has six, and calculating the revolved fluid volume requires
numerical integration. This issue will be discussed in further detail in chapter 3.

In addition, the mesh size varies with the coordinate $r$. The coarse cells far from the origin yield lower accuracy in interface normal and curvature calculations, while the fine cells near the origin place severe limits on the time step size used to calculate unsteady flows [29, 38].

An oft-cited advantage of the finite volume method is that the discretized equations remain fully conservative. However, when expanding the convective and viscous terms in spherical coordinates, extra curvilinear terms appear that cannot be treated conservatively. There are ways to avoid the curvilinear terms, such as expressing the velocity components in Cartesian coordinates [35], or discretizing the Navier-Stokes equation in its vector form [71], or introducing local base vectors at the cell centers, and expressing the direction vectors at other points, such as at cell faces, in terms of the base vectors at the cell centers and appropriate direction cosines [38, 68]. To avoid unnecessary complexity, the curvilinear terms are not treated conservatively, but it will be shown (in chapter 4, Validation) that it seems an adequate approach for this model.

Finally, applying outflow boundary conditions to the spherical domain is not a trivial task. Since the coordinate axes change directions, it is impossible to align the grid lines at the outflow boundary in the stream-wise direction. For uniform flow over an immersed object, some earlier work (e.g. [19, 31, 33]) set the outer boundary, $r = r_{\infty}$, sufficiently far from the object that the flow was assumed to have returned to a uniform one. Then the boundary conditions on both the inflow and outflow sides of the domain were set to the specified uniform external velocity. A more sophisticated approach divides the outer boundary into two sections: the upstream that is unaffected by the immersed object, on which is specified a uniform external velocity, and the downstream that is influenced by the object, in which the boundary variables are extrapolated from upstream values [5, 30, 34]. This thesis implements the latter approach, and the downstream section has the parabolic boundary conditions given by Magnaudet et al. [36].
1.6 Objectives

The objectives of this thesis were:

1. to develop a Navier-Stokes flow solver including a VOF implementation in 2D spherical coordinates;

2. to validate the numerical model using existing experimental and numerical results;

3. and to apply the numerical model to study oil/water/particle separation in a uniform laminar flow, and in particular, to examine the influence of interfacial tension, contact angle, initial oil volume, and external velocity.

1.7 Overview

The remainder of this thesis is organized in the following manner: chapter 2 describes the finite volume discretization of the governing equations, chapter 3 presents details of the VOF method implemented in the spherical coordinate system, chapter 4 presents validation of the model, chapter 5 presents the results, and chapter 6 summarizes the main findings and future work.
Chapter 2

Numerical Flow Solver

In this chapter, the numerical model for oil/water/particle separation is presented. The oil and water are assumed to be incompressible, Newtonian and have constant density and viscosity. The flow is assumed to be laminar and axisymmetric in the $\phi$ direction. The governing equations are described first (section 2.1), followed by the choice of numerical grid, boundary conditions (section 2.2), the overall mathematical model (section 2.3), the discretization of each term (sections 2.3.1, 2.3.2, 2.3.3, and 2.3.4), and finally a complete timestep (section 2.3.5).

2.1 Governing Equations

The flow of oil and water is described by the Navier-Stokes equations for conservation of mass and momentum:

$$\nabla \cdot \vec{V} = 0,$$

$$\frac{\partial (\rho \vec{V})}{\partial t} + \nabla \cdot (\rho \vec{V} \vec{V}) = -\nabla P + \nabla \cdot \vec{\tau} + \rho \vec{g} + \vec{F}_{st}$$

where $\vec{V}=(u,v,w)$ represents the velocity in $\vec{x}(r,\theta,\phi)$, $P$ the pressure, $t$ the time, $\rho$ the density, $\vec{g}$ the gravitational acceleration, $\vec{F}_{st}$ the surface tension force, and $\vec{\tau}$ the shear
stress tensor. For Newtonian fluids, \( \tilde{\tau} \) is given by

\[
\tilde{\tau} = \mu (\nabla \vec{V} + (\nabla \vec{V})^T)
\]

(2.3)

where \( \mu \) represents the dynamic viscosity.

Although there are two fluids, oil and water, in the model, Eqs. (2.1) to (2.3) are solved over the whole domain (a “one-fluid” approach); the separate oil and water phases are defined solely by variations in physical properties. The interfaces between the water and oil are indicated by a scalar function \( f \), defined as:

\[
f = \begin{cases} 
1 & \text{within oil} \\
0 & \text{within water} 
\end{cases}
\]

where \( f \) is advected with the flow according to:

\[
\frac{\partial f}{\partial t} + (\vec{V} \cdot \nabla) f = 0
\]

(2.4)

### 2.2 Numerical Grid

The equations are solved in the spherical coordinate system shown in Fig. 2.1(a). The flow is assumed axisymmetric in the \( \phi \) direction; thus the domain is two-dimensional \((r, \theta)\). The equations are discretized via a finite volume scheme on a staggered mesh, with the velocity components located at the cell faces and pressure at the cell centers, Fig. 2.1(b). A staggered mesh allows the velocity and pressure fields to be tightly coupled, and is suitable for the fractional-step discretization method, described in section 2.3. In addition, it avoids the possibility of the “checkboard” pressure field - in which pressures at neighbouring nodes can have different values, yet the apparent pressure gradients in the discretized equations are zero.
Figure 2.1: (a) The spherical coordinate system superimposed onto the Cartesian one; (b) the staggered mesh.
At the solid particle boundary, \( r = r_{sph} \), the velocity components adhere to the no-slip and no-penetration conditions:

\[
\begin{align*}
    u_{sph} &= 0 \\
    v_{sph} &= 0
\end{align*}
\] (2.5) (2.6)

where the subscript \( sph \) denotes values at the spherical particle surface. Note that at all boundaries where the normal velocity is explicitly specified, the pressure gradient in the direction normal to the boundary is set to zero.

At the symmetric boundaries (\( \theta = 0 \) and \( \theta = \pi \)), the velocity components adhere to the free-slip and no-penetration conditions:

\[
\begin{align*}
    \left( \frac{\partial u}{\partial \theta} \right)_{sym} &= 0 \\
    v_{sym} &= 0
\end{align*}
\] (2.7) (2.8)

where the subscript \( sym \) denotes values at the symmetric boundary.

The outer boundary, at \( r = r_{\infty} \), must be sufficiently far from the solid particle to not influence the results, and so is divided into two sections as per Li and Boulos [34], shown in Fig. 2.2(a). On the first section, from \( \theta = 0 \) to \( \theta = 3\pi/4 \), the uniform external velocity, \( \vec{V}_{\infty} = -V_{\infty} \hat{e}_z \), is specified, and thus:

\[
\begin{align*}
    u_{\infty,1} &= -V_{\infty} \cos \theta \\
    v_{\infty,1} &= V_{\infty} \sin \theta
\end{align*}
\] (2.9) (2.10)

where the subscript \((\infty, 1)\) denotes values at the first section of the outer boundary.

The downstream section, from \( \theta = 3\pi/4 \) to \( \theta = \pi \), is an outflow boundary, with the flow influenced by the solid particle. The outflow boundary conditions were adopted from Magnaudet et al. [36], which are not physically meaningful, but are designed to reduce the disturbance to the upstream flow. At the outer boundary, a row of ghost cells - temporary cells beyond the domain - is introduced, Fig. 2.2(b). The velocity components
and pressure in this row of cells are determined using the information upstream via the following approximations:

\[
\begin{align*}
\left(\frac{\partial^2 u}{\partial r^2}\right)_{\infty,2} &= 0 \\
\left(\frac{\partial v}{\partial r}\right)_{\infty,2} &= 0 \\
\left(\frac{\partial^2 P}{\partial \theta \partial r}\right)_{\infty,2} &= 0
\end{align*}
\]

where the subscript \((\infty, 2)\) denotes values at the downstream section of the outer boundary. Now that the original boundary cells, those within the domain, have neighbouring cells in all directions, they can be treated in the same way as other interior cells.

![Diagram](image)

Figure 2.2: (a) The boundaries of the domain; (b) the row of ghost cells introduced at the outflow boundary.
Chapter 2. Numerical Flow Solver

2.3 Discretized Equations

This section presents the details of the numerical methodology for discretizing and solving Eqs. (2.1) and (2.2). First of all, the volume fraction, $f_{i,j}$, for each cell is calculated by integrating the scalar function $f$ over the cell volume:

$$f_{i,j} = \frac{1}{\Omega_{i,j}} \int_{\Omega_{i,j}} f \, d\Omega$$  \hspace{1cm} (2.11)

where $\Omega_{i,j}$ is the volume of the cell with index $i, j$. The volume fraction represents the fraction of a cell volume occupied by, in this case, the oil. $f_{i,j} = 1$ indicates the cell is full of oil, $f_{i,j} = 0$ indicates the cell is full of water, and $0 < f_{i,j} < 1$ implies an oil/water interface. The advection of the volume fractions, the discretization of Eq. (2.4) is presented in the next chapter. The volume fractions are used to approximate the fluid properties in each cell:

$$\rho_{i,j} = f_{i,j} \rho_1 + (1 - f_{i,j}) \rho_2 \hspace{1cm} (2.12)$$

$$\mu_{i,j} = f_{i,j} \mu_1 + (1 - f_{i,j}) \mu_2 \hspace{1cm} (2.13)$$

where $\rho_1$, $\rho_2$, and $\mu_1$, $\mu_2$ are the densities and dynamic viscosities of oil and water, respectively.

The fractional step method implemented here utilizes the Crank-Nicolson scheme for the time discretization of Eq. (2.2), similar to [11, 21]:

$$\frac{1}{\Delta t} (\rho^{n+1} \tilde{V}^* - \rho^n \tilde{V}^n) + \frac{1}{2} \left[ \nabla \cdot (\rho^{n+1} \tilde{V}^* \tilde{V}^*) + \nabla \cdot (\rho^n \tilde{V}^n \tilde{V}^n) \right] = \frac{1}{2} (\nabla \cdot \tilde{\tau}^n + \nabla \cdot \tilde{\tau}^n) - \nabla P^n + \bar{F}^n_{st} + \frac{1}{2} (\rho^{n+1} + \rho^n) \ddot{g} \hspace{1cm} (2.14)$$

$$\frac{1}{\Delta t} (\rho^{n+1} \tilde{V}^{**} - \rho^{n+1} \tilde{V}^*) = \nabla P^n - \bar{F}^n_{st} + \bar{F}^{n+1}_{st} \hspace{1cm} (2.15)$$

$$\frac{1}{\Delta t} (\rho^{n+1} \tilde{V}^{n+1} - \rho^{n+1} \tilde{V}^{**}) = -\nabla P^{n+1} \hspace{1cm} (2.16)$$

where the superscripts $n$ and $n + 1$ represent values at the current and next timesteps, and the superscripts * and ** represent interim values. Eq. (2.14) predicts an interim
velocity field, with the convective, viscous, and gravitational terms discretized in time by the Crank-Nicolson scheme. Note that \( \mathbf{g} \) only appears for the validation cases; it was set to zero for the results presented in chapter 5. Eq. (2.15) modifies \( \mathbf{V}^* \) by subtracting the pressure contribution at time \( n \), and replacing the contribution of the surface tension force with the time \( n+1 \) value. The latter is carried out in order to treat the surface tension force and pressure gradient more consistently to reduce spurious currents [23]. Finally, in Eq. (2.16), the pressure contribution at \( n + 1 \) is added to \( \mathbf{V}^{**} \) to complete the conservation of momentum equation.

As \( \mathbf{V}^* \) and \( \mathbf{V}^{**} \) are not divergence-free, \( \nabla P^{n+1} \) is used to enforce continuity. Taking the divergence of both sides of Eq. (2.16), and setting \( \nabla \cdot \mathbf{V}^{n+1} = 0 \) yields the following Poisson equation:

\[
\nabla \cdot \mathbf{V}^{**} = \nabla \cdot \left( \frac{\Delta t}{\rho^{n+1}} \nabla P^{n+1} \right)
\]

(2.17)

that is solved for \( \nabla P^{n+1} \).

The spatial discretization of the terms in the Navier-Stokes equations is presented next. In a finite volume method, the terms in the Navier-Stokes equations are integrated over the cell volume. The unsteady term and other source terms are integrated assuming their value at the cell center prevails over the entire volume, thus:

\[
\int_{\Omega_{i,j}} S d\Omega = S_P \Omega_{i,j}
\]

(2.18)

where \( S \) is any source term, and \( S_P \) is the value of the source term at the cell center. The discretizations of the convective, viscous, surface tension, and pressure terms are presented in the following sections.

### 2.3.1 Convective Term

The convective term \( \nabla \cdot (\rho \mathbf{V} \mathbf{V}) \), when expanded in spherical coordinates, takes the following form:

\[
(\nabla \cdot (\rho \mathbf{V} \mathbf{V}))_r = \frac{1}{r^2 \sin \theta} \left[ \frac{\partial}{\partial r} \left( r^2 \sin \theta \rho uu \right) + \frac{\partial}{\partial \theta} \left( r \sin \theta \rho uv \right) \right]
\]
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\[ + \frac{\partial}{\partial \phi} \left( r \rho w u \right) - \frac{\rho v v}{r} - \frac{\rho w w}{r} = \nabla \cdot \left( \rho u \vec{V} \right) - \frac{\rho v v}{r} - \frac{\rho w w}{r} \]  
(2.19)

\[ \left( \nabla \cdot \left( \rho \vec{V} \vec{V} \right) \right)_\theta = \frac{1}{r^2 \sin \theta} \left[ \frac{\partial}{\partial r} \left( r^2 \sin \theta \rho u v \right) + \frac{\partial}{\partial \theta} \left( r \sin \theta \rho u v \right) + \frac{\partial}{\partial \phi} \left( r \rho w v \right) \right] + \frac{\rho w v}{r} - \frac{\rho w w}{r} \cot \theta \]

\[ = \nabla \cdot \left( \rho u \vec{V} \right) + \frac{\rho w v}{r} - \frac{\rho w w}{r} \cot \theta \]  
(2.20)

for the \( r \) and \( \theta \) directions, respectively. Note that as the flow is axisymmetric, terms involving \( w \) and the partial derivatives in the \( \phi \) direction, \( \partial / \partial \phi \), are equal to zero. In the finite volume method, the momentum equations are integrated over the control volume. If all the terms are expressed as the divergence of a vector or a tensor - the strong conservation form [68], by applying the Gauss Divergence Theorem, the volume integrals can be transformed into surface integrals. Thus what leaves the surface of one cell enters through the surface of the adjacent cell. This fully conservative property is one of the advantages of the finite volume method. Unfortunately, when the direction of the vector components is not fixed, as in the spherical coordinate system, extra curvilinear terms arise, such as \( -\rho v v / r \) in Eq. (2.19) and \( \rho w v / r \) in Eq. (2.20), which cannot be treated conservatively. For this work, to maintain simplicity of implementation, the equations are left in the weak conservative form. The curvilinear terms are treated as source terms using Eq. (2.18), while the volume integral of the divergence term is converted into a surface integral, via Gauss’ Theorem as follows:

\[ \int_{\Omega} \nabla \cdot \left( \rho u \vec{V} \right) d\Omega = \int_{A} \rho u \left( \vec{V} \cdot \hat{n} \right) dA \]  
(2.21)

for the \( r \)-direction, where \( A \) is the cell surface area and \( \hat{n} \) is the outward unit normal from the surface. Eq. (2.21) can be discretized into:

\[ \int_{A} \rho u \left( \vec{V} \cdot \hat{n} \right) dA \simeq \sum_{f} \left( \rho \langle u \rangle \right) V^{f} A \]  
(2.22)
where the index $f$ denotes summation over the four cell faces, $V^f l A$ is the volume flow rate leaving a cell face, and $\rho(u)$ is $u$-momentum per unit volume. Continuity is enforced for the pressure cells, but not for the staggered velocity cells. Nevertheless, the velocity components at the velocity cell faces can be made divergence-free by averaging the volume flow rates across the neighbouring pressure cell faces \[24\]. This yields the following interpolation for the flux velocity $V^f l$, refer to Fig. 2.3(a):

\[
\begin{align*}
u^f l_{i,j} & = \frac{u_{i,j+\frac{1}{2}} A_{i,j+\frac{1}{2}} + u_{i,j-\frac{1}{2}} A_{i,j-\frac{1}{2}}}{2A_{i,j}} \\
v^f l_{i+\frac{1}{2},j+\frac{1}{2}} & = \frac{v_{i+\frac{1}{2},j+1} A_{i+\frac{1}{2},j+1} + v_{i+\frac{1}{2},j} A_{i+\frac{1}{2},j}}{2A_{i+\frac{1}{2},j+\frac{1}{2}}} 
\end{align*}
\]

(2.23)

where $u^f l_{i,j}$ refers to the flux velocity at the bottom face and $v^f l_{i+\frac{1}{2},j+\frac{1}{2}}$ at the left face.

The flux quantity $\langle u \rangle$ is approximated using the second order van Leer method \[67\]. For example, $\langle u \rangle_{i,j}$ at the bottom face is approximated as:

\[
\langle u \rangle_{i,j} = \begin{cases} 
  u_{i,j-\frac{1}{2}} + \frac{\Delta r_j}{2} \alpha^L \left( \frac{\delta u}{\delta r} \right)_{i,j-\frac{1}{2}} \left[ 1 - \frac{u^f l_{i,j} \Delta t}{\Delta r_j} \right], & u^f l_{i,j} > 0 \\
  u_{i,j+\frac{1}{2}} - \frac{\Delta r_j}{2} \alpha^L \left( \frac{\delta u}{\delta r} \right)_{i,j+\frac{1}{2}} \left[ 1 + \frac{u^f l_{i,j} \Delta t}{\Delta r_j} \right], & u^f l_{i,j} < 0
\end{cases}
\]

(2.24)

where the velocity gradients are approximated as:

\[
\left( \frac{\partial u}{\partial r} \right)_{i,j-\frac{1}{2}} = \frac{u_{i,j+\frac{1}{2}} - u_{i,j-\frac{1}{2}}}{\Delta r_j + \Delta r_{j-1}}
\]

(2.25)

and

\[
\left( \frac{\partial u}{\partial r} \right)_{i,j+\frac{1}{2}} = \frac{u_{i,j+\frac{3}{2}} - u_{i,j-\frac{1}{2}}}{\Delta r_j + \Delta r_{j+1}}
\]

(2.26)

and $\alpha^L$ is the van Leer limiter introduced to avoid oscillations in the velocity distribution that might occur for any second or higher order approximations. Refer to \[6\] for a more complete description of the method and the derivation of $\alpha^L$. To improve numerical
stability, the van Leer approximation is implemented as a first order upwind scheme with a second order correction, as described in [43]. In other words, the second term on the right hand side of Eq. (2.24) is applied using the deferred correction method [43].

Corresponding equations for the discretized form of the convective term in the \( \theta \)-direction are derived in a similar way to the equations in the \( r \)-direction, and so not presented here.

\subsection*{2.3.2 Viscous Term}

The viscous term \( \nabla \cdot \tilde{\tau} \), when expanded in spherical coordinates, takes the form:

\[
\begin{align*}
(\nabla \cdot \tilde{\tau})_r & = \nabla \cdot (\tilde{\tau} \cdot \hat{e}_r) - \frac{\tau_{\theta \theta}}{r} - \frac{\tau_{\phi \phi}}{r} \\
(\nabla \cdot \tilde{\tau})_\theta & = \nabla \cdot (\tilde{\tau} \cdot \hat{e}_\theta) + \frac{\tau_{\theta r}}{r} - \frac{\tau_{\phi \phi}}{r} \cot \theta
\end{align*}
\]

where the shear stress \( \tilde{\tau} = \mu \left( \nabla \hat{V} + \left( \nabla \hat{V} \right)^T \right) \) is a symmetric tensor, expressed, in spherical coordinates, as:

\[
\tilde{\tau} = \begin{bmatrix}
2\mu \frac{\partial u}{\partial r} & \mu \left( \frac{1}{r} \frac{\partial u}{\partial \theta} + r \frac{\partial}{\partial r} \left( \frac{v}{r} \right) \right) & \mu \left( \frac{1}{r \sin \theta} \frac{\partial u}{\partial \phi} + \frac{r}{r} \frac{\partial}{\partial \phi} \left( \frac{w}{r} \right) \right) \\
\mu \left( \frac{1}{r} \frac{\partial u}{\partial \theta} + r \frac{\partial}{\partial r} \left( \frac{v}{r} \right) \right) & 2\mu \frac{\partial v}{\partial r} + u & \mu \left( \frac{1}{r \sin \theta} \frac{\partial u}{\partial \phi} + \frac{\sin \theta}{r \partial \phi} \left( \frac{w}{\sin \theta} \right) \right) \\
\mu \left( \frac{1}{r \sin \theta} \frac{\partial u}{\partial \phi} + r \frac{\partial}{\partial r} \left( \frac{w}{r} \right) \right) & \mu \left( \frac{1}{r \sin \theta} \frac{\partial v}{\partial \phi} + \frac{\sin \theta}{r \partial \phi} \left( \frac{w}{\sin \theta} \right) \right) & 2\mu \frac{\partial w}{\partial r} + \frac{u}{r} + v \cot \theta
\end{bmatrix}
\]

Similar to the approach taken for the convective terms, Eqs. (2.27) and (2.28) are integrated over the cell volume. Again, the curvilinear terms are treated as source terms, while the volume integral of the divergence term is converted into surface integral, via Gauss’ Theorem as follows:

\[
\int_{\Omega} \nabla \cdot (\tilde{\tau} \cdot \hat{e}_r) \, d\Omega = \int_{A} (\tilde{\tau} \cdot \hat{e}_r) \cdot \hat{n} \, dA
\]

where \( A \) is the cell surface area and \( \hat{n} \) is the outward unit normal from the surface.

Eq. (2.30) can be discretized into:

\[
\int_{A} (\tilde{\tau} \cdot \hat{e}_r) \cdot \hat{n} \, dA \simeq (\tau_{rr})_{i,j+1} A_{i,j+1} - (\tau_{rr})_{i,j} A_{i,j} + (\tau_{\theta r})_{i+\frac{1}{2},j+\frac{1}{2}} A_{i+\frac{1}{2},j+\frac{1}{2}} - (\tau_{\theta r})_{i-\frac{1}{2},j+\frac{1}{2}} A_{i-\frac{1}{2},j+\frac{1}{2}}
\]

(2.31)
Figure 2.3: The indexes used for a staggered velocity cell in the (a) $r$ and (b) $\theta$ directions.
A similar equation can be derived for the $\theta$-direction.

The partial derivatives are approximated using the finite difference scheme. In the $r$-direction, the terms in the stress tensor are approximated as follows, refer to Fig. 2.3(a):

\[
\left( \frac{\partial u}{\partial r} \right)_{i,j} = \frac{u_{i,j+\frac{1}{2}} - u_{i,j-\frac{1}{2}}}{\Delta r_j} \quad (2.32)
\]

\[
\left( \frac{1}{r} \frac{\partial u}{\partial \theta} \right)_{i+\frac{1}{2},j+\frac{1}{2}} = \frac{2 \left( u_{i+1,j+\frac{1}{2}} - u_{i,j+\frac{1}{2}} \right)}{r_j + \frac{1}{2} \left( \Delta \theta_{i+1} + \Delta \theta_i \right)} \quad (2.33)
\]

\[
\left[ \frac{r}{\partial r} \left( \frac{v}{r} \right) \right]_{i+\frac{1}{2},j+\frac{1}{2}} = \left( \frac{\partial v}{\partial r} - \frac{v}{r} \right)_{i+\frac{1}{2},j+\frac{1}{2}} = \frac{v_{i+\frac{1}{2},j+1} - v_{i+\frac{1}{2},j}}{r_j + 1 - r_j} - \frac{v_{i+\frac{1}{2},j+1} + v_{i+\frac{1}{2},j}}{2r_j + 1} \quad (2.34)
\]

The values of the source terms at the center of the cell are approximated as:

\[
\left( \frac{1}{r} \frac{\partial v}{\partial \theta} \right)_{i,j+\frac{1}{2}} = \frac{1}{2} \left( v_{i+\frac{1}{2},j+1} + v_{i+\frac{1}{2},j} \right) - \left( v_{i-\frac{1}{2},j+1} + v_{i-\frac{1}{2},j} \right) \quad (2.35)
\]

\[
v_{i,j+\frac{1}{2}} = \frac{v_{i+\frac{1}{2},j} + v_{i+\frac{1}{2},j+1} + v_{i-\frac{1}{2},j} + v_{i-\frac{1}{2},j+1}}{4} \quad (2.36)
\]

In the $\theta$-direction, the terms in the stress tensor are approximated as follows, refer to Fig. 2.3(b):

\[
\left[ \frac{r}{\partial r} \left( \frac{v}{r} \right) \right]_{i+\frac{1}{2},j+\frac{1}{2}} = \frac{v_{i+\frac{1}{2},j+1} - v_{i+\frac{1}{2},j}}{r_j + 1 - r_j} - \frac{v_{i+\frac{1}{2},j+1} + v_{i+\frac{1}{2},j}}{2r_j + 1} \quad (2.37)
\]

\[
\left( \frac{1}{r} \frac{\partial u}{\partial \theta} \right)_{i+\frac{1}{2},j+\frac{1}{2}} = \frac{2 \left( u_{i+1,j+\frac{1}{2}} - u_{i,j+\frac{1}{2}} \right)}{r_j + \frac{1}{2} \left( \Delta \theta_i + \Delta \theta_{i+1} \right)} \quad (2.38)
\]

\[
\left( \frac{1}{r} \frac{\partial v}{\partial \theta} \right)_{i,j} = \frac{v_{i+\frac{1}{2},j} - v_{i-\frac{1}{2},j}}{r_j \Delta \theta_i} \quad (2.39)
\]

\[
\left( \frac{u}{r} \right)_{i,j} = \frac{u_{i,j+\frac{1}{2}} + u_{i,j-\frac{1}{2}}}{2r_j} \quad (2.40)
\]

The values of the source terms at the center of the cell are approximated as:

\[
\left( \frac{1}{r} \frac{\partial u}{\partial \theta} \right)_{i+\frac{1}{2},j} = \frac{\left( u_{i+1,j-\frac{1}{2}} + u_{i+1,j+\frac{1}{2}} \right) - \left( u_{i,j-\frac{1}{2}} + u_{i,j+\frac{1}{2}} \right)}{r_j \left( \Delta \theta_i + \Delta \theta_{i+1} \right)} \quad (2.41)
\]

\[
\left[ \frac{r}{\partial r} \left( \frac{v}{r} \right) \right]_{i+\frac{1}{2},j} = \frac{v_{i+\frac{1}{2},j+1} - v_{i+\frac{1}{2},j-1}}{r_j + 1 - r_j} - \frac{v_{i+\frac{1}{2},j}}{r_j} \quad (2.42)
\]

\[
u_{i+\frac{1}{2},j} = \frac{u_{i,j-\frac{1}{2}} + u_{i,j+\frac{1}{2}} + u_{i+1,j-\frac{1}{2}} + u_{i+1,j+\frac{1}{2}}}{4} \quad (2.43)
\]
2.3.3 Surface Tension

At the interface between two static fluids, and in the absence of any external force, a boundary condition requires the surface tension to be balanced by a pressure difference according to the Young-Laplace equation [32]:

$$\Delta P_{\text{surface}} = \sigma \kappa$$

(2.44)

where $\sigma$ is the surface tension coefficient and $\kappa$ is the local curvature of the interface defined by:

$$\kappa = \frac{1}{R_1} + \frac{1}{R_2}$$

(2.45)

where $R_1$ and $R_2$ represent the principal radii of curvature.

An alternative treatment of the surface tension is the continuum surface force (CSF) model of Brackbill et al. [4]. In this model, surface tension is represented by a volume force that resembles the induced pressure difference in Eq. (2.44):

$$F_{st} = \sigma \kappa \nabla f$$

(2.46)

where $\nabla f$ is the volume fraction gradient and is approximated as:

$$(\nabla f)_{i,j+\frac{1}{2}} = \frac{f_{i,j+1} - f_{i,j}}{r_{j+1} - r_j}$$

(2.47)

$$(\nabla f)_{i+\frac{1}{2},j} = \frac{f_{i+1,j} - f_{i,j}}{r_j (\theta_{i+1} - \theta_i)}$$

(2.48)

A well-known drawback of this method is the introduction of numerical spurious currents near the interface, that can be problematic in surface tension dominant flows [23]. The spurious currents can result from inaccurate representations of the surface tension force, and/or an incompatible treatment of the surface tension and pressure gradient terms, which for a static spherical bubble, should exactly balance each other. The former can be improved by a better curvature approximation, which is described in section 3.1.5. The latter can be improved by using the balanced-force approach proposed by Francois et al. [23]. The basic idea behind this approach is to discretize $\nabla P$ (in Eq. (2.14)) and
\( \nabla f \) (in Eq. (2.46)) in the same manner and at the same location, i.e. at cell faces. \( \vec{F}_{st} \) is non-zero only at cell faces when an interface lies in one or both of the adjacent cell volumes or coincides with the cell face, i.e. \( \nabla f \neq 0 \).

Finally, since the surface tension force is calculated at cell faces, the curvature at cell centers must be interpolated to cell faces. For example, the curvature at the \( j + \frac{1}{2} \) face is evaluated as:

\[
\kappa_{i,j}^{\frac{1}{2}} = \begin{cases} 
\frac{\kappa_{i,j} + \kappa_{i,j+1}}{2} & \text{if } 0 < f_{i,j} < 1 \text{ and } f_{i,j+1} = 0 \text{ or } 1 \\
\kappa_{i,j} & \text{if } 0 < f_{i,j} < 1 \text{ and } f_{i,j+1} = 0 \text{ or } 1 \\
\kappa_{i,j+1} & \text{if } 0 < f_{i,j+1} < 1 \text{ and } f_{i,j} = 0 \text{ or } 1 
\end{cases}
\]

### 2.3.4 Pressure Term

The pressure field is determined by discretizing Eq. (2.17) and solving the set of algebraic equations:

\[
a_{i,j} P_{i,j} = b_{i,j} - \sum_{nb} a_{nb} P_{nb} \tag{2.49}
\]

where the index \( nb \) represents the four neighboring cells, and the coefficients are as follows:

\[
a_{i+\frac{1}{2},j} = \frac{A_{i+\frac{1}{2},j}}{\rho_{i+\frac{1}{2},j} r_j (\theta_{i+1} - \theta_i)} \\
a_{i-\frac{1}{2},j} = \frac{A_{i-\frac{1}{2},j}}{\rho_{i-\frac{1}{2},j} r_j (\theta_i - \theta_{i-1})} \\
a_{i,j+\frac{1}{2}} = \frac{A_{i,j+\frac{1}{2}}}{\rho_{i,j+\frac{1}{2}} (r_{j+1} - r_j)} \\
a_{i,j-\frac{1}{2}} = \frac{A_{i,j-\frac{1}{2}}}{\rho_{i,j-\frac{1}{2}} (r_j - r_{j-1})} \\
a_{i,j} = -a_{i+\frac{1}{2},j} - a_{i-\frac{1}{2},j} - a_{i,j+\frac{1}{2}} - a_{i,j-\frac{1}{2}} \\
b_{i,j} = \frac{1}{\Delta t} \left( v_{i+\frac{1}{2},j} A_{i+\frac{1}{2},j} - v_{i-\frac{1}{2},j} A_{i-\frac{1}{2},j} + u_{i,j+\frac{1}{2}} A_{i,j+\frac{1}{2}} - u_{i,j-\frac{1}{2}} A_{i,j-\frac{1}{2}} \right) \tag{2.50}
\]

Eq. (2.49) is solved using the Bi-Conjugate Gradient Stabilized method [43].
2.3.5 Complete Timestep

One complete timestep, from $t^n$ to $t^{n+1} = t^n + \Delta t$, involves the following operations, where $\rho^n, \mu^n, \kappa^n, f^n, u^n, v^n$, and $P^n$ are known, either as initialized values or from a previous timestep:

1. reconstruct interfaces from volume fractions $f^n$

2. advect $f^n$ to $f^{n+1}$ using $u^n$ and $v^n$

3. calculate $\rho^{n+1}, \mu^{n+1},$ and $\kappa^{n+1}$ from $f^{n+1}$

4. solve Eq. (2.14) to determine the interim velocity field $\vec{V}^*$

5. solve Eq. (2.15) to determine the interim velocity field $\vec{V}^{**}$

6. solve the Poisson equation, Eq. (2.17), to determine $\nabla P^{n+1}$

7. solve Eq. (2.16) to determine $\vec{V}^{n+1}$
Chapter 3

The Volume-of-Fluid Method in Spherical Coordinates

The VOF method is an interface capturing technique that tracks fluid volume instead of an interface directly, by accounting for the volume fraction $f$ of one of the fluids - say oil - in each computational cell. $f = 1$ and $f = 0$ imply that a cell is full of oil and water, respectively; $0 < f < 1$ implies the existence of an “interface cell.”

A VOF method consists of two operations per timestep: reconstruction and advection. A brief description will be first given in Cartesian coordinates before introducing a more detailed description in the spherical coordinate system, illustrated in Fig. 2.1(a). Due to the axisymmetric assumption in the $\phi$ direction, the implementation is simplified to two dimensions, $r$ and $\theta$ on the $x$-$z$ plane.

State-of-the-art VOF methods reconstruct interfaces in a piecewise linear (PLIC) manner in each interface cell, which requires an estimate of an interface normal and a calculated line constant. In the Cartesian coordinate system, the reconstructed line segment can be expressed as:

$$x = -\frac{n_z}{n_x}z + L$$  \hspace{1cm} (3.1)

where $\vec{n} = n_x \hat{i} + n_z \hat{k}$ is the calculated normal, and $L$ the line constant, which determines
the position of the segment within the cell. There are then two types of interface cells: 
the interface either intersects two opposite cell faces or two adjacent ones, as shown in 
Fig. 3.1(a).

In the spherical system, each interface segment is similarly represented by a normal 
and a line constant, which can be expressed as:

\[
r = \frac{n_x L}{n_z \cos \theta + n_x \sin \theta}
\]  

(3.2)

Notice that the normal components are specified in Cartesian coordinates for reasons of 
convenience in calculating fluid volumes.

The curved cell faces at constant \( r \) complicate the calculation of \( L \). Instead of two 
prototypical interface cells, there are six in the spherical system, illustrated in Fig. 3.1(b), 
which will be further discussed in section 3.1.3. (Note that in this figure and some others, 
the curvature of the \( r \) faces has been exaggerated for purposes of clarity.)
Figure 3.1: (a) The two types of interface cells in Cartesian coordinates; (b) the six types in spherical coordinates.
Moreover, fluid volume is calculated by revolving areas about the $z$-axis, as shown in Fig. 3.2(a). As a result, unlike in the 2D Cartesian system, a volume fraction does not correspond to a single projected area fraction, as illustrated in Fig. 3.2(b). Instead, the closer the fluid volume in a cell is to the $z$-axis, the larger is the projected area. Section 3.1 presents a methodology for reconstructing interfaces in spherical coordinates, including details of calculating normals, line constants, and reconstructed volumes.

Figure 3.2: (a) Volume revolved about the $z$-axis. (b) For the same volume fraction $f = 0.25$, for a cell centered at $(r=0.2125, \theta=0.7461)$, the projected area fraction depends on the position of the interface. The illustrated area fractions are (1) 0.261, (2) 0.239, (3) 0.258, and (4) 0.242.
Following reconstruction in each interface cell, fluid volume is advected according to Eq. (2.4), which is repeated here:

\[
\frac{\partial f}{\partial t} + (\vec{V} \cdot \nabla) f = 0
\]

where \(\vec{V}\) is the divergence-free velocity field determined using the finite volume flow solver (chapter 2). Discretization of this equation will be discussed in section 3.2.

### 3.1 Reconstruction

The details presented here are for a uniform spherical mesh of size \((\Delta r, \Delta \theta)\); the extension to a non-uniform mesh is relatively straightforward. Interfaces must be reconstructed both in interface cells \((0 < f < 1)\) and in the flux volumes that are a part of the volume advection calculation (described in section 3.2). Reconstruction requires determination of a normal and a line constant for each interface cell. Here, the normal is calculated using the so-called height function method [23], which has recently been shown to yield much more accurate normals than commonly used methods based on calculating \(\nabla f\) (e.g. [72]). Then the line constant \(L\) is solved iteratively (section 3.1.2) to yield a reconstructed volume fraction (section 3.1.3) that matches the known value. (Note that in Cartesian coordinates one can easily calculate \(L\) directly [54]; but an iterative scheme is necessary in the spherical system, for reasons of geometric complexity.) For the special case of reconstructing near a contact line, some modifications are necessary (section 3.1.4). In addition, interface curvature (section 3.1.5), which is required to determine the surface tension force, is also calculated using the height function method.

Finally, note that the work up to section 3.1.3 was completed prior to beginning my M.A.Sc. program, but is included here for completion.
3.1.1 Calculating Normals

The height function method for calculating an interface normal $\vec{n}$ from volume fractions has previously been applied to Cartesian coordinates; the spherical implementation is somewhat more complicated. As illustrated in Fig. 3.3, the method involves constructing a $7 \times 3$ stencil about each interface cell $(i, j)$, and then determining fluid “heights” $R$ or $\Theta$ (depending on the orientation) along three columns of the stencil. The preferred orientation for calculating $\vec{n}$ is determined only after heights in both directions have been calculated.

For stencils oriented in the $r$ direction about a cell $(i, j)$, Fig. 3.3(a), one discretely sums the volume of one of the fluids in each of three columns, and then determines the height, $R_i$, that yields an equivalent total volume:

$$
\int_0^{2\pi} \int_{\theta}^{\theta + \Delta \theta} \int_{r_b}^{R_i} r^2 |\sin \theta| \, dr \, d\theta \, d\phi = \sum_{a=j-3}^{j+3} f_{i,a} \Omega_{i,a} \tag{3.3}
$$

$r_b$ is the distance from the origin to the base of the stencil, and $\Omega_{i,a}$ and $f_{i,a}$ are the volume and volume fraction of cell $(i, a)$, respectively. Rearranging this equation yields:

$$
R_i = 3 \left[ \sum_{a=i-3}^{i+3} \frac{3 \sum_{a=j-3}^{j+3} f_{i,a} \Omega_{i,a}}{2\pi [\cos \theta - \cos (\theta + \Delta \theta)]} + r_b^3 \right]^{1/3} \tag{3.4}
$$

Occasionally, in under-resolved regions of a domain, a height function stencil may intersect more than one interface, evidenced by a non-monotonic change in volume fraction along any column. Such situations are handled similarly to [37].

Alternatively, for stencils oriented in the $\theta$ direction, Fig. 3.3(b), the height $\Theta_j$ (in radians) is calculated by equating:

$$
\int_0^{2\pi} \int_{\theta}^{\Theta_j} \int_{r}^{r + \Delta r} r^2 |\sin \theta| \, dr \, d\theta \, d\phi = \sum_{a=i-3}^{i+3} f_{a,j} \Omega_{a,j} \tag{3.5}
$$

where $\theta_b$ is the angle from the positive $z$-axis to the base of the stencil. Rearranging this equation yields:

$$
\Theta_j = \cos^{-1} \left\{ \cos \theta_b - \frac{3 [\sum_{a=i-3}^{i+3} f_{a,j} \Omega_{a,j}]}{2\pi [ (r + \Delta r)^3 - r^3]} \right\} \tag{3.6}
$$
Figure 3.3: A $7 \times 3$ stencil oriented in the (a) $r$ and (b) $\theta$ directions.
Having determined fluid heights in both directions, the stencil “more normal” to the interface is then used to calculate $\vec{n}$: if $|R_{i+1} - R_{i-1}|/\Delta r \leq |\Theta_{j+1} - \Theta_{j-1}|/\Delta \theta$, the stencil oriented in the $r$ direction is used; otherwise, the $\theta$ stencil is used. If the stencil is oriented in the $r$ direction, the normal is then calculated as:

$$\vec{n} = -R_i \hat{e}_r + R_\theta \hat{e}_\theta$$

(3.7)

where $\hat{e}_r$ and $\hat{e}_\theta$ are unit vectors in the $r$ and $\theta$ directions, and $R_\theta$ denotes the partial derivative $\partial R/\partial \theta$, approximated by:

$$R_\theta = \frac{R_{i+1} - R_{i-1}}{2\Delta \theta}$$

(3.8)

Otherwise, if the stencil is oriented in the $\theta$ direction, the normal is determined as:

$$\vec{n} = r_j \Theta_r \hat{e}_r - \hat{e}_\theta$$

(3.9)

where $\Theta_r$ denotes $\partial \Theta/\partial r$, approximated by:

$$\Theta_r = \frac{\Theta_{j+1} - \Theta_{j-1}}{2\Delta r}$$

(3.10)

Finally, the normals are converted to Cartesian components:

$$n_z = n_r \cos \theta - n_\theta \sin \theta$$

(3.11)

$$n_x = n_r \sin \theta + n_\theta \cos \theta$$

(3.12)
3.1.2 Calculating the Line Constant $L$

Given a normal $\vec{n}$, a line constant $L$ must be determined that yields a revolved volume equal to the known fluid volume $f_{i,j}\Omega_{i,j}$; this is done iteratively here via the bisection method [16]. The initial limits of $L$ correspond to $f = 0$ and $f = 1$; the first guess of $L$ is the average of the two limits. Depending on whether the corresponding volume is greater or less than the actual value, one of the limits of $L$ is then reset to the guessed value, and a new guess is calculated. The process repeats until the difference between the calculated and known fluid volumes is less than some cutoff value.

To determine the initial upper and lower limits of $L$, the orientation of the interface, $\theta_m$, is compared to the orientation of the right and left cell faces, $\theta_r$ and $\theta_l$, defined in Fig. 3.4. Three cases exist, as shown in Fig. 3.5. In case 1, $L_{\text{lower}}$ corresponds to the interface that intersects the inner right corner; $L_{\text{upper}}$ is either tangent to the outer $r$ face or intersects the outer left corner of the cell. In case 2, the $L_{\text{lower}}$ interface intersects the inner left corner; the other interface is either tangent to the outer $r$ face or intersects the
outer right corner. In case 3, the bounding interfaces will intersect the two corners of the outer $r$ face.

Figure 3.5: The three cases for determining the limiting values of the line constant $L$: (a) $\theta_m < \theta_r$, (b) $\theta_l < \theta_m$, and (c) $\theta_r \leq \theta_m \leq \theta_l$

### 3.1.3 Calculating the Reconstructed Volume

Given $\vec{n}$ and a guessed value of $L$, the reconstructed fluid volume must be calculated. In a 2D spherical system, a typical cell is illustrated in Fig. 3.4(b): two of the faces are linear segments, $\theta_r$ and $\theta_l$; two are circular arcs, $r_i$ and $r_o$. Returning to Fig. 3.1(b), notice that an interface can intersect: (1) the two linear $\theta$ faces, (2) the two curvilinear $r$ faces, (3) a $\theta$ and a $r$ face, (4) the outer $r$ face twice, (5) the inner $r$ face twice and the two $\theta$ faces, and (6) the inner $r$ face twice and the outer $r$ face. Note that case 6 is a special instance of case 5 that will only occur when reconstructing an advected flux volume (described in section 3.2), characterized by $\Delta r \ll r \Delta \theta$. For a given interface cell,
to determine the intersection type and to calculate the revolved volume associated with \( \vec{n} \) and \( L \), a number of geometric functions are utilized repeatedly to calculate various quantities; these functions are similar in spirit to the geometric toolkit of Rider and Kothe [50].

1. The **line-line intersection** function determines the point of intersection of an interface and a \( \theta \) face; the intersection is only of interest if it lies on the cell face (i.e. between \( r_i \) and \( r_o \)).

2. The **line-curve intersection** function determines the intersection of an interface and one of the \( r \) faces, by simultaneously solving the equations of a line and a circle. The intersection is only of interest if it lies between \( \theta_r \) and \( \theta_\ell \).

3. The **tangent to a curve** function locates the tangent point of a line of specified slope and a \( r \) face, if it lies between \( \theta_r \) and \( \theta_\ell \). The line constant of the tangent line is then:

\[
L = \sqrt{r^2 \left[ \left( \frac{n_z}{n_x} \right)^2 + 1 \right]} \tag{3.13}
\]

4. The **location of a point** function is used to determine whether a specified point in an interface cell is within oil or water. Since \( \vec{n} \) points towards oil, we evaluate the dot product of \( \vec{n} \) and a vector from a point on the interface to the point of interest; if positive, then the specified point is in oil, else the point is in water.

The final two functions are used to calculate revolved volumes.

5. The **volume of a full cell**, bounded by \( \theta_r \), \( \theta_\ell \), \( r_i \), and \( r_o \), is:

\[
\Omega = \int_0^{2\pi} \int_{\theta_r}^{\theta_\ell} \int_{r_i}^{r_o} r^2 |\sin \theta| \, dr \, d\theta \, d\phi \tag{3.14}
\]

which simplifies to:

\[
\Omega = \frac{2\pi}{3} (r_o^3 - r_i^3) (\cos \theta_r - \cos \theta_\ell) \tag{3.15}
\]
6. For a cell with an interface that only intersects the two $\theta$ faces (i.e. type 1), the volume above/below an interface is calculated by replacing either $r_i$ or $r_o$ in Eq. (3.14) by the line equation of the interface, Eq. (3.2). Thus the volumes above and below an interface are:

$$
\Omega_{\text{above}} = \int_{\theta_e}^{\theta_i} \frac{2\pi}{3} \left[ r_o^3 - \frac{(n_x \cdot L)^3}{(n_z \cos \theta + n_x \sin \theta)^3} \right] |\sin \theta| \, d\theta \quad (3.16)
$$

and

$$
\Omega_{\text{below}} = \int_{\theta_e}^{\theta_i} \frac{2\pi}{3} \left[ \frac{(n_x \cdot L)^3}{(n_z \cos \theta + n_x \sin \theta)^3} - r_i^3 \right] |\sin \theta| \, d\theta \quad (3.17)
$$

respectively. These equations are integrated numerically using Gaussian quadrature [16].

For a given $\vec{n}$ and a guessed $L$, the reconstructed fluid volume can be determined using these functions in a systematic way. First the intersection type (see Fig. 3.1(b)) can be identified using functions 1 and 2. The fluid orientation relative to the interface can then be determined via function 4. Finally, the revolved fluid volume can be determined by manipulating Eqs. (3.15), (3.16), and (3.17) (via functions 5 and 6). For example, Fig. 3.6 illustrates an interface that intersects the $r_o$ and $\theta_{\ell}$ faces (case 3), with oil to the right of the interface. The revolved volume of oil can be calculated by partitioning the cell into two subcells: one full and one with fluid below the interface; hence the fluid volume can be calculated by summing Eqs. (3.15) and (3.17).

### 3.1.4 Special Case: Reconstructing Near a Contact Line

When an interface intersects a solid surface, the orientation of the interface is specified as a known contact angle $\alpha$, which in turn affects the reconstruction of cells in the vicinity of the contact line. An approach to applying contact angles in the context of height functions in a 2D Cartesian system is described by Afkhami and Bussmann [1]. An analogous approach is applied in this case to the 2D spherical system.
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Figure 3.6: Calculation of the revolved reconstructed volume in an interface cell, by partitioning the cell into two subcells.

A contact line appears as a point on the projected 2D $r - \theta$ plane. Since VOF does not explicitly track an interface, the contact line location must be identified implicitly. A contact line cell - a cell that contains the contact line - is defined as an interface cell along a solid surface that neighbours an empty cell. $\alpha$ is the angle between the normal to the interface and the normal to the solid surface at the contact line point, Fig. 3.7(a). The contact line position is then determined iteratively. With each guess of the contact line position within the cell and the specified $\alpha$, the interface normal, line constant, and the resultant fluid volume are calculated and compared to the known fluid volume. Note that the normal in this cell is not calculated from height functions.

Once $\vec{n}$ and $L$ for the contact line cell have been determined, the heights $R_{i-1}$ for the empty neighbouring column and $\Theta_{j-1}$ within the solid boundary (refer to Fig. 3.7) can be calculated, in order to calculate the contact line value of $\kappa$. To calculate $R_{i-1}$,
Figure 3.7: (a) The contact angle $\alpha$ is the angle between the normal to the interface and the normal to the solid boundary; (b) contact-line stencil in the $r$-direction, the fluid volume in the ghost cells (hatched) is determined by extending the interface into the solid boundary; (c) contact-line stencil in the $\theta$-direction.
the reconstructed interface in the contact line cell is extended into the solid boundary, and the corresponding volume fractions in the “ghost cells” (i.e. the neighbouring cells within the solid boundary) are calculated based on the extended interface (the hatched volumes in Fig. 3.7(b). Heights $R_{i+1}$ and $R_i$ are calculated from volume fractions as before, except that they include the ghost cell values. Finally, $R_{i-1}$ is defined such that $\alpha$ can be approximately satisfied at the contact line:

$$R_{i-1} = R_i - r_{sph} (\theta_i - \theta_{i-1}) \tan (\alpha - \Delta \theta_c)$$

(3.18)

where $\Delta \theta_c$ is the value of $\theta$ at the contact line point subtract the value at the cell center. Similarly, for a contact line oriented more normal to the $\theta$-direction, given $\Theta_j$, $\Theta_{j-1}$ can be calculated such that $\alpha$ can be approximately satisfied at the contact line:

$$\Theta_{j-1} = \Theta_j - \frac{(r_j - r_{j-1}) \cos (\alpha - \Delta \theta_c)}{r_{sph} \sin (\alpha - \Delta \theta_c)}$$

(3.19)

Finally, a major obstacle to contact line simulations is that in the region near the contact line cell, the height function stencil can sometimes be under-resolved, by allowing the interface to cross the bottom/top of the stencil, as shown in Fig. 3.8(a). This leads to either a large under- or overestimation of the height in that column. For example, consider Fig. 3.8(a). If $\Theta_{j+1}$ is determined using Eq. (3.6), its value will be greatly over-predicted leading to a larger calculated $r$-component of the normal in cell $(i, j)$, as illustrated in the poor reconstruction in Fig. 3.8(c). To circumvent this problem, Ferdowsi and Bussmann [20] suggested that instead of calculating height $\Theta_{j+1}$ in column $j + 1$, one should calculate a radial height $R_{i+1}$ in row $i + 1$, and then substitute $\theta_{i+1}$ for $\Theta_{j+1}$ and $(R_{i+1} - r_{j-1})$ for $2\Delta r$ in Eq. (3.10) to calculate the normal components.

A similar approach is applied here, but instead of replacing $\Theta_{j+1}$ with $\theta_{i+1}$, $\Theta_{j+1}$ is calculated in a modified column whose width is defined by $r_{trunc}$, as shown in Fig. 3.8(b). In this case, $r_{trunc}$ corresponds to the radial height in row $i + 3$, in other words $R_{i+3}$. Then, $2\Delta r$ is replaced by $0.5 \left( r_{j+1/2} + r_{trunc} \right) - r_{j-1}$. Fig. 3.8(d) illustrates an improved
reconstruction using the new approach. An under-resolved stencil in the $r$-direction can be handled analogously.

Figure 3.8: (a) An under-resolved stencil where the interface crossed the top of the stencil; (b) an alternative way of defining the stencil; (c) interface reconstruction using the old stencil; (d) interface reconstruction using the new stencil.
3.1.5 Curvature Calculation

The height function method which is used to calculate the interface normal is also used to calculate interface curvature. This allows the heights determined to calculate normals to be reused for curvatures. The equations for the curvature are derived from the fundamental magnitudes of second order (see Appendix A). For a stencil oriented in the $r$-direction, the curvature is calculated as:

$$
\kappa = \frac{\text{sign}(n_r)}{\left(R^2 R_\theta^2 \sin^2 \theta + R^4 \sin^2 \theta\right)^{3/2}} \left(R^2 R_\theta^2 \sin^2 \theta \cos \theta - 3R^3 R_\theta^2 \sin^3 \theta + R^4 R_\theta \sin^3 \theta\right) + R^4 R_\theta \sin^2 \theta \cos \theta - 2R^5 \sin^3 \theta + R^4 R_\theta \sin^3 \theta\right) \right)^{3/2}
$$

where $\text{sign}(n_r)$ denotes only the sign of the $r$ component of the normal, and $R_{\theta \theta}$ denotes the second partial derivative $\partial^2 R/\partial \theta^2$, approximated by:

$$
R_{\theta \theta} = \frac{R_{i+1} - 2R_i + R_{i-1}}{\Delta \theta^2}
$$

On the other hand, for a stencil oriented in the $\theta$-direction, the curvature is calculated by:

$$
\kappa = \frac{\text{sign}(n_\theta)}{\left(r^2 \sin^2 \Theta + r^4 \Theta_r^2 \sin^2 \Theta\right)^{3/2}} \left(2r^5 \Theta_r^3 \sin^3 \Theta + 3r^3 \Theta_r \sin^3 \Theta + r^4 \Theta_r \sin^3 \Theta - r^2 \sin^2 \Theta \cos \Theta - r^4 \Theta_r^2 \sin^2 \Theta \cos \Theta\right) \right)^{3/2}
$$

where $\text{sign}(n_\theta)$ denotes only the sign of the $\theta$ component of the normal, and $\Theta_{rr}$ denotes $\partial^2 \Theta/\partial r^2$, approximated by:

$$
\Theta_{rr} = \frac{\Theta_{j+1} - 2\Theta_j + \Theta_{j-1}}{\Delta r^2}
$$

This concludes the presentation of the reconstruction methodology. The following section focuses on the second operation in the VOF method, namely advection.
Given a divergence-free velocity field $\vec{V}$, advection is governed by Eq. (2.4). For discrete volume fractions, Youngs [72] discretized this equation in an operator-split manner, advecting $f$ separately in each orthogonal direction once per timestep $\Delta t$. Applied to the spherical coordinate system, Eq. (2.4) is discretized as:

$$f_{i,j}^* = f_{i,j}^n \Omega_{i,j} - \left( u_{i,j+\frac{1}{2}} \langle f \rangle_{i,j+\frac{1}{2}} A_{i,j+\frac{1}{2}} - u_{i,j-\frac{1}{2}} \langle f \rangle_{i,j-\frac{1}{2}} A_{i,j-\frac{1}{2}} \right) \Delta t$$

(3.24)

$$f_{i,j}^{n+1} = f_{i,j}^* \Omega_{i,j}^* - \left( v_{i+\frac{1}{2},j} \langle f \rangle_{i+\frac{1}{2},j} A_{i+\frac{1}{2},j} - v_{i-\frac{1}{2},j} \langle f \rangle_{i-\frac{1}{2},j} A_{i-\frac{1}{2},j} \right) \Delta t$$

(3.25)

where $f_{i,j}^n$, $f_{i,j}^*$, $f_{i,j}^{n+1}$ are the volume fractions at timestep $n$, after advection in one direction, and at timestep $n + 1$, respectively; $u$ and $v$ are average face velocities in the $r$ and $\theta$ directions, calculated using the finite volume flow solver; $\Omega$ and $\Omega^*$ are the cell volumes at timestep $n$ and after advection in one direction, respectively, determined using Eq. (3.15), and $A$ is the surface area of a cell face, calculated as:

$$A = \int_0^{2\pi} \int_{\theta_i}^{\theta_o} r^2 |\sin \theta| d\theta d\phi$$

(3.26)

for $r$ faces ($A_{i,j+1/2}$ and $A_{i,j-1/2}$), and

$$A = \int_0^{2\pi} \int_{r_i}^{r_o} r |\sin \theta| dr d\phi$$

(3.27)

for $\theta$ faces ($A_{i+1/2,j}$ and $A_{i-1/2,j}$). $\langle f \rangle$ is the volume fraction of oil in a flux volume, determined by geometrically reconstructing the interface inside the region enclosed by the dashed lines in Fig. 3.9. Note that after the first half step, the interface cells are reconstructed using the $f^*$ values in the original cell volumes $\Omega$. The order of advection is alternated every timestep to minimize directional bias.

This concludes the presentation of the methodology of the two operations at each timestep of the VOF method, namely reconstruction and advection. The next chapter presents validations of the numerical model.
Figure 3.9: \( \langle f \rangle \) is the volume fraction of fluid 1 within the flux volume (region inside the dashed line).
Chapter 4

Validation

The numerical model was validated by a series of test cases before it was applied to model the oil/water/particle separation. The flow code solver and the VOF algorithm were first validated independently. Then the combined model was validated by reproducing the equilibrium configurations of an axisymmetric oil-coated particle acted upon by gravity.

4.1 Flow Code Solver

The following test cases were used to validate the flow code solver: uniform flow over a solid sphere (section 4.1.1), uniform flow over a spherical bubble (section 4.1.2), and linearly accelerating flow over a solid sphere (section 4.1.3). For each test case, for Re < 1, the domain size was $r_\infty/r_{sph} \approx 68$, for $1 \leq Re < 10$, $r_\infty/r_{sph} \approx 33$, and for Re $\geq 10$, $r_\infty/r_{sph} = 16$.

4.1.1 Uniform Flow Over a Solid Sphere

The flow solver was first validated for uniform flow over a solid sphere, which has been studied numerically and experimentally by many authors [15, 22, 30, 33, 36, 48, 49, 51, 64]. At a critical Reynolds number, a recirculation region develops behind the solid
sphere. The angle at which the flow separates, Fig. 4.1(a), the distance at which the flow reattaches, Fig. 4.1(b), the vortex position, Fig. 4.1(c), and the surface drag coefficient, Fig. 4.1(d), are plotted versus Reynolds number up to 300. In addition, the surface pressure, Fig. 4.2, and vorticity, Fig. 4.3 are plotted at Re = 1, 10, 100, and 300 (Here \( \theta = 0^\circ \) corresponds to the front stagnation point). The reattachment length and vortex positions are non-dimensionalized by the sphere diameter, \( d \), the relative pressure \( (P-P_o) \), where \( P_o \) is the pressure at a point on the upstream boundary, by \( \rho V_\infty^2/2 \), the viscosity by \( 2V_\infty/d \), and the surface drag coefficient is defined as:

\[
C_d = \frac{F}{\pi d^2 \rho V_\infty^2/8}
\]  

(4.1)

Note that some data for this and the following test cases were only available in graphical form presented in Magnaudet et al. [36], Johnson and Patel [30], and Chang and Maxey [9], and were retrieved by digitizing the graphs using GetData Graph Digitizer 2.24. For most cases, the computed results agree very well with the literature data, especially those of Le Clair et al. [33] and Magnaudet et al. [36]. This is most likely because the outer boundary conditions are adapted from the ones defined by Magnaudet et al. [36]. The scatter in the reattachment length beginning at Re = 200 exists even between among published data, likely because, as Johnson and Patel [30] reported, the flow is no longer axisymmetric at Re \( \geq 211 \).
Figure 4.1: (a) Separation angle, (b) reattachment length, (c) vortex position, and (d) drag coefficient for uniform flow over a solid sphere.
Figure 4.2: Surface pressure distributions on the solid sphere at (a) $Re=1$, (b) $Re=10$, (c) $Re=100$, and (d) $Re=300$. 
Figure 4.3: Surface vorticity distributions on the solid sphere at (a) Re=1, (b) Re=10, (c) Re=100, and (d) Re=300.
4.1.2 Uniform Flow Over a Spherical Bubble

The flow solver was further validated for uniform flow over a spherical bubble. Shear-free boundary conditions were applied at the bubble surface (at \( r = r_{sph} \)):

\[
    u_{sph} = 0 \tag{4.2}
\]

\[
    \left( \frac{\partial v}{\partial r} - \frac{v}{r} \right)_{sph} = 0 \tag{4.3}
\]

The drag coefficient is plotted for \( Re \) up to 300, Fig. 4.4, and the surface pressure, Fig. 4.5, and vorticity, Fig. 4.6, are plotted for \( Re = 1, 10, 100, \) and 300. Again, the results agree well with existing data from [3, 36, 44, 53, 65], especially that of Magnaudet et al. [36].

![Figure 4.4: Drag coefficient for uniform flow over a spherical bubble.](image-url)
Figure 4.5: Surface pressure distributions on the spherical bubble at (a) $Re=1$, (b) $Re=10$, (c) $Re=100$, and (d) $Re=300$. 
Figure 4.6: Surface vorticity distributions on the spherical bubble at (a) \( \text{Re}=1 \), (b) \( \text{Re}=10 \), (c) \( \text{Re}=100 \), and (d) \( \text{Re}=300 \).
4.1.3 Linearly Accelerating Flow Over a Solid Sphere

The uniform flow over a solid sphere and bubble are steady state cases. To test the time discretization, linear accelerating flow over a solid sphere was simulated and the results compared to those of Chang and Maxey [9]. The external velocity $V_\infty(t)$ accelerates linearly:

$$
V_\infty(t) = \begin{cases} 
  c_1 & t \leq t_s \\
  c_1 + A_c(t - t_s) & t_s < t \leq t_e \\
  c_2 & t > t_e
\end{cases}
$$

where $t_s$ and $t_e$ are the time when acceleration begins and ends, respectively, $c_1$ and $c_2$ are constants between zero and one, $A_c$ is the dimensionless acceleration number (its dimensional form is given by $A_c V_{\text{max}}^2 / r_{\text{sph}}$), and $V_{\text{max}} = \max(V_\infty(t))$ is the maximum external velocity. Note that for this test case only, the flow is from left to right, and thus $\theta = 0^\circ$ corresponds to the rear stagnation point. The surface pressure, measured relative to the value at the front stagnation point, is non-dimensionalized by $\rho V_{\text{max}}^2 / 2$; viscosity by $V_{\text{max}} / r_{\text{sph}}$, Re is defined as $2 \rho V_{\text{max}} r_{\text{sph}} / \mu$, and the surface drag coefficient is defined as:

$$
C_d = \frac{F}{\pi \rho r_{\text{sph}}^2 V_{\text{max}}^2} \quad (4.4)
$$

The first case corresponds to $c_1 = 0.5$, $c_2 = 1$, Re = 10 and $A_c = 1$. The drag coefficients (viscous drag $C_f$, pressure drag $C_p$, and total drag $C_d$), surface pressure, and surface vorticity are plotted in Figs. 4.7(a), 4.8, and 4.9, respectively. The results are in close agreement with those presented by Chang and Maxey [9], except for the pressure distribution at the instant after acceleration ceases, at which time the pressure changes abruptly, Fig. 4.8(d). One factor that contributes to the discrepancy is that the short time, $\Delta t$, that elapses after acceleration ceases, was not specified in Chang and Maxey’s paper; all they mentioned was that a time step of the order of $10^{-6}$ is not uncommon, and so $\Delta t$ was set to $10^{-6}$ for the present study.
Figure 4.7: Surface drag coefficients at Re=10, and (a) Ac=1 and (b) Ac=-1.
Figure 4.8: Surface pressure distributions at Re=10 and A_c=1 when (a) $V_\infty(t)=0.5$, (b) $V_\infty(t)=0.75$, (c) $V_\infty(t_e-\Delta t)<1$, (d) the instant after acceleration ceases $V_\infty(t_e+\Delta t)=1$, and (e) $V_\infty(t_e+1)=1$. 
Figure 4.9: Surface vorticity distributions at $Re=10$ and $A_c=1$ when (a) $V_\infty(t)=0.5$, (b) $V_\infty(t)=0.75$, (c) the instant after acceleration ceases $V_\infty(t_e+\Delta t)=1$, and (d) $V_\infty(t_e+1)=1$. 
The second test corresponds to $c_1 = 1$, $c_2 = 0.5$, $Re = 10$ and $A_c = -1$, corresponding to a decelerating $V_\infty$. There are inconsistencies in the surface pressure distributions at the instants right after the deceleration begins, Fig. 4.10(b), and ceases, Fig. 4.10(e), but again, $\Delta t$ was not specified. In addition, the distribution does not agree well when $V_\infty(t) = 0.68$, Fig. 4.10(d), but coincidentally, Chang and Maxey’s curve for $V_\infty(t) = 0.68$ closely matches with the present data for the instant before deceleration ceases, $V_\infty(t_e - \Delta t) \approx 0.5$. On the other hand, the results for drag coefficients, Fig. 4.7(b), and surface vorticity, Fig. 4.11, are in excellent agreement.
Figure 4.10: Surface pressure distributions at Re=10 and $A_c=-1$ when (a) $V_\infty(t_s)=1$, (b) the instant after deceleration begins $V_\infty(t_s + \Delta t) < 1$, (c) $V_\infty(t)=0.75$, (d) $V_\infty(t)=0.68$, and (e) the instant after deceleration ceases $V_\infty(t_e + \Delta t)=0.5$. 
Figure 4.11: Surface vorticity distributions at Re=10 and $A_c=-1$ when (a) $V_\infty(t_s)=1$, (b) $V_\infty(t)=0.75$, and (c) the instant after deceleration ceases $V_\infty(t_c + \Delta t)=0.5$. 

(a) 

(b) 

(c)
4.2 VOF Algorithm

The VOF methodology was extensively tested on uniform meshes of radius $r_\infty = 1$. Results of both reconstruction and advection tests are detailed below. The following three norms were defined for errors $\varepsilon_{i,j}$ calculated in each of $N$ interface cells:

\[ L_1 = \frac{1}{N} \sum_{i,j} \varepsilon_{i,j} \]
\[ L_2 = \sqrt{\frac{1}{N} \sum_{i,j} \varepsilon_{i,j}^2} \]
\[ L_\infty = \max(\varepsilon_{i,j}) \]

4.2.1 Reconstruction Tests

To test reconstruction, several simple geometries were examined. In terms of the projected area, a semi-circle centered at the origin and one centered at (-0.6, 0), a circle, a semi-ellipse, and a plane bounded by a line parallel to and one by a line oblique to the $z$-axis, were examined. The dimensions of each shape are listed in Table 4.1, and the reconstructed geometries are illustrated in Fig. 4.12 at a mesh resolution of $40 \times 40$, and correspond to two spheres, a torus, an ellipsoid, a cylinder, and a cone. The reconstruction error was evaluated as the angular difference (in radians) between the calculated normal and the correct one. For the circles, the correct normal was assumed to be a vector from the center of a cell to the center of the circle. Note that the errors at cells adjacent to the origin and the outer boundary were not included, since the height function stencils for these cells are missing one column.

Tables 4.2 and 4.3 list the normal and curvature errors for each case as a function of mesh size. The circle centered at the origin is reconstructed to machine precision, as the height function technique in this case calculates normals and curvatures that are exact. On the other hand, the curvature for the oblique line (constant $\theta$), corresponding to a cone, is calculated to machine precision, but the normal error depends on the difference
between the incline angle and the angle at the center of the interface cell; hence refining the mesh does not necessarily reduce the error. For the other cases, the calculated normals converge with approximately first-order accuracy, while the calculated curvatures converge with approximately first to second-order accuracy.

Figure 4.12: The projected areas associated with six reconstruction tests, illustrated on a $40 \times 40$ mesh of unit radius. These areas correspond to (a,b) a sphere, (c) a torus, (d) an ellipsoid, (e) a cylinder, and (f) a cone.
## Table 4.1: Dimensions of each geometry.

<table>
<thead>
<tr>
<th>Case</th>
<th>Projected Shape</th>
<th>Center</th>
<th>Dimension(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Sphere</td>
<td>Semi-Circle</td>
<td>(0,0)</td>
<td>Radius=0.37</td>
</tr>
<tr>
<td>2. Sphere</td>
<td>Semi-Circle</td>
<td>(-0.6,0)</td>
<td>Radius=0.3</td>
</tr>
<tr>
<td>3. Torus</td>
<td>Circle</td>
<td>(0,0.6)</td>
<td>Radius=0.3</td>
</tr>
<tr>
<td>4. Ellipsoid</td>
<td>Semi-Ellipse</td>
<td>(0,0)</td>
<td>Semimajor axis=0.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Semiminor axis=0.2</td>
</tr>
<tr>
<td>5. Cylinder</td>
<td>Plane bounded by</td>
<td>N/A</td>
<td>Height=0.3</td>
</tr>
<tr>
<td></td>
<td>Horizontal Line</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6. Cone</td>
<td>Plane bounded by</td>
<td>N/A</td>
<td>Incline angle=0.35 rad</td>
</tr>
<tr>
<td></td>
<td>Oblique Line</td>
<td></td>
<td></td>
</tr>
<tr>
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<td>Resolution</td>
<td>$L_1$</td>
<td>$L_2$</td>
</tr>
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<td>------------</td>
<td>---------</td>
<td>---------</td>
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<td>2.30E-02</td>
<td>3.40E-02</td>
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<td>2.81E-02</td>
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<td>3.43E-03</td>
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Table 4.2: Summary of reconstruction errors.
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<th>$L_2$</th>
<th>$L_\infty$</th>
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<td>1.16E-15</td>
<td>2.66E-15</td>
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<td>1.96E-02</td>
<td>3.43E-02</td>
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<td>3. Torus</td>
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<td>4.94E-01</td>
<td>2.29E+00</td>
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<td>5. Cylinder</td>
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Table 4.3: Summary of curvature errors.
4.2.2 Advection Tests

To test the whole volume tracker, including reconstruction and advection at multiple timesteps, the sphere and the torus were advected in a horizontal velocity field, and the advection error was evaluated as the difference between the calculated and the expected exact fluid volumes at the end of each simulation. Table 4.4 lists the errors for each case as a function of mesh size. Each case was run at two different resolutions.

For the first case, a sphere with a radius of 0.37 and centered at the origin is translated horizontally in a velocity field of 0.02 for 3700 timesteps with a timestep size of 0.005, as shown in Fig. 4.13. For the second case, a torus with a tube radius of 0.37, and a center of torus to center of tube distance of 0.42, is translated under the same velocity field for 3700 timesteps to the right and then 3700 more to the left, to return the torus to the origin, as shown in Fig. 4.14. Overall, the error norms decrease by a factor of at least five as the resolution increases from $40 \times 40$ to $80 \times 80$.

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Resolution</th>
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<th>$L_2$</th>
<th>$L_{\infty}$</th>
</tr>
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Table 4.4: Summary of advection errors.
Chapter 4. Validation

Figure 4.13: A sphere of radius 0.37 translates to the right, at timesteps (a) 0, (b) 925, (c) 1850, (d) 2775, and (e,f) 3700. The resolution of (a) to (e) is $80 \times 80$; (f) is at $40 \times 40$. 
Figure 4.14: A torus with a tube radius of 0.37 translates to the right and then returns to its initial position, at timesteps (a) 0, (b) 1230, (c) 2460, (d) 3700, and (e,f) 7400. The resolution of (a) to (e) is $80 \times 80$; (f) is at $40 \times 40$. 
4.3 Flow Solver Combined with the VOF Algorithm

Finally, the combined flow solver and VOF methodology was validated by reproducing some of the results of Smith and van de Ven [60], of an axisymmetric oil-coated particle acted upon only by gravity and surface tension. The results are plotted as curves of contact angle, $\alpha$, versus the equilibrium position of the contact line as defined by the filling angle $\psi$, and compared with the results at constant Bond number, $\lambda$, and dimensionless oil volume, $\zeta$. The results for $\zeta = 3$ and $\lambda = 0, 0.3$ and $0.5$ are shown in Fig. 4.15. In Figs. 4.15(b) and (c), Smith and van de Ven [60] calculated two equilibrium values of $\psi$ for each $\alpha$, and the present model yields good predictions of one of the two positions.
Figure 4.15: Contact angle $\alpha$ versus equilibrium position $\psi$ at $\zeta=3$, and (a) $\lambda=0$, (b) $\lambda=0.3$, and (c) $\lambda=0.5$. 
Chapter 5

Results

The second focus of this thesis, after a description of the model that was developed, is a presentation of results of a study that examined the fate of an oil-coated particle immersed in a uniform laminar flow, and in particular, to predict the conditions at which separation occurs. The following list itemizes the values assigned to various parameters:

- The particle size relevant to oil sands range from 1 to 1000 microns [14, 62]. However, it has been found that particles smaller than 10µm (fine solids) tend to be retained in a continuous solvent + bitumen (oil) phase during the extraction, which is a different problem to that studied in this work [62]. To this end, the range of coarse solids (10µm-1000µm) was represented by an intermediate size of 100µm.

- By the addition of solvents, the oil phase density and dynamic viscosity can approach values associated with water; for simplicity, for this preliminary study, these values are assumed to be the same: \( \rho = 1000 \text{kg/m}^3 \) and \( \mu = 0.001 \text{Pa·s} \), respectively.

- The ratio of oil to oil + particle volume \( \eta \) varies from 20% to 60%.

- The interfacial tension of the oil/water interface \( \sigma \) is assumed constant, and ranges from 0.01mN/m to 50mN/m. This range was chosen to illustrate the effect of ultra-low interfacial tension achieved by adding surfactants.
• The contact angle $\alpha$, measured through the oil, is either $30^\circ$ or $90^\circ$, which represent a wetting and a non-wetting case.

• The uniform external velocity $V_\infty$ is $10\text{mm/s}$, approximately the terminal velocity of the particle falling through water.

These conditions correspond to the following dimensionless parameters:

$$\frac{\mu_1}{\mu_2} = 1$$
$$\frac{\rho_1}{\rho_2} = 1$$
$$\text{Re} = \frac{\rho_2 V_\infty d}{\mu_2} = 1$$
$$\text{Ca} = \frac{\mu_2 V_\infty}{\sigma} = 2 \times 10^{-4} \text{ to } 1$$
$$\alpha = 30^\circ \text{ or } 90^\circ$$
$$\eta = 0.20 \text{ to } 0.60$$

where subscripts 1 and 2 correspond to oil and water, respectively. Although Johnson and Patel [30] reported that a uniform flow over a solid sphere remains axisymmetric up to a Reynolds number of 210, it must be acknowledged that this is a major assumption when the oil phase is also present.

The VOF algorithm requires that the CFL number be less than $1/2$ for each of the two advection steps, and so for all results presented in this chapter, $\Delta t$ was set such that the flux volume across each cell face was less than half of the cell volume. In addition, $\Delta t$ was chosen to avoid numerical instabilities due to the interfacial tension term. $\Delta t$ was set to $1\mu\text{s}$ when $\sigma \leq 10\text{mN/m}$, and $0.1\mu\text{s}$ otherwise.

The domain was discretized by 60 control volumes in each of the $r$ and $\theta$ directions, and the mesh was non-uniform in the $r$ direction: for the first cell, $\Delta r_1 = 2.121\mu\text{m}$ and $\Delta r$ then increased geometrically at a ratio of 1.05 to a final domain size $r_\infty = 16r_{\text{sph}}$.

The equilibrium positions for $\text{Re} = 1$, $\alpha = 90^\circ$, and $\eta = 0.2$ (presented in section 5.1)
were also calculated for a domain size of $r_\infty \approx 33r_{sph}$, but values of $\psi$ differed by less than 1% from the values calculated on the smaller domain, as illustrated in Fig. 5.1. As a result, the domain size for all subsequent simulations was set to $r_\infty = 16r_{sph}$.

Figure 5.1: Comparison of equilibrium positions at Re=1, $\alpha = 90^\circ$, and $\eta = 0.2$, for domain sizes $r_\infty = 16$ and $r_\infty \approx 33$ times the sphere radius.

Section 5.1 examines whether an equilibrium configuration is possible within a uniform flow for different values of Ca, $\eta$, and $\alpha$. Section 5.2 presents results of oil/water/particle simulations where the oil film initially coats the particle, to assess when the oil phase separates or reaches an equilibrium configuration.

5.1 Equilibrium Configuration of an Oil Drop

This section presents results of simulations that examine possible equilibrium oil/particle configurations within a uniform aqueous flow, as a function of Ca, $\eta$, and $\alpha$. In order to eliminate the dynamic effects associated with film rupturing and initial rapid de-wetting (e.g. under high interfacial tension) of the oil phase that initially envelops the particle, these simulations were initialized with a configuration already close to equilibrium: specifically, the spherical cap configuration with $\psi$ determined from Eq. (1.1). The flow
was initially stationary, and at $t = 0$, an external velocity $\vec{V}_\infty$ was imposed at the outer boundary.

Fig. 5.2(a) illustrates the equilibrium configurations of the oil at Re = 1, $\alpha = 90^\circ$, $\eta = 0.2$, for values of Ca = 0, 0.001, 0.01, 0.1 and 0.2 (corresponding to $\sigma = \infty$, 10, 1, 0.1 and 0.05mN/m). The equilibrium configurations at Ca = 0.001 and 0.01 overlap the Ca = 0 profile, or the spherical cap configuration at zero shear. This implies that the interfacial tension is sufficiently strong that the external shear is effectively negligible. As Ca increases ($\sigma$ decreases), the oil configuration begins to deviate from the spherical cap, as the effect of the external shear becomes more important. Finally, at a critical $0.2 < Ca \leq 1$, the interfacial tension force can no longer hold the oil drop together. The oil stretches into a long thread, see Fig. 5.3(a), and it is reasonable to assume that it will eventually rupture/separate, although the simulation was not run long enough to see that happen. Nevertheless, no equilibrium configuration was predicted.

Figs. 5.2(b) and (c) illustrate the equilibrium configurations at $\eta = 0.4$ and 0.6, respectively. The observed trends are similar to the case for $\eta = 0.2$; that is, as Ca increases, the drop deviates more from the spherical cap configuration. However, the critical value of Ca at which an equilibrium configuration can still be observed decreases as $\eta$ increases (separation occurs between Ca = 0.1 and 0.2).

Fig. 5.4(a) is a plot of $\psi$ versus Ca for the three values of $\eta$. The horizontal lines correspond to $\psi$ at Ca = 0, which are calculated using Eq. (1.1), except $\eta = \zeta/(\zeta+4\pi/3)$. These are the maximum possible values of $\psi$ for each $\eta$, since any shear ($Ca > 0$) will cause the oil to de-wet further, and hence $\psi$ can only decrease. Note that some equilibrium positions lie slightly above the horizontal line, e.g. at low Ca, $\eta = 0.4$. This can only be due to numerical errors (e.g. errors in $\kappa$ calculated via height functions, that affect the calculated interfacial tension force). For $\eta = 0.2$, the external shear is negligible at $Ca \leq 0.01$, as the $\psi$ data points coincide with the horizontal line; at the other extreme, no data point is plotted for $Ca \geq 1$, when the first instance of oil phase rupturing was
observed. At larger values of \( \eta \), shear forces are more noticeable starting at lower values of Ca, because for the same \( \sigma \), a larger droplet has a smaller curvature (interfacial tension force is proportional to \( \sigma \kappa \)), and a larger surface on which the shear force can act. In these cases, the first instance of oil phase rupturing was observed at \( \text{Ca} = 0.2 \).

A corresponding set of simulations was run for \( \alpha = 30^\circ \), illustrated in Fig. 5.5. The main difference between the \( \alpha = 30^\circ \) and \( 90^\circ \) results is that all else being equal, \( \psi \) is larger when \( \alpha = 30^\circ \), as shown in Fig. 5.4. In other words, the oil at a smaller contact angle will wet a larger portion of the particle surface, and so the oil becomes more difficult to remove. Note that at \( \text{Ca} = 1 \), irrespective of \( \alpha \), the oil phase stretches to form a long neck and eventually, at least a fraction of the oil will pinch off, as the shear force overcomes the interfacial force.

Note also that at \( \text{Ca} = 0.2 \), the external shear and interfacial tension forces are of comparable magnitude. As mentioned previously, de-wetting the solid occurs more easily at \( \alpha = 90^\circ \). For \( \eta = 0.4 \) and 0.6, as the oil phase is drawn downstream by the external shear, the contact line de-wets until the oil phase separates (when \( \psi \) is close to 0). This is different than the separation behaviour at \( \text{Ca} = 1 \), in that the oil phase is still round in shape, as shown in Fig. 5.3(b). This behaviour was not observed when \( \alpha = 30^\circ \).
Figure 5.2: Equilibrium configurations at Re=1, $\alpha = 90^\circ$, (a) $\eta=0.2$, (b) 0.4, and (c) 0.6
Figure 5.3: (a) Oil phase stretching into a long thread and eventually rupturing; (b) oil phase rupturing while maintaining a round shape.
Figure 5.4: Equilibrium position versus Ca at Re=1, (a) $\alpha = 90^\circ$, and (b) $\alpha = 30^\circ$. Horizontal lines represent the limiting positions in the absence of flow.
Figure 5.5: Equilibrium configurations at $\text{Re}=1$, $\alpha = 30^\circ$, (a) $\eta=0.2$, (b) 0.4, and (c) 0.6.
5.2 Dynamic Effects on the Separation Process

Having examined possible equilibrium configurations, this section presents results of complete simulations. The oil is initially a thin film coating the solid particle, when a uniform external velocity $\vec{V}_\infty$ is imposed at the upstream boundary at $t = 0$. The oil film on the front side of the sphere then decreases in thickness until the film ruptures and a contact line forms. Unfortunately, the thickness at which this occurs is unknown. Many existing models simply assume that rupture occurs when the film is less than one mesh cell thick (e.g. [47]), but this yields results that are grid-dependent. The results presented here are based on an assumption that rupture occurs when the film thickness is less than an arbitrary specified value, which was chosen to be $2.5\mu m$. Once the film ruptures, a hole forms. The initial hole radius was heuristically chosen large enough so that once formed, the hole did not immediately close back up. The initial hole radius was specified as approximately $3\mu m$ for the $\alpha = 90^\circ$ case and $6\mu m$ for the $\alpha = 30^\circ$ case. Section 5.2.1 presents simulation results at $Re = 1$, $\alpha = 90^\circ$, $\eta = 0.2$, for $0.0002 \leq Ca \leq 1$ by modifying values of $\sigma$; section 5.2.2 presents the results at $\alpha = 30^\circ$ (note that these cases were also presented in section 5.1 without the dynamic effects); finally, section 5.2.3 examines the effects of modifying $\vec{V}_\infty$, which changes the values of $Re$ and $Ca$ simultaneously.

5.2.1 $Re = 1$, $\alpha = 90^\circ$, and $\eta = 0.2$

Fig. 5.6 illustrates results for $Ca = 0.001$. Once the film ruptures, the oil de-wets rapidly. The contact line overshoots its equilibrium position, see Fig. 5.6(e), and then moves back in the opposite direction to reach its equilibrium position. Additional simulations were run for $0.0002 \leq Ca \leq 1$ by changing values of $\sigma$. The equilibrium contact line positions are plotted and compared with the results of section 5.1 in Fig. 5.7(a). For $0.0003 \leq Ca \leq 0.2$, where the oil film can attain a stabilized configuration, the equilibrium contact line positions are the same as those predicted when the oil was initialized as a drop. Fig. 5.8
shows that at $Ca = 0.4$, the interfacial tension can no longer hold the oil together, as the oil stretches until rupture. This $Ca$ value, at which rupture occurs, is also consistent with the value presented in section 5.1.

Recall that in section 5.1, it was shown that at low values of $Ca$, when the oil film is initialized as a drop, that the external shear is negligible and that the oil retains a spherical shape. By contrast, when the oil is initialized as a thin film coating the particle, the oil does not reach an equilibrium configuration, but instead, the film can rupture so that most of the oil separates from the particle. An example at $Ca = 0.00025$ is illustrated in Fig. 5.9. To understand this better, the contact line velocity is plotted against contact line position, $\psi'$, in Fig. 5.10, for $0.001 \leq Ca \leq 0.00025$. At these values of $Ca$, once the contact line forms, it rapidly de-wets due to the high interfacial tension force (recall that the external water velocity is only 10mm/s). The oscillation in velocity is due to discretization errors in calculating the interfacial tension force; in fact, the wavelength of the oscillations is related to the mesh cell size. In addition, the initial scattering of velocity data is due to the approximation made of the oil film shape near the contact line when it forms. At $Ca = 0.001$, refer to Fig. 5.10(a), it can be observed that the contact line overshoots its equilibrium position (indicated by the red dashed line), then reverses direction and oscillates, until eventually it stabilizes at the equilibrium position. Another important observation is the existence of a steep negative slope, $dV/d\psi'$, a rapid deceleration with respect to contact line position that begins just before the contact line crosses the equilibrium position, indicated by the green dotted line. At lower values of $Ca$, see Fig. 5.10(b)-(d), not only does the contact line velocity increase, but the initiation of the rapid deceleration happens after the contact line passes the equilibrium position. Consequently, at $Ca = 0.00025$, see Fig. 5.10(d), the oil overshoots the equilibrium configuration so much that the film de-wets until separation occurs.

In summary, the separation mechanism at low $Ca$ is different than at high $Ca$. At high $Ca$, the shear force is responsible for the separation because it overcomes the interfacial
force holding the oil together. At low Ca, the high interfacial tension force induces rapid contact line motion, such that the oil film speeds past its equilibrium configuration to such an extent that some or all of the oil detaches. If the contact line motion was to be slowed down (for example, by increasing the oil viscosity or decreasing the contact angle), then this type of separation might not occur. In fact, no separation was observed at Ca = 0.00025 when $\mu_{oil}$ was increased by a factor of ten, or when $\alpha$ was set to 30°.
Figure 5.6: The behaviour of a thin oil film around a rigid particle, $Re=1$, $\alpha=90^\circ$, $\eta=0.2$, $Ca=0.001$, at (a) $t=0$ms, (b) $t=12$ms, (c) $t=12.2$ms, (d) $t=12.4$ms, (e) $t=12.6$ms, and (f) $t=20$ms.
Figure 5.7: Comparison of equilibrium positions versus Ca for the oil initialized as a thin film and as a spherical drop; Re=1 for (a) $\alpha = 90^\circ$, and (b) $\alpha=30^\circ$. Horizontal lines represent the maximum values of $\psi$ in the absence of flow.
Figure 5.8: The behaviour of a thin oil film around a rigid particle, \(\text{Re}=1, \alpha=90^\circ, \eta=0.2,\) \(\text{Ca}=0.4,\) at (a) \(t=0\) ms, (b) \(t=35\) ms, (c) \(t=70\) ms, (d) \(t=105\) ms, (e) \(t=140\) ms, and (f) \(t=156\) ms.
Figure 5.9: The behaviour of a thin oil film around a rigid particle, $Re=1$, $\alpha=90^\circ$, $\eta=0.2$, $Ca=0.00025$, at (a) $t=0\text{ ms}$, (b) $t=11.5\text{ ms}$, (c) $t=11.55\text{ ms}$, (d) $t=11.6\text{ ms}$, (e) $t=11.65\text{ ms}$, and (f) $t=11.71\text{ ms}$.
Figure 5.10: Contact line velocity versus position at Re=1, α=90°, η=0.2, (a) Ca=0.001, (b) Ca=0.0005, (c) Ca=0.0003, and (d) Ca=0.00025. Red dashed line represents equilibrium position, and green dotted line represents beginning of rapid deceleration with respect to contact line position. ψ’ denotes the instantaneous contact line position.
5.2.2 Re = 1, $\alpha = 30^\circ$, and $\eta = 0.2$

A corresponding set of simulations was run for $\alpha = 30^\circ$. Fig. 5.11 illustrates results for $Ca = 0.001$. Fig. 5.7(b) plots the equilibrium contact line positions for $0.0002 \leq Ca \leq 0.4$, and the results are consistent with those of section 5.1, with a slight discrepancy of 1.73% at $Ca = 0.01$, due to the discretization error in calculating the interfacial tension force near the contact line. No equilibrium configurations exist for $Ca \geq 1$. The main difference between the $\alpha = 30^\circ$ and $90^\circ$ results is that under the same flow conditions, $\psi$ is larger when $\alpha = 30^\circ$, as mentioned in section 5.1. In addition, the contact line motion is slower when $\alpha = 30^\circ$, and therefore, equilibrium configurations exist even at the lowest value of $Ca$ considered, that is, $Ca = 0.0002$. This implies the interfacial tension driven separation is harder to achieve at low contact angles.
Figure 5.11: The behaviour of a thin oil film around a rigid particle, $Re=1$, $\alpha=30^\circ$, $\eta=0.2$, $Ca=0.001$, at (a) $t=0$ ms, (b) $t=12$ ms, (c) $t=15$ ms, (d) $t=18$ ms, (e) $t=21$ ms, and (f) $t=24$ ms.
5.2.3 Increasing External Velocity

Finally, the effect of increasing $V_\infty$ was studied. Varying $V_\infty$ affects both Re and Ca. Simulations were run for $\alpha = 90^\circ$, $\eta = 0.2$, and $\sigma = 10 \text{mN/m}$, for $10 \text{mm/s} \leq V_\infty \leq 1000 \text{mm/s}$, corresponding to $1 \leq \text{Re} \leq 100$ and $0.001 \leq \text{Ca} \leq 0.1$. Increasing $V_\infty$ increases the external shear force on the oil film, so one would expect the oil to de-wet further along the sphere, i.e. $\psi$ will decrease. Fig. 5.12(a) shows the equilibrium configurations for Re = 0, 1, 50, and 100 (Ca = 0, 0.001, 0.05 and 0.1). Clearly, increasing $V_\infty$ by a factor of up to 50 has little effect on the equilibrium configuration. This is because both $\sigma$ and $\kappa$ are large (the latter due to the small oil volume), and thus the resulting interfacial tension force dominates, holding the oil tightly into a spherical shape. Further increasing $V_\infty$ by a factor of 100 not only does not trigger any separation process, but also unexpectedly causes the oil to wet a slightly larger portion of the particle surface. Figs. 5.12(b) and (c) shows the velocity streamlines for Re = 1 and Re = 100, respectively. At Re = 1, the water flows only in the stream-wise direction, while at Re = 100, separation/recirculation regions appear, one on the particle before the contact line and one behind the oil drop, which seem to be the reason that the oil wets more of the particle surface. Fig. 5.13(a) displays the equilibrium position $\psi$ versus Re. At $\eta = 0.2$, $\psi$ remains nearly coincident with the horizontal line, $\psi$ at zero shear, up to Re = 60, and that is approximately when the front separation begins to be noticeable, i.e. Re between 60 and 70. For Re $\geq 70$, the oil begins to wet a larger surface than the limiting case at zero shear. The rear recirculation appears at approximately Re = 90.

Simulations were also run for $\eta = 0.4$ and $\eta = 0.6$. At $\eta = 0.4$, increasing velocity up to $V_\infty = 1000 \text{mm/s}$ has little effect on the separation, and does not result in a monotonic reduction in $\psi$. At $\eta = 0.6$, the predicted trend was observed, i.e. increasing velocity facilitates oil de-wetting. In this case, the larger oil volume results in a smaller interface curvature and a larger surface for the shear force to act on, and thus oil separation was observed at Re = 70. Fig. 5.13(b) plots the equilibrium position $\psi$ versus Ca,
superimposed onto the data presented in section 5.1. At $\eta = 0.6$, increasing Ca, whether by increasing $V_\infty$ or decreasing $\sigma$, facilitates oil de-wetting; at lower oil volume ratios, $\eta = 0.2$ and 0.4, the trends when increasing the capillary number begin to diverge around Ca = 0.02.

Figure 5.12: (a) Equilibrium configurations at $\alpha=90^\circ$, $\eta=0.2$, and Re=0, 1, 50 and 100 (Ca=0, 0.001, 0.05 and 0.1). Streamline plots at $\alpha=90^\circ$, $\eta=0.2$, (b) Re=1 (Ca=0.001), and (c) Re=100 (Ca=0.1).
Figure 5.13: (a) Equilibrium position versus Re at $\alpha=90^\circ$, and $\sigma=10\text{mN/m}$; (b) equilibrium position versus Ca at $\alpha=90^\circ$, and $\sigma=10\text{mN/m}$, superimposed onto the results of section 5.1.
Chapter 6

Conclusion

6.1 Summary

This thesis presents a Navier-Stokes interfacial flow solver developed in 2D spherical coordinates. The governing equations are discretized using the Finite Volume approach; fluid interfaces are represented using the VOF method and reconstructed in a piecewise linear (PLIC) manner. This novel implementation utilizes the height function method to calculate interface normals and curvatures, and an iterative approach to calculate the line constants. The interfacial tension force is imposed via the continuum surface force (CSF) model of Brackbill et al. [4]. The flow solver and the VOF algorithm have been validated both separately and together, and the results generally agree well with available experimental and numerical data.

The numerical model was applied to study oil/water/particle separation in a uniform laminar flow. The study was divided into two parts. The first examined the possible equilibrium configurations of the oil phase, in which the oil was initialized as a spherical droplet partially coating the particle. It was observed that at $\text{Re} = 1$ and at low $\text{Ca}$, the effect of external shear is negligible, and the oil retains the spherical cap configu-
ration. As Ca increases, i.e. by decreasing the interfacial tension, the shape of the oil begins to deviate from a spherical cap. At Ca \( \approx 1 \), the interfacial tension can no longer hold the oil together, as the oil stretches out as a long thread behind the particle, and eventually ruptures. Finally, it was observed that increasing the contact angle facilitates oil de-wetting, which can lead to separation at lower Ca, where the oil separates while maintaining a round shape.

In the second part, the oil was initialized as a thin film coating the entire particle to study the dynamic effects associated with film rupturing and de-wetting. The equilibrium configurations are consistent with the first part of the study except at low values of Ca and at a high contact angle \( \alpha = 90^\circ \). Under these conditions, once a contact line forms, the high interfacial tension induces rapid de-wetting, which causes the contact line to overshoot its equilibrium position. Thus, at some point, the contact line velocity that decreases from the time the contact film forms, increases again until rupture occurs. Similar velocity patterns were observed in Smith and van de Ven’s experiment for liquid/liquid/particle separation under gravity [60]. Increasing oil viscosity or decreasing contact angle will suppress the interfacial tension driven separation by slowing down the contact line motion. Finally, increasing the external fluid velocity was observed to aid separation for larger volume oil droplets.

It is known in extraction processes that decreasing interfacial tension [55] or increasing contact angle [60] will improve separation efficiency. With an idealized situation of a single particle within a uniform flow, this work illustrates the underlying mechanisms: lowering the interfacial tension facilitates the “snap-off” mechanism [10] where portion of the oil ruptures and separates; while increasing contact angle helps de-wetting and promotes interfacial tension driven separations.
6.2 Future Work

The following list presents a number of opportunities for improving and further developing this work:

1. The current model makes assumptions regarding the thickness at which an oil film ruptures, and of the initial oil film profile once the contact line forms. A better approach would be to incorporate the actual physics to determine when and how the film ruptures, and how the resultant contact line forms. For example, Sharma and Ruckenstein [57] derived simple relations of the critical film thickness at which rupture occurs to the radius of the hole that forms, for a given contact angle, by comparing the change in free energy. Similarly, when the oil stretches into a long thread, the model again assumes the thread radius at which rupture occurs. To model the situation more accurately, the next step would be to replace these assumptions with analytical relations, or perhaps experimental correlations.

2. The model applies a constant (equilibrium) contact angle, but since the contact line is in motion, it would be more appropriate to apply a dynamic contact angle.

3. Finer cells are required to properly capture the contact line and high interface curvatures. Thus the numerical model could be improved by utilizing an adaptive refinement scheme, i.e., refining the mesh locally at regions of interest, rather than the entire mesh. This would allow better use of computational resources.

4. Athabasca oil sands are hydrophilic and generally considered to be water-wet such that a film of water lies between the bitumen and the sand particle [13, 63]. A next step would be to initialize the model with a thin water film between the oil and particle surface, and examine the effect of this water layer on the separation process. But as the oil would no longer be in direct contact with the particle surface, it would be harder to decide when and how the oil film initially ruptures.
Adaptive refinement would be especially useful for capturing the initial oil profile once rupture occurred.

5. Finally, the current model is implemented in a 2D spherical coordinate system. One could extend this model to a 3D spherical coordinate system, in order to study more complicated flows not limited by the axisymmetric assumption.
Appendix A

For a surface $F(u, v)$, the fundamental magnitudes of first order are determined by [70]:

\[
\begin{align*}
E &= \frac{\partial \vec{r}}{\partial u} \cdot \frac{\partial \vec{r}}{\partial u} \\
F &= \frac{\partial \vec{r}}{\partial u} \cdot \frac{\partial \vec{r}}{\partial v} \\
G &= \frac{\partial \vec{r}}{\partial v} \cdot \frac{\partial \vec{r}}{\partial v} \\
H^2 &= EG - F^2
\end{align*}
\]

where $\vec{r}$ is the position vector at a point on the surface. The unit normal is calculated by:

\[
\hat{n} = \frac{1}{H} \frac{\partial \vec{r}}{\partial u} \times \frac{\partial \vec{r}}{\partial v}
\]

The fundamental magnitudes of the second order are determined by:

\[
\begin{align*}
L &= \hat{n} \cdot \frac{\partial^2 \vec{r}}{\partial u^2} \\
M &= \hat{n} \cdot \frac{\partial^2 \vec{r}}{\partial u \partial v} \\
N &= \hat{n} \cdot \frac{\partial^2 \vec{r}}{\partial v^2}
\end{align*}
\]

Finally, the curvature of the surface can be determined from the fundamental magnitudes of first and second order by:

\[
\kappa = \kappa_1 + \kappa_2 = \frac{EN - 2FM + GL}{H^2}
\]

where $\kappa_1$ and $\kappa_2$ are the curvatures in the two principal directions.
Bibliography


