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Laminar Plunging Jets - Interfacial Rupture and Inception of Entrainment

A dissertation submitted to the Graduate School of the University of Cincinnati
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in the Department of Mechanical and Materials Engineering of the College of Engineering and Applied Science by

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ABSTRACT

Laminar Plunging Jets - Interfacial Rupture and 
Inception of Entrainment

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Doctor of Philosophy

Interfacial rupture and entrainment are commonly observed, e.g., air bubbles within a container being filled with water from a faucet. The example involves a liquid jet (density, \(\rho\), and viscosity, \(\eta\)) plunging into a receiving pool of liquid. Below a critical liquid-jet velocity, the interface develops a cusp-like shape within the receiving pool. The cusp becomes sharper with increasing liquid-jet velocity, and at a critical velocity \((V_c)\), the interface between the liquid and the surrounding fluid (density, \(\rho_0\), and viscosity, \(\eta_0\)) ruptures. Interfacial tension can no longer preserve the integrity of the interface between the two immiscible fluids, and the plunging jet drags/entrains surrounding fluid into the receiving pool. Subsequently, the entrained fluid breaks up into bubbles within the receiving pool.

The focus of this dissertation is the numerical prediction of the critical entrainment inception velocities for laminar plunging jets using the Volume-Of-Fluid (VOF) method, a Computational Fluid Dynamics (CFD) method to simulate multi-fluid flows.

Canonical to bottle-filling operations in the industry is the plunging-jet configuration - the liquid jet issues from a nozzle and plunges into a container filled with liquid. Simulations of this configuration require capturing flow phenomena over a large range of length scales (4 orders of magnitude). Results
show severe under-prediction of critical entrainment velocities when the maximum resolution is insufficient to capture the sharpening, and eventual rupture, of the interfacial cusp. Higher resolutions resulted in computational meshes with prohibitively large number of cells, and a drastic reduction in time-step values.

Experimental results in the literature suggest at least a 100-fold increase in the smallest length scale when the entrained fluid is a liquid instead of air. This narrows the range of length scales in the problem. We exploit the experimental correlation between critical capillary number, \( Ca_c = \frac{\eta V_c}{\sigma} \), and viscosity ratio, \( \frac{\eta_0}{\eta} \), in postulating an alternate approach involving scaling of the pertinent physics by using liquids as entrained fluids.

The scaling approach is tested using a rotating cylinder placed at the interface between two fluids. A mesh-independence study using successively finer meshes predicted critical entrainment velocity values within about 1% of each other. Numerical predictions compared well with experimental data, with less than 1% difference in the case where exact experimental data was available, and a maximum of 6% difference for cases where experimental data was extrapolated to make the comparison. These results lend credibility to our approach.

The effect of densities of the two fluids in contact manifests as buoyancy force at the interfacial cusp. Remarkably, contrary to a priori notions, we observed that as \( \Delta \rho \) increased, the effect of buoyancy decreased relative to other forces at the interfacial cusp. Finally, we propose an empirical correlation between \( Ca_c \) and \( \frac{\eta_0}{\eta} \) which allows extrapolation of critical entrainment conditions between the rotating-cylinder configuration (with liquids being entrained) to the plunging-jet configuration (with air being entrained).
The primary contribution of this research is the physics-based scaling approach utilized to overcome the simulation challenges posed by the physics of interface rupture and entrainment.
This thesis is dedicated to Drs. Shantha & G. Vijayaraghavan
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*It’s time for new beginnings! Cheers!*
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Nomenclature

\( \alpha, \gamma \) \hspace{1cm} \text{Volume fraction of a fluid in a computational cell}

\( \eta \) \hspace{1cm} \text{Viscosity of liquid that forms the plunging jet}

\( \eta_0 \) \hspace{1cm} \text{Viscosity of entrained fluid}

\( \kappa \) \hspace{1cm} \text{Mean interfacial surface curvature}

\( \rho \) \hspace{1cm} \text{Density of liquid that forms the plunging jet}

\( \rho_0 \) \hspace{1cm} \text{Density of entrained fluid}

\( \sigma \) \hspace{1cm} \text{Interfacial tension between plunging-jet liquid and entrained fluid}

\( \mathbf{v} \) \hspace{1cm} \text{Velocity of fluid}

\( \Delta \rho \) \hspace{1cm} \( \rho - \rho_0 \)

\( Bo_c = \frac{\Delta \rho g L^2}{\sigma} \) \hspace{1cm} \text{Critical Bond number}

\( Ca_c = \frac{\eta V_c}{\sigma} \) \hspace{1cm} \text{Critical capillary number}

\( D_p \) \hspace{1cm} \text{Diameter of liquid jet at the plunging point}

\( Fr_o = \frac{V_o^2}{gZ} \) \hspace{1cm} \text{Froude number of plunging jet}

\( p \) \hspace{1cm} \text{Static pressure of fluid}

\( Re_p = \frac{D_p V_e \rho}{\eta} \) \hspace{1cm} \text{Reynolds number of plunging jet}

\( V_e, V_c \) \hspace{1cm} \text{Minimum/critical entrainment velocity}

\( V_o \) \hspace{1cm} \text{Velocity of plunging jet at nozzle exit}

\( We_p = \frac{D_p V_e^2 \rho}{\sigma} \) \hspace{1cm} \text{Weber number of plunging jet}

\( Z \) \hspace{1cm} \text{Jet length, measured between nozzle exit and plunging point}
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Chapter 1

Introduction

The focus of this dissertation is the numerical simulation of laminar plunging jets and the associated phenomenon of interfacial rupture and entrainment. This chapter presents introductory descriptions of the key ideas involved in this dissertation, namely, “entrainment,” “plunging jet,” and “modeling and simulation.”

1.1 Entrainment

The phenomenon of entrainment is fundamental, and rich in the physics it exhibits. We encounter entrainment on an everyday basis - filling a glass of water from a faucet, aerating coffee by pouring the coffee into a ‘tumbler’ from a height (a particularly south-Indian way of drinking coffee), giving a milk-shake its texture, diving into a swimming pool, releasing flavor in a pour of wine, etc. The common denominator in all the the aforementioned examples, irrespective of the causal action/forces, is surrounding air being drawn into the liquid as bubbles. This phenomenon where surrounding fluid (in most cases, air) penetrates through a liquid surface is called entrainment. In all the examples just mentioned, the surface tension forces are not
1.1 Entrainment

sufficient to prevent the rupture of the liquid surface, resulting in entrainment of air.

Entrainment occurs, both, in nature, and in industrial applications. Examples in nature are “white-water” formation in rapids, and frothing on ocean surfaces. The process of entrainment plays a vital role in sustaining life in oceans, rivers and streams; it acts as a mode of mass transfer for oxygen from the atmosphere into the liquid body. Entrainment also plays a role in releasing carbon dioxide from the ocean surface to the atmosphere, thereby playing a part in the study of global climate change and green-house effects.

In the industry, many processes involve entrainment of air. Air bubbles trapped while pouring concrete give concrete its durability in climates with repeating freeze-thaw cycles [U.S. Dept. of Transportation] [(Narayanan & Ramamurthy, 2000)]. The effects of entrainment have also proved important in naval hydrodynamics - as a source of noise when bubbles formed due to entrainment burst at the water surface, and affecting performance/efficiencies of sea faring vessels (Kiger & Duncan, 2012). Other examples include liquid-gas reactors, mixing tanks, entry of missiles into water, and waste-water treatment.

The filling of bottles with a viscous liquid is frequently encountered in the consumer goods industry. Hair-care products (shampoos, conditioners, etc.), cleaning liquids (detergents, dish-washing liquids, etc.), pharmaceutical products (cough expectorants, liquid antacids, etc.) are examples of consumer products that involve filling bottles with liquids using nozzles. During the filling process, entrainment of air is undesirable. The entrained air frequently causes foam formation which, in turn, causes overflow. Cleaning operations add to production costs. In time, the foam settles, and leaves a volume of air at the top of the bottles (under fill). Hence, there is also additional plastic used than is necessary. Additional plastic not only impacts monetary costs, but also impacts the environment. Recent research and development
1.2 Plunging Jets

Efforts in the industry have identified understanding the entrainment phenomenon as an important step in the design of filling processes. The work presented in this dissertation is closely aligned with the process of bottle filling.

The entrainment phenomenon described in this section is frequently associated with plunging jets. The next section provides a description of plunging jets.

1.2 Plunging Jets

A plunging jet involves a vertical liquid jet emanating from a nozzle, and entering a container holding the same liquid. In this dissertation, the container with the liquid in it is termed the receiving pool. This geometric configuration with the jet issuing from a nozzle and plunging into a container filled with liquid is called the plunging-jet configuration. A characteristic physical process observed in plunging jets is the entrainment of air into the receiving pool due to the penetrating liquid jet. The photograph [Fig. 1.1] shows air bubbles being formed in the receiving pool due to a plunging jet. Beyond certain critical conditions, the liquid-air interface ruptures, and the liquid jet drags air from its surroundings into the receiving pool. Subsequently, the air pulled into the receiving pool breaks up into bubbles.

Plunging jets have been studied in the context of air entrainment by ocean/sea waves. An example is the work conducted by Chanson & Jaw-Fang (1997) on the plunging-jet characteristics of plunging breakers. As shown in Fig. 1.2, waves form a plunging jet, and impinge upon the water free surface (plunging breakers), thereby causing entrainment of air. Plunging jets have also been studied as canonical problems to understand the entrainment/aeration seen in hydraulic structures such as spillways, dams, etc. (Chanson, 1996).

The plunging-jet configuration is canonical to bottle-filling processes in the indus-
1.2 Plunging Jets

Figure 1.1 Entrainment of Air by a Plunging Jet [adapted from Jesse Belden (NUWC) and Tadd T. Truscott (BYU)]

Figure 1.2 Schematic of plunging breaker (plunging wave) showing entrainment of air under the ocean/sea surface (adapted from Chanson & Jaw-Fang (1997))
try. Bottle-filling processes involve a nozzle issuing liquids to fill containers/bottles, and as mentioned in Section 1.1, entrainment is undesirable. Since this work is aligned with studying entrainment with respect to bottle filling, we use the plunging-jet configuration to understand the entrainment phenomenon better.

We have now introduced the important terms in the title, namely - entrainment, and plunging jets. In the following section, we briefly describe “modeling and simulation,” - the approach we use in the present work to investigate the entrainment phenomenon.

### 1.3 Modeling and Simulation

Modeling and simulation involves recreating the real world using mathematical equations that represent the governing dynamics/physics, and solving these equations using computers. The phrase Computational Fluid Dynamics (CFD) is used when the mathematical equations pertain to the dynamics of fluids. In the present work, CFD is used to simulate the flow field of interest. Frequently, CFD allows for better insight into the evolution of the flow field, and is cost-effective in studying complex systems when compared to experimental methods.

A number of commercial software packages (FLUENT, Flow3D, CFX, etc.) exist that allow a user to simulate fluid flows. They have been continually developed over a number of years. Commercial software bring a number of advantages - years of meticulous development and dedicated customer support. Companies depend on commercial software for their modeling and simulation needs to a large extent. Along with the advantages comes the huge cost of licensing fees levied upon customers by top-flight commercial software vendors. In the present work, we use an open-source CFD tool-kit called OpenFOAM. FOAM stands for Field Operation And Manipula-
OpenFOAM was initially developed at Imperial College, London, UK, in the late 1980s, and was written in C++ due to C++’s modularity and object-oriented programming features. The developers subsequently posted the code online, and researchers from across the world were able to download the source code, and work with it to improve the CFD tool-kit - hence the term “open.” This strategy is closely aligned with the way Linux operating systems evolve - free access, open-source, and community-based development. In addition, OpenFOAM is massively parallelizable. Continuous improvement in OpenFOAM’s capabilities and the associated lowering of costs has resulted in increased use of OpenFOAM in companies like Volkswagen Group, Ford Motor Co., Daimler-Chrysler, and P&G. In this work, we explore the use of OpenFOAM to simulate our problem of interest, namely, the entrainment phenomenon observed when a laminar jet plunges into a receiving pool.

1.4 Thesis Organization

This dissertation is organized as follows: in Chapter 2, we present the background, followed by the specific objectives of the present work. Chapter 3 outlines the numerical framework used to carry out the simulations. In Chapter 4, we describe simulations of the plunging-jet configuration, results obtained, and the challenges posed by the physics on the numerical framework used. Chapter 5 begins with describing the background to an alternate approach based on scaling of the physics. We further describe how the approach addresses the challenges identified at the end of Chapter 4. We then formally propose this scaling approach. In Chapters 6 and 7, we discuss the results obtained from using the scaling approach. Chapter 8 draws conclusions from the work, presents an overall summary, and outlines avenues for further investigation to expand the scope of this work.
1.5 Closure

In this chapter, we introduced the key phrases in the title of this work - “interfacial rupture and entrainment” and “plunging jets.” We have also introduced the idea of “modeling and simulation,” - the approach we take to investigate the entrainment phenomenon. We then described how the rest of this document is organized. In the next chapter, we provide the reader a background into the research that has been conducted by others, followed by the specific objectives of our work.
Chapter 2

Background and Specific Objectives

This chapter describes background information followed by the research objectives of the current work. The background information is presented in two sections. The first section is a review of pertinent literature on experimental and theoretical work. In the second section, we discuss research published in the area of numerical simulations of the entrainment phenomenon. While we conveyed the motivation for our work in the previous chapter, this chapter puts the present work in perspective with regard to the research that has been conducted and published by others.

2.1 Background: Theory and Experiments

Lin & Donnelly (1966) observe that prior to their research publication, very little exploratory work had been done in the area of air entrainment by plunging jets. Although entrainment had been an established phenomenon, little or no research had been conducted to explain the mechanism of air entrainment. The research published
2.1 Background: Theory and Experiments

Figure 2.1 Laminar plunging jet - illustration of entrainment mechanism showing the unstable collar-like gas-film. (Lin & Donnelly, 1966)

by Lin & Donnelly (1966) was one of the first to explore the physics of air entrainment associated with plunging jets. The focus of their work was on the laminar plunging jet, since, up until then, air entrainment associated with laminar plunging jets had not been recorded experimentally. They observed that the mechanisms for air entrainment were different for laminar and turbulent plunging jets. Figure 2.1 shows a schematic representation of a laminar plunging jet entraining air into the receiving pool. The jet issues from a nozzle. Beyond a certain critical jet velocity, the interface between the liquid and air ruptures, and the surrounding air is entrained into the liquid. A collar-like gas-film is formed which quickly becomes unstable and breaks up into air bubbles. The bubbles thus formed rise to the liquid surface due to buoyancy.

Figure 2.2 shows a schematic representation of a turbulent plunging jet entraining
2.1 Background: Theory and Experiments

Figure 2.2 Turbulent plunging jet - illustration of entrainment mechanism showing surface undulations that cause air carry-under, (Lin & Donnelly, 1966)

air. The entrainment mechanism is different from that observed in laminar plunging jets. Here, the entrainment is due to disturbances that form on the jet surface. These disturbances hold pockets of air which are then entrained into the receiving pool. A stark difference between the laminar and turbulent plunging jets is the depth to which the bubbles penetrate the receiving pool. In the case of the laminar jet, the depth is much greater due to the penetration of the gas film into the liquid. In the case of the turbulent jet, there is no gas film formation, and hence, the bubbles are much closer to the surface of the receiving pool.

In Chapter 1, we introduced the air entrainment phenomenon as fundamental to a number of applications. Subsequent to Lin & Donnelly (1966)’s work, a number of researchers have explored the air entrainment phenomenon associated with plunging-
2.1 Background: Theory and Experiments

jet configurations using experimental and theoretical methods. In the interest of
brevity, we present only the literature relevant to the our work, and that is used herein.
Where required, we refer to published literature that provide additional information
on a particular topic.

2.1.1 Laminar Plunging Jets

Figure 2.3 shows two distinct modes that have been observed with regard to laminar
plunging jets. The first mode involves the formation of a steady interfacial cusp
in the receiving pool, with no air being entrained. This occurs when the liquid jet
velocity is below the critical entrainment velocity. The second mode occurs when the
liquid jet velocity is equal to, or greater than, the critical entrainment velocity. The
surface-tension force at the liquid surface (interface) is no longer able to preserve the
integrity of the interface. The interface ruptures and causes entrainment of air into
the receiving pool. The critical conditions at which the transition from one mode to
another occurs is our topic of interest.

Various studies on plunging jets in the literature suggest the existence of a spe-
cific velocity at which entrainment begins. This velocity is termed as the minimum
entrainment velocity, $V_e$, or the critical entrainment velocity, $V_c$. To the best of the
author’s knowledge, a theoretical approach to accurately predict the minimum en-
trainment velocity of a laminar plunging jet has still not been developed. Lin &
Donnelly (1966) presented an empirical correlation which allowed for estimating the
critical entrainment velocity for laminar, viscous, Newtonian liquids. Their data is
shown in Fig. 2.4. According to Lin & Donnelly (1966), $V_e$ depends on liquid prop-
erties and flow variables as shown in Eq. (2.1).

$$V_e = f(\eta, \sigma, \rho, D_p),$$

(2.1)
2.1 Background: Theory and Experiments

Figure 2.3 Photographs of the transition from steady mode to entrainment mode. a. steady cusp formation, b. inception of entrainment, c. breaking of gas film into bubbles (Reyssat et al., 2008)
where $\eta$ is the viscosity of the liquid, $\rho$ is the density of the liquid, $\sigma$ is the interfacial tension, and $D_p$ is the diameter of the jet at the point of intersection with the receiving pool (plunging point).

Equation (2.1) does not include the nozzle diameter, $D_o$, and jet length, $Z$. Jet length is the distance between the nozzle and the receiving pool. Changing the jet length and/or the nozzle diameter are only important in so far as to produce a change in the values of $D_p$, and hence, are accounted for in Eq. (2.1). An empirical relationship between the jet Weber number, $(We)_p$, and the jet Reynolds number, $(Re)_p$ was proposed by Lin & Donnelly (1966) [Eq. (2.2)].

$$
(We)_p = 10((Re)_p)^{0.74},
$$

(2.2)

where $(Re)_p$ is the Reynolds number of the jet at the plunging point ($(Re)_p = \frac{D_p V_e \rho}{\eta}$), and $(We)_p$ is the Weber number of the jet at the plunging point ($(We)_p = \frac{D_p V_e^2 \rho}{\sigma}$).

Equation (2.2) was arrived at by curve-fitting a line through the data obtained from experiments with liquids whose densities ranged from 846 to 1246 kg/m$^3$, whose surface-tension coefficients ranged from 0.03 to 0.063 N/m, and viscosities ranged from 25 to 400 mPas. Perry (1967) conducted experiments with aqueous glycerol solutions and found Eq. (2.2) to hold good for his data as well. Lin & Donnelly (1966)’s data is of particular interest to us since industrial bottle-filling processes involve liquids whose properties are within the range of liquid properties used in Lin & Donnelly (1966)’s work.

In the literature, along with minimum entrainment velocity, experimental data has been published with regard to the volume flow-rate of the air entrained, bubble-size distribution, and depth of penetration of the bubbles. For more information, the reader is referred to a comprehensive review of previous experimental research in the area of entrainment by plunging jets conducted by Bin (1993).
Figure 2.4 Empirical correlation proposed by Lin & Donnelly (1966) by curve fitting through experimental data points.
2.2 Background: Modeling and Simulation

In this section, the equations governing fluid flow are presented, followed by background on modeling and simulation of interfacial flows.

2.2.1 Governing Equations

Navier-Stokes equations are a set of equations that mathematically represent fundamental conservation principles in the realm of Newtonian physics. The equations separately represent conservation of mass, and conservation of momentum. Computational fluid dynamics involves solving these equations, along with the conservation of energy equation, using numerical methods to obtain the flow-field solution for a particular problem. In the present work, the conservation of mass [Eq. (2.3)], and momentum [Eq. (2.4)] equations for incompressible, Newtonian fluids are solved.

\[
\nabla \cdot \mathbf{v} = 0 \quad (2.3)
\]

\[
\rho \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla p + \eta \nabla^2 \mathbf{v} + f_{\text{surface tension}} + f_{\text{gravity}} \quad (2.4)
\]

where \( \mathbf{v} \) is the velocity of the fluid, \( \rho \) is the density of the fluid, \( \eta \) is the dynamic viscosity of the fluid, and \( p \) is the static pressure of the fluid. The equation for the conservation of mass is a mathematical representation of the fundamental law - mass can neither be created nor destroyed. The conservation of momentum is a force balance. In this work, the momentum equation represents a balance of the persisting forces in our problem, namely, inertia, shear (viscous forces), surface tension and gravity.

The conservation equations describe fluid flow as a continuum. The equations are non-linear partial differential equations, which do not lend themselves to being solved
2.2 Background: Modeling and Simulation

exactly except in a few simple cases. In order solve these equations, they are cast into discrete form such that the solution to the now ‘discretized’ equations closely approximate (what would have been) the solution to the continuous problem that the PDEs represent at discrete points in space and time.

2.2.2 Discretization

Discretization is the procedure used to cast the governing equations in discrete form, thereby converting them into a system of algebraic equations that are to be solved for flow variables that are now assumed to exist at discrete points in space and time. Several methods for the discretization of governing equations have been developed. Historically, the finite-differencing method of discretization has been used extensively for fluid dynamics problems. Other, more recent methods are the finite-volume method and the finite-element method. A detailed description of the finite-differencing method and how it is employed in solving fluid-flow problems is provided by Pletcher et al. (2010). The finite-element method had been traditionally used in solving problems related to structural mechanics before being applied to fluid dynamics. The beginnings of applying the finite-element method to solving fluid dynamics problems is described by Shen (1977). Since then, a number of researchers have successfully applied the method to solving a diverse set of fluid dynamics problems.

In the present work, the finite-volume method is used. The governing PDEs are written in integral form, over a control volume. A number of such control volumes stacked together in different coordinate directions make up the computational domain. A fundamental difference between the finite-volume method and other methods is how the physical laws that the equations represent play into the discretization process. The finite-volume method is locally conservative, in that, the flux balance over every control-volume is, by definition, satisfied.
As an example, consider the equation for the conservation of mass for an incompressible fluid with velocity, \( \mathbf{v} \), over a control volume, \( CV \) [Fig. 2.5].

\[
\nabla \cdot (\mathbf{v}) = 0 \tag{2.5}
\]

Integrating the equation over the control volume, we get

\[
\int_{CV} (\nabla \cdot \mathbf{v}) dV = 0 \tag{2.6}
\]

Using the divergence theorem, the above equation can be rewritten as

\[
\int_{S} (\mathbf{v} \cdot \mathbf{n}) dS = 0 \tag{2.7}
\]

The divergence of mass in the control volume, \( CV \), is equal to the net flux of mass through the boundaries, \( S \), of the control volume. \( \mathbf{n} \) is the unit normal vector of the bounding surfaces of the control volume facing outward. Equation (2.7) represents a local flux balance over a single control volume. The integrals thus arrived at can
2.2 Background: Modeling and Simulation

Consider a computational domain that consists of regular, unit-spaced control volumes stacked together [Fig 2.6]. For simplicity, assume the orientation of the control volumes to be along Cartesian coordinates. Let the intersection of solid lines be cell centers, and the intersections of dashed lines be face centers. Faces f1, f2, f3, and f4, form faces of one control volume with cell center P. Let neighbouring cell centers of the control volume of interest be N (north), S (south), E (east), and W (west). Let $\phi$ be a flow-field variable. The flow-field variables are stored at cell centers ($\phi_P$ and $\phi_{Neighbours}$). In the finite-volume framework, we need a method to obtain face-centered values, so that fluxes at the control-volume faces can be determined. Various interpolation schemes are used to obtain face-centered values from cell-centered values. Schemes such as the Upwind-Differencing scheme (UDS), the Central-Differencing Scheme (CDS), a combination of the upwind and the central differencing schemes be evaluated using various numerical integration methods such as the Simpson’s rule and the Trapezoidal rule.

Figure 2.6 Control Volume with cell center P, and neighbours, North, South, East, and West. f1, f2, f3, f4 are faces of the control volume
2.2 Background: Modeling and Simulation

- such as the QUICK (Quadratic Upwind Interpolation for Convection Kinematics) scheme (Leonard, 1979), are used in order to carry out the interpolation so that the fluxes at the face centers can be evaluated. As an example, consider face $f1$. The upwind (first-order accurate) and central (second-order accurate) approximations of $\phi_{f1}$ are as follows:

- Upwind-difference approximation: $\phi_{f1} = \begin{cases} 
\phi_P & \text{if flux across } f1 \geq 0, \\
\phi_N & \text{if flux across } f1 < 0 
\end{cases}$

- Central-difference approximation: $\phi_{f1} = \frac{\phi_P + \phi_N}{2}$

The momentum and energy conservation equations can be discretized in a similar manner, thereby providing a system of algebraic equations that represent the governing PDEs. The equations thus obtained can be solved based on specific initial and boundary conditions relevant to the physical problem at hand. A detailed account of the finite-volume method is provided by Versteeg & Malalasekera (2007).

The problem of interest in this study further involves the complexity of modeling an interface between two fluids. The different numerical approaches developed to model and simulate an interface are briefly outlined in the next section.

2.2.3 Modeling of Interfaces

Modeling interfacial phenomena inherently poses numerical challenges since the solution methodology is required to capture/track discontinuities. Apart from interfaces between two fluids, the same challenges are seen in modeling Mach shocks and material interfaces. Special mathematical treatment is required for numerically modeling the spatial and temporal evolution of such discontinuities.

Numerical simulation capabilities for two-fluid systems can be broadly classified into two categories: interface-fitting methods (surface methods), and interface-
2.2 Background: Modeling and Simulation

Figure 2.7 Methods of representing an interface between two fluids [(Ub-bink, 1997)]


A fundamental limitation of interface-fitting methods is their failure to simulate interface coalescence and rupture. In the present work, we use an interface-capturing method called the Volume-Of-Fluid (VOF) method. The VOF method falls within the category of interface capturing methods. The VOF method was first developed by Hirt & Nichols (1981). In a seminal paper, they proposed using fluid volume fraction to track the evolution of the interface between two fluids. The volume fraction is bounded between 0 and 1, where a value of 0 would indicate the presence of one fluid, and a value of 1 would indicate the presence of the other fluid. In this way, the interface between the fluids (regions where the volume fraction has values between 0 and 1) is clearly demarcated. The spatial and temporal evolution of the interface results from the volume fraction being advected using the local velocity field [Eq. (2.8)].

\[
\frac{\partial \gamma}{\partial t} + \nabla \cdot (\mathbf{v} \gamma) = 0
\] (2.8)

Much like the level-set method [(Sethian, 1996), (Osher & Sethian, 1988)], the
2.2 Background: Modeling and Simulation

VOF method can be used to capture the evolution of interfaces in an Eulerian framework (i.e., the mesh does not need to be aligned with the interface at each point in time). The VOF method can inherently simulate interface rupture and coalescence. Another advantage is that the VOF method can handle large topological changes of the interface better than other methods.

A number of ways of implementing the VOF method have been devised. Gopala & van Wachem (2008) compare the advantages and disadvantages of four of the methods using test-cases, namely, flux-corrected transport (FCT) by Boris & Book (1973), lagrangian piecewise linear interface construction (L-PLIC) by Van Wachem & Schouten (2002), compressive interface capturing scheme for arbitrary meshes (CICSAM) by (Ubbink, 1997), and inter-gamma scheme by Jasak & Weller (1995).

While the basic premise of the VOF method remains the same in all the methods listed above, the differences arise from the different numerical schemes employed in the advection of the volume fraction. The CICSAM and the Inter-gamma differencing schemes employ compressive characteristics in order to avoid a diffused interface. Also, both the compressive schemes are constructed using Normalized Variable diagram (NVD) concepts introduced by Leonard to ensure boundedness of the volume-fraction.

In our work, the ability to simulate interface rupture is central to study of entrainment inception. In addition, the two-fluid solver in OpenFOAM is written based on the VOF method.

2.2.4 Modeling and Simulation of Entrainment

In the literature, most attempts at numerically modeling and simulation of the entrainment phenomenon are related to aeration encountered in hydraulic systems like spillways (Aydin & Ozturk, 2009), and breaking waves on ocean surfaces (Moraga
2.2 Background: Modeling and Simulation

et al., 2008; Lubin et al., 2006). The flow field is turbulent and the mechanism of entrainment is different as compared to that of a laminar jet plunging into a reservoir of liquid.

Sene (1988) published a phenomenological model based on turbulent characteristics of the flow field that can be incorporated within numerical simulations for the prediction of entrainment by turbulent plunging jets. The model proposed by Sene (1988) was employed by Ma et al. (2010) as a sub-grid model in their simulations, and they found the predicted rates of entrainment compared well with experimental results. A similar model has been incorporated within Flow3D to simulate entrainment by turbulent plunging jets (Hirt, 2003). The deformation of the jet surface is a result of the imbalance between the turbulent intensity and the surface-smoothening forces of surface tension and gravity. When the turbulent intensity is large, surface deformations cause entrainment, as seen in Fig. 2.2. Hence, within Flow3D, a turbulence model is invoked in addition to the entrainment model, to simulate the entrainment phenomenon.

To the best of the author’s knowledge, no such phenomenological models exist for laminar plunging jets, be it for a Newtonian or a non-Newtonian liquid. The entrainment mechanism observed in laminar plunging jets does not lend itself to a similar analysis as that employed in the case of entrainment observed with turbulent plunging jets. Since no phenomenological models exist, our aim is to use the VOF method to explicitly capture the inception of entrainment.

Next, we list the specific objectives of the present study.
2.3 Specific Objectives

1. Conduct simulations of the plunging-jet configuration using the VOF method and capture the inception of entrainment.

2. Identify the challenges that the physics poses on the numerical methodology in carrying out simulations mentioned in Objective 1.

3. Explore a new approach to simulate entrainment inception of the laminar plunging jet. The new approach must address the challenges identified in Objective 2.

4. Provide evidence to support the efficacy of the new approach by simulating a simple validation case. The validation case must exhibit similar physics as observed in the plunging-jet configuration.

2.4 Closure

In this chapter, we presented pertinent background information with respect to modeling of the entrainment phenomenon as associated with laminar plunging jets. Also, we listed the specific objectives that we aim to achieve. This sets the stage for describing the numerical framework employed in the present study in the next chapter.
Chapter 3

Numerical Framework and Methodology

This chapter describes the numerical framework and methodology used in the present dissertation. As described in Chapter 2, fluid flow is characterized by the Navier-Stokes (NS) equations. Our interest is in numerically solving these equations to determine the temporal and spatial evolution of the interface between two immiscible fluids. The Volume-Of-Fluid (VOF) framework is used to simulate the evolving interface. In the VOF approach, a scalar advection equation is solved in conjunction with “modified” NS equations (modified in a manner that allows for the simulation of two/multiple fluids using a single set of equations). The equations are discretized using the finite-volume technique described in Chapter 2.

The following sections describe the VOF approach, and since OpenFOAM is used to conduct the simulations, we also describe the numerics that form the two-fluid solver in OpenFOAM, namely, interFoam.
3.1 Volume Of Fluid (VOF) Method

Consider two immiscible fluids, Fluid 1 and Fluid 2, sharing a physical domain as shown in Fig. 3.1. We define a variable, $\gamma$, such that:

1. $\gamma = 1$ in all regions that contain only Fluid 1 in the physical domain,
2. $\gamma = 0$ in all regions that contain only Fluid 2 in the physical domain,

where $\gamma$ is known as the volume fraction, color function or an indicator function (Gopala & van Wachem, 2008). The interface is a singularity, i.e., the value of $\gamma$ changes abruptly from zero to unity across it. In order to use numerical methods to capture interfacial phenomena (as opposed to using interfacial fitting methods), the singularity is assumed to be spread over a small, but finite thickness over which $\gamma$ varies continuously from one value to another. Under this assumption, the same stringent characteristics of boundedness and non-oscillatory behaviour are required.

**Figure 3.1** Designated volume-fraction values: $\gamma = 1$ implies presence of Fluid 1, $\gamma = 0$ implies presence of Fluid 2, $0 < \gamma < 1$ implies interface between Fluid 1 and Fluid 2
3.1 Volume Of Fluid (VOF) Method

of the numerical methods as in the modeling of other physical phenomena such as capturing Mach shocks. For the case of two-fluid flows, the interface is the thin region where $\gamma$ varies continuously from 0 to 1 [Fig. 3.1]. Hence, the interface between the two immiscible fluids is defined as the region where $0 < \gamma < 1$.

Employing the definition of volume fraction, the continuity and momentum equations can be cast in a composite manner such that the solution to the entire two-fluid flow field can be obtained using a single set of equations [Eq. (3.1), Eq. (3.2)], without having to solve two different sets of equations for the two different fluids. A single set of equations is arrived at by defining a single density, $\rho$, and a single viscosity, $\eta$, as shown in Eq. (3.3) and Eq. (3.4), respectively.

Continuity equation:

$$\nabla \cdot \mathbf{v} = 0, \quad (3.1)$$

Momentum equation:

$$\rho \left\{ \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right\} = -\nabla p + \eta \nabla^2 \mathbf{v} + f_{\text{surface tension}} + f_{\text{gravity}}, \quad (3.2)$$

where,

$$\rho = \gamma \rho_{\text{Fluid 1}} + (1 - \gamma) \rho_{\text{Fluid 2}} \quad (3.3)$$

$$\eta = \gamma \eta_{\text{Fluid 1}} + (1 - \gamma) \eta_{\text{Fluid 2}} \quad (3.4)$$

Hence, $\gamma = 1$ implies $\rho = \rho_{\text{Fluid 1}}$, and $\eta = \eta_{\text{Fluid 1}}$; $\gamma = 0$ implies $\rho = \rho_{\text{Fluid 2}}$, and $\eta = \eta_{\text{Fluid 2}}$. Across the interface, where $0 < \gamma < 1$, $\rho$ and $\eta$ are linear combinations of properties of the two fluids.

An additional advection equation [Eq. (3.5)] is solved for the volume fraction, $\gamma$, to account for the temporal and spatial evolution of the interface between the two fluids:

$$\frac{\partial \gamma}{\partial t} + \nabla \cdot (\mathbf{v} \gamma) = 0. \quad (3.5)$$
3.1 Volume Of Fluid (VOF) Method

Solving Eq. (3.5) is not trivial. The discontinuity at the interface poses a numerical challenge, in that, lower-order accurate schemes are stable but numerically diffusive, whereas higher-order accurate schemes preserve a sharp interface but are numerically unstable.

The following sections describe the numerical methods employed to solve the set of governing equations.

3.1.1 Solution Methodology: Temporal Evolution

Both, the Navier Stokes equations and the scalar advection equation, contain a time-derivative term. Determining the temporal evolution of the flow field requires a numerical method/scheme that advances the solution of these equations in time. A number of numerical methods have been developed, e.g., forward Euler, Crank-Nicholson, implicit Euler. In the present work, we use the Crank-Nicholson method as it is an implicit method, and formally second-order accurate in time. The next paragraph describes the Crank-Nicholson scheme in further detail.

Consider the general partial differential equation of the form \( \frac{\partial \phi}{\partial t} = f(\phi, x, t, \frac{\partial \phi}{\partial x}, \frac{\partial^2 \phi}{\partial x^2}) \) for a dependent variable \( \phi \). The computational stencil for the Crank-Nicholson scheme is shown in Fig. 3.2. The subscripts \( i \) and \( n \) represent counters for the discretized \( x \) and \( t \), respectively. The Crank-Nicholson scheme for representing the time derivative of \( \phi \) is shown in Eq (3.6).

\[
\left( \frac{\partial \phi}{\partial t} \right)_{i}^{n+1} \approx \frac{\phi_{i}^{n+1} - \phi_{i}^{n}}{\Delta t} = \frac{1}{2} \left[ f_{i}^{n+1}(\phi, x, t, \frac{\partial \phi}{\partial x}, \frac{\partial^2 \phi}{\partial x^2}) + f_{i}^{n}(\phi, x, t, \frac{\partial \phi}{\partial x}, \frac{\partial^2 \phi}{\partial x^2}) \right] \quad (3.6)
\]

In this section, we presented the method/scheme employed to advance the solution in time. In the following sections, we describe the solution methodology used to solve for the flow variables within one time step.
3.1 Volume Of Fluid (VOF) Method

3.1.2 Solution Methodology: Scalar-Advection Equation

Recently, Deshpande et al. (2012) provided a detailed description of the interFoam solver. The following description of interFoam parallels that presented in their work. The scalar-advection equation [Eq. (3.7)] mathematically represents the temporal and spatial advection of the volume fraction using the local velocity field. For finite-volume discretization, we integrate Eq. (3.7) over a control volume, $dV$, [Eq. (3.8)], and using the divergence theorem for the second term on the left-hand side, we obtain Eq. (3.9).

\[
\frac{\partial \gamma}{\partial t} + \nabla \cdot (v \gamma) = 0 \quad (3.7)
\]

\[
\int_V \frac{\partial \gamma}{\partial t} dV + \int_V \nabla \cdot (v \gamma)dV = 0 \quad (3.8)
\]

\[
\int_V \frac{\partial \gamma}{\partial t} dV + \int_S (v \gamma) \cdot n dS = 0, \quad (3.9)
\]

where $dS$ is the elemental surface bounding the elemental volume $dV$. 

![Computational stencil for Crank-Nicholson scheme](image)

Figure 3.2 Computational stencil for Crank-Nicholson scheme
The first term on the left-hand side of Eq. (3.9) can be numerically evaluated using one of the methods mentioned in Section 3.1.1. The second term on the left-hand side of Eq. (3.9) requires close attention, since the treatment of this term must ensure that $\gamma$ is bounded, and at the same time, the interface is minimally diffused. Modeling convective terms to capture other discontinuous phenomena, such as Mach shocks, involves dealing with similar constraints on the numerical method.

To complete the discretization of Eq. (3.9), at a particular time level, $n$, let the second term on the left-hand side of Eq. (3.9) be written in the form shown in Eq. (3.10).

$$
\int_S (\mathbf{v}_s \cdot \mathbf{n}) dS \equiv \sum_{\text{cell faces}, f} (F_u + \lambda_m F_c) (3.10)
$$

where the advective fluxes, $F_u$ and $F_c$, are defined as follows:

$$
F_u = \phi_f \gamma_f, \text{upwind}, (3.11)
$$

Figure 3.3 Face owned by cell P and neighbour cell, N
3.1 Volume Of Fluid (VOF) Method

\[ F_c = \phi_f \gamma_f + \phi_r f \gamma_r f (1 - \gamma)_{rf} - F_u, \quad (3.12) \]

where volume flux is \( \phi_f = v_f S_f \), and \( S_f = n dS \).

Here, \( \lambda_m \) acts as a delimiter. At any point in the domain where \( \gamma = 0 \) or \( \gamma = 1 \), \( \lambda_m = 0 \). For all points in the domain with \( \gamma \in (0, 1) \) (note: this signifies the interface), \( \lambda_m = 1 \). Hence, at all computational-domain points in the region of only one fluid or the other, the advection term is treated using an upwind scheme alone [Eq. (3.13)].

\[ (F_u + \lambda_m F_c) = \phi_f \gamma_{f, \text{upwind}} \quad (3.13) \]

At all computational points in the region of the interface \( 0 < \gamma < 1 \), the advection term is treated as shown in Eq. (3.14). Higher-order bounded schemes are used for \( \phi_f \gamma_f \). The second term on the right-hand side of Eq. (3.14) corresponds to an artificial term (interface compression term) introduced to ensure the interface remains sharp.

\[ (F_u + \lambda_m F_c) = \phi_f \gamma_f + \phi_r f \gamma_r f (1 - \gamma)_{rf} \quad (3.14) \]

In order to compute the first term on the right-hand side of Eq. (3.14), \( \phi_f \gamma_f \), \( v_f \) and \( \gamma_f \) are evaluated at face centers [refer Fig. 3.3]. For simplicity, let us assume uniform grid spacing, and linear interpolation for the velocity field in order to arrive at face-centered values from cell-centered values [Eq. (3.15)]:

\[ v_f = \frac{v_P + v_N}{2}. \quad (3.15) \]

In order to arrive at face-centered values of \( \gamma \), \( \gamma_f \) is computed using a combination of upwind and central interpolation/differences using values at cell centers [Eq. (3.16)]
3.1 Volume Of Fluid (VOF) Method

so that,

\[ \gamma_f = (1 - \lambda_\gamma)(\gamma_f)_{UD} + \lambda_\gamma(\gamma_f)_{CD} \]  \hspace{1cm} (3.16)

where

\[ (\gamma_f)_{UD} = \begin{cases} \gamma_P & \text{for } \phi_f \geq 0, \\ \gamma_N & \text{for } \phi_f < 0 \end{cases} \]  \hspace{1cm} (3.17)

and

\[ (\gamma_f)_{CD} = \frac{\gamma_P + \gamma_N}{2}. \]  \hspace{1cm} (3.18)

The limiter \( \lambda_\gamma \) is chosen based on the specific high-order scheme used, such as the Van Leer scheme, the SuperBee scheme, the Minmod scheme, the QUICK scheme, or the gamma-differencing schemes. In the present work, we use the Van Leer scheme to obtain \( \gamma_f \).

Now, Eqs. (3.16), (3.17), and (3.18) can be combined into a single expression using a switch (a sign function), \( \varsigma(\phi_f) \), as follows:

\[ \gamma_f = \gamma_P + \frac{\gamma_N - \gamma_P}{2}[1 - \varsigma(\phi_f)(1 - \lambda_\gamma)], \]  \hspace{1cm} (3.19)

where \( \varsigma(\phi_f) \) is defined in the following manner:

\[ \varsigma(\phi_f) = \begin{cases} 1 & \text{for } \phi_f \geq 0, \\ -1 & \text{for } \phi_f < 0. \end{cases} \]  \hspace{1cm} (3.20)

We have now described a way to obtain the face-centered values for \( \phi_f \gamma_f \) from cell-centered values, with the ability to use high-order schemes for the interpolation process. These schemes play a vital part in keeping \( \gamma_f \) bounded.
Next, we focus on the second term on the right-hand side of Eq. (3.14), i.e., the artificial interface compression term introduced into the scalar-advection equation so that the interface remains sharp. To evaluate $\phi_{rf}\gamma_{rf}(1 - \gamma)_{rf}$, $\phi_{rf}$ is calculated using Eqs. (3.21),(3.22), and (3.23):

$$\phi_{rf} = \min(C_{\gamma}\frac{|\phi_f|}{|S_f|}, \max[|\phi_f|/|S_f|])(n_f.S_f), \quad (3.21)$$

where

$$n_f = \frac{\nabla(\nabla \gamma)}{|\nabla(\nabla \gamma)|} \quad (3.22)$$

$n_f$ is the unit vector parallel to $(\nabla \gamma)_f$,

and interpolating for $(\nabla \gamma)_f$ from cell centered-values [refer Fig. 3.3]

$$(\nabla \gamma)_f = \frac{(\nabla \gamma)_P + (\nabla \gamma)_N}{2} \quad (3.23)$$

Now, only $\gamma_{rf}$ remains to be determined in order to completely evaluate the interface compression term in Eq. (3.14). $\gamma_{rf}$ is determined using existing values of $\gamma$ at cell centers, and the previously calculated value of $\phi_f$ [Eq. (3.24)].

$$\gamma_{rf} = \gamma_P + \frac{(\gamma_N - \gamma_P)}{2}[1 - \varsigma(\phi_f)(1 - \lambda_{\gamma r})], \quad (3.24)$$

where $\lambda_{\gamma r}$ is the limiter that is estimated based on Eq. (3.25) as

$$\lambda_{\gamma r} = \min\{\max(1 - \max[(1 - (4\gamma_P(1 - \gamma_P))^2, (1 - (4\gamma_N(1 - \gamma_N))^2)], 0), 1\} \quad (3.25)$$

This brings to close our discussion on the discretization and interpolation schemes used to solve the scalar-advection equation. Next we describe the solution methodology to calculate the flow variables - velocity and pressure. The velocity and pressure fields in the computational domain are determined by solving fundamental conservation equations for mass and momentum.
3.1.3 Solution Methodology: Mass and Momentum Conservation Equations

The Navier-Stokes equations describing the flow of incompressible fluids - the conservation of mass [Eq. (2.3)] and momentum [Eq. (2.4)] equations, involve two quantities that need to be determined, the velocity field, $v$, and the pressure field $p$. The conservation of mass, also called the continuity equation, involves only the velocity field. In the momentum equation, the pressure field appears only as a source term on the right-hand side. Given these observations, solving for the velocity and pressure field requires attention.

For two-dimensional problems, the \textit{vorticity-stream function approach} is often used to solve the incompressible Navier-Stokes equations. The approach involves recasting the governing equations in terms of transformed variables (vorticity and stream function). This leads to a parabolic vorticity-transport equation and an elliptic Poisson equation for stream function, and these provide the solution for the velocity field. The advantage of this approach is that pressure is totally decoupled from the equations, and can be computed by solving a separate Poisson equation following the determination of the velocity field \cite{Pletcher2010} for details on deriving the transformed equations]. The \textit{vorticity-stream function} approach is particularly advantageous for two-dimensional problems but is not as straightforward for three-dimensional flows since two stream-functions are needed to represent the velocity field in a three-dimensional flow field.

Another class of solution methods consists of directly solving for the velocity field and the pressure field. These methods are classified as primitive-variable approaches. For incompressible flows, the \textit{artificial compressibility method} developed by Chorin (1967) involves introducing an artificial time derivative of density in the continuity
3.1 Volume Of Fluid (VOF) Method

equation (mass conservation equation) \(- (\frac{\partial \rho}{\partial t})_{\text{artificial}}\). The artificial density is related to the pressure through an artificial equation of state \(- p = \frac{\rho_{\text{artificial}}}{\beta}\), where \(\beta\) is an artificial compressibility factor (Pletcher et al., 2010). As the flow field reaches a steady state, the contribution of the artificial time-derivative term tends to 0. Hence, the term changes the path to solution, but does not affect the final solution.

To retain the coupling between velocity and pressure, Patankar & Spalding (1972) proposed the SIMPLE (Semi-Implicit Method for Pressure Linked Equations) scheme. The SIMPLE scheme and its variations (SIMPLER, SIMPLE-C, PISO, etc.) proposed subsequently are predictor-corrector methods. The equations are solved for primitive variables - velocity and pressure. In the present work, the PISO (Pressure Implicit with Splitting of Operators) scheme (Issa, 1986) is used for the pressure-velocity coupling. Details of the implementation of the PISO algorithm within the VOF framework are provided by Ubbink (1997).

3.1.4 Solution Methodology: Calculating Surface-tension Forces

An important aspect of VOF computations is the calculation of surface-tension forces. Laplace’s theorem states that the increase in hydrostatic pressure \(\Delta P\) that occurs upon traversing the boundary between the two fluids is equal to the product of the surface tension \(\sigma\) and the curvature of the surface \(C = \frac{1}{R} + \frac{1}{R'}\) (De Gennes et al., 2004, p. 8):

\[
\Delta P = \sigma \left( \frac{1}{R} + \frac{1}{R'} \right) = \sigma \kappa
\]

where \(\sigma\) is defined as the energy that must be supplied to increase the surface area by one unit (De Gennes et al., 2004, p. 4), and \(\kappa\) is the mean surface curvature. \(R\) and \(R'\) are the principle radii of curvature.
3.1 Volume Of Fluid (VOF) Method

The issues in evaluating surface-tension forces in the VOF framework are succinctly explained by Ubbink (1997). Physically, the pressure across an interface due to surface tension is discontinuous, but in order to include the effect of surface tension, the pressure jump needs to be expressed as a gradient in the momentum conservation equation. In addition, the VOF method treats the two fluids as one mixture. Hence, the solution methodology needs to also include a way to allow for the surface-tension based pressure gradient to be 0 everywhere except at the interface.

In OpenFOAM, the surface-tension force is calculated using the Continuous Surface Force (CSF) formulation. The CSF formulation was proposed by Brackbill et al. (1992). Ubbink (1997)'s description of Brackbill et al. (1992)'s formulation is repeated here. The indicator function, $\alpha$, in Ubbink’s writeup is equivalent to the volume fraction, $\gamma$, in our work.

Figure 3.4(a) shows the schematic of the transitional region where $\alpha(x, y, z) = c$, where $0 < c < 1$. In the transitional region, $\alpha$ is a continuous and twice differentiable, implying a smooth variation between 0 and 1. Hence, different values of $\alpha$ or $c$ denote different layers in the transition region, as shown in Fig. 3.4(a). The line $ab$ is perpendicular to every layer of the interface and spans the transitional region. Figure 3.4(b) shows the smooth variation of pressure and the indicator function across the line $ab$.

Gradient of $\alpha$, $\nabla \alpha$, is the vector normal to the layers of constant $\alpha$ in the transitional region, and is 0 everywhere in the computational domain except in the transitional region. The curvature of the interface layers is then calculated as the divergence of the unit normal vector [Eq (3.27)].

$$
\kappa = - \nabla \cdot \left( \frac{\nabla \alpha}{|\nabla \alpha|} \right) 
$$

(3.27)

The surface-tension-induced pressure change in the transitional region along the
3.2 Solution Algorithm

The iterative process carried out by OpenFOAM’s two-fluid solver, interFoam, is as follows:

1. All the variables are initialized at $t = 0$

2. The scalar-advection equation is solved for new values of the volume fraction at $t + \Delta t$ using the fluxes calculated at $t$.

3. The values of $\gamma$ at $t + \Delta t$ are then used to obtain new values for mixture density and viscosity.

\[ f_{\text{surface tension}} = \nabla P = -\sigma \kappa (\nabla \alpha). \]  

(3.28)

Figure 3.4 Schematic representation of the transition region at a fluid-fluid interface (Ubbink, 1997)

line $ab$ is calculated as $P_t = P_a + \sigma \kappa (\alpha_t - \alpha_a)$, where subscript $t$ denotes any point on the line $ab$ between $a$ and $b$. This can be generalized to calculate the surface tension force, $f_{\text{surface tension}}$, present in the conservation of momentum equation as
4. The PISO algorithm is invoked to solve for the velocity and pressure fields at $t + \Delta t$. The surface-tension force is calculated based on the CSF formulation described in Section 3.1.4.

5. Steps 2, 3, and 4 are repeated to solve for the time-dependent evolution of the flow field.

In the next section, we discuss requirements placed on the solution algorithm for stable computations.

### 3.3 Courant Number Restriction

The discretized equations are approximations of the partial differential equations (PDEs) we want to solve. The discretization process must ensure that the discretized equations are consistent with the PDEs they approximate, but consistency does not necessarily mean convergence to the solution. For initial-value problems which are solved using marching techniques, the evolution of error is an important factor that decides whether the numerical method used to solve the discretized equation is stable or unstable. Numerical methods that are stable do not allow for small errors in the calculation process to amplify.

The Fourier/von Neumann analysis ((Pletcher et al., 2010), sec.3-6.1) is based on the premise that the numerical solution and associated error must satisfy the same discretized equation, and evolve in time in the same manner. An amplification factor can be derived from such an analysis which characterizes the behaviour of error in time, such that, any small change in the input values either leads to unbounded growth of error, or stable computations.

The numerical stability requirement for a number of explicit numerical methods for solving hyperbolic PDEs is the Courant-Friedrichs-Lewy (CFL) number.
3.4 Closure

The CFL number, also called the Courant number, identifies the relationship between velocity, distance between discrete, computational points, and time step. The Courant number for a first-order, one-dimensional, wave equation takes the form: Courant Number = \( \frac{c \Delta t}{\Delta x} \), where \( c \) is the wave speed, \( \Delta t \) is the time step, and \( \Delta x \) is the distance between discrete, computational points. The stability condition can be derived to be \( |\text{Courant number}| \leq 1 \).

In multiple dimensions, the stability condition becomes even more stringent. Gopala & van Wachem (2008) discuss the CFL/Courant Number stability criterion for compressive schemes (such as used in the present work, see Section 3.1.2), and state that, for numerical stability in three dimensions, it is necessary to limit the Courant number to \(< 1/3 \). In all our simulations, we use time-step values that ensure this condition is met.

3.4 Closure

In this chapter, we have described the numerical framework/methodology employed in the present work. In summary, the two-fluid solver is based on the Volume-Of-Fluid (VOF) method, which incorporates a scalar-advection equation along with the Navier-Stokes equations (conservation of mass and momentum) to model the spatial and temporal evolution of interfacial flows.

In the next chapter, we describe use of this numerical framework to conduct simulations of the plunging-jet configuration to capture interfacial rupture and entrainment.
Chapter 4

Simulations of Plunging-Jet Configuration

In this chapter, we present details of our simulations of the plunging-jet configuration and the associated phenomenon of entrainment. The objective is to use the numerical framework described in Chapter 3, and capture the entrainment phenomenon, specifically, the transition from steady filling to air bubbles being entrained. Since an explicit model is not available to provide critical conditions for entrainment inception observed in laminar plunging jets (explicit models presume critical conditions to be known a priori, and provide these conditions to the solution process), we require our calculations to capture the entrainment phenomenon implicitly, i.e, as a consequence of solving the governing equations.

We described the plunging-jet configuration in Chapter 2, Section 2.1. To reiterate, the plunging-jet configuration involves a liquid jet issuing from a nozzle, and impinging into a container filled with liquid. In most practical situations, the liquid forming the jet and the liquid in the container are the same, and this is the assumption we make in this study as well.
4.1 Simulation Details

The following sections provide details of our simulations. The key questions we address are how accurate are our simulations, and to what extent can we predict the critical conditions for entrainment inception with the chosen numerical framework. Answers to these questions will prove critical in identifying a new approach to simulate interface rupture and entrainment.

4.1 Simulation Details

In this section, we describe the simulations undertaken to predict critical entrainment conditions associated with the laminar plunging-jet configuration. Lin & Donnelly (1966) presented a correlation between critical Weber number, $W_{ep}$, and critical Reynolds number, $Re_p$. These non-dimensional variables were calculated using the velocity of the jet at which entrainment inception occurs, $V_e$. Their correlation was constructed using data from experiments where the critical conditions were recorded for different liquids issuing from nozzles of different diameters. We pick one such experimental data point (8G200A) from Lin & Donnelly (1966)’s data. This data point corresponds to an Aqueous Glycerol liquid jet with a viscosity of 0.2 Pas, and issuing from a nozzle with diameter of 8 mm. According to Lin & Donnelly (1966)’s correlation, entrainment inception for 8G200A occurs at $Re_p = 40$ [Fig. 4.1]. Additional liquid properties required to simulate the flow field are density, $\rho$, = 1120 $kg/m^3$, and interfacial tension between the liquid and air, $\sigma$, = 0.059 $N/m$.

The computational domain employed is shown in Fig. 4.2. The liquid jet issues from the nozzle, and plunges into the container filled with the same liquid. The container filled with liquid forms the receiving pool. This weir-like set-up allows for excess liquid to flow over the sides of the container. This ensures that the distance, $Z$, between the nozzle and the point at which the liquid jet plunges into the receiving
4.1 Simulation Details

**Figure 4.1** Minimum entrainment velocity correlation (Lin & Donnelly, 1966); experimental data point chosen for simulations: 8G200A at $Re_p = 40$

pool is constant with respect to time.

As described in Chapter 2, the subscript $p$ denotes the plunging point - the point at which the liquid jet meets the interface at the receiving pool. Let subscript $o$ denote conditions at the nozzle exit (see Fig. 4.3). The Reynolds number, $Re_o$, and the Weber number, $We_o$, at the nozzle exit can be evaluated using a simplistic energy balance, $V_p^2 = V_o^2 + 2gZ$, and a mass balance, $V_oD_o^2 = V_pD_p^2$. Introducing a Froude number, $Fr_o$, defined as $Fr_o = \frac{V_o^2}{gZ}$, we can relate the non-dimensional variables defined at the two locations, the plunging point and at the nozzle exit, using the Froude number, $Fr_o$ [Eqs. (4.1) and (4.2)].

$$Re_p = Re_o(1 + \frac{2}{Fr_o})^{1/4} \quad (4.1)$$
4.1 Simulation Details

Figure 4.2 Computational domain of the plunging-jet configuration; a. three-dimensional domain showing container filled with liquid, b. two-dimensional section which when rotated 360 degrees forms the three-dimensional computational domain. All dimensions are non-dimensionalized using diameter of nozzle

Figure 4.3 Plunging liquid jet issuing from nozzle exit, and impinging into receiving pool at plunging point
4.1 Simulation Details

\[ W_{\epsilon_p} = W_{\epsilon_o}(1 + \frac{2}{Fr_o})^{3/4} \] (4.2)

For the data point corresponding to 8G200A with \( (R_e)_{p} = 40 \), using the simplistic mass and energy balance relations, we calculate that \( V_o = 0.705 \text{ m/s} \) and \( Z = 4.9D_o \).

The 3-D computational meshes are created using Gridgen (a commercial CFD preprocessor). Since the nozzle and the container are cylindrical, the computational meshes are constructed using cylindrical cells so that the computational meshes are boundary-fitted. Also, the Volume-Of-Fluid (VOF) method used to conduct the present simulations is known to be grid-topology biased; i.e., a greater number of rectangular cells is required to capture a cylindrical jet accurately (without distorting the interface) than the number of cylindrical cells, since cylindrical cells conform to the cylindrical jet boundary.

In order to investigate the effect of mesh resolution on the flow field solution, three meshes, successively refined, are constructed. The coarsest mesh has a resolution of 1 mm, and the finest mesh has a resolution of 0.25 mm. As we will see in the next section, the mesh resolution afforded by even the finest mesh is not adequate to accurately capture the entrainment phenomenon. Further refinement of the 3-D computational mesh leads to prohibitively large number of cells, and consequently, high computational costs and wall-clock times. Lin & Donnelly (1966) observed from their experiments that, within the container, once entrainment has occurred, the collar-like air film that is entrained remains axisymmetric until a steady depth is reached, beyond which oscillations set in, and the film breaks up into bubbles. Hence, for the time period prior to the onset of these oscillations, we take advantage of the axisymmetric nature of the flow field and perform the simulations on a single-cell thick axisymmetric section of the 3-D domain. This enables further fine mesh resolutions, while also maintaining reasonable total computational times. Axisymmetric
4.2 Results

Simulation results obtained from using the 3-D computational mesh show an air film being formed beneath the surface of the liquid in the container. The observed features of the flow field closely resemble the expected physics - surrounding air is entrained into the receiving pool by the liquid jet, and an air film is formed, which subsequently breaks up into bubbles [Fig. 4.5]. This simulation corresponds to using the estimated (from empirical data provided by Lin & Donnelly (1966)) critical liquid-jet velocity at which entrainment occurs. A test to evaluate our simulations is to conduct another simulation with a liquid-jet velocity less than the critical value. At velocities less than the critical entrainment velocity, a steady cusp should be observed, with no air entrained into the receiving pool [Fig. 4.4]. A simulation with $V_o = 0.5$ m/s is undertaken to determine if the numerical computations capture a steady cusp.

**Figure 4.4** Schematic of plunging-jet configuration; a) steady interfacial cusp at sub-critical conditions, b) air film entrained into receiving pool at critical entrainment conditions (adapted from Lorenceau et al. (2004)).
4.2 Results

formation. Figure 4.6 shows an air film being entrained, and a few bubbles as well. These results are aphysical, and indicate the lack of sufficient mesh resolution to capture the entrainment phenomenon.

Comparing the simulation results obtained using three different mesh resolutions also provides evidence of the inadequacy of the mesh resolution to capture the entrainment phenomenon. The coarsest mesh is of 1 mm resolution, and the finest mesh is of 0.25 mm resolution. Figure 4.7 shows the spatial location of the interface (defined as the locus of points where volume fraction equals 0.5) predicted by simulations at the same time instant \( (t = 20T) \), where \( T \) is the time taken for the liquid jet to traverse from the nozzle exit to the receiving pool. The coarsest mesh is denoted by Mesh 1, and the finest mesh by Mesh 3. We observe that the spatial locations of the interface are markedly different from one mesh to another. These results suggest that greater mesh resolution is required to obtain a mesh-independent solution. Refining the 3-D domain further resulted in computational meshes with prohibitively large number of cells.

Taking advantage of the axisymmetry in the flow field prior to the onset of oscillations of the entrained air film, axisymmetric simulations are conducted with a greater mesh resolution of 0.1 mm. The axisymmetric computational domain is a 1-cell thick sector of the 3-d domain and 1 cell thick. This leads to a reduction in the total number of computational cells as compared the number of cells needed for the 3-D simulations. Again, as in the case of the 3-D computations, two cases are investigated. The first case corresponds to the jet velocity equal to the critical velocity for entrainment to occur \( ((Re)_p = 35.18, (We)_p = 108.43) \). The second case corresponds to a jet velocity being lower than the critical entrainment velocity \( ((Re)_p = 11.74, (We)_p = 24.33) \). In the first case, simulation results show an air film being formed beneath the surface of the receiving pool, and subsequently breaking up
Figure 4.5 Simulation of entrainment in a 3-D computational domain; a 2-D section shows entrained air-film along with formation of air bubbles. Gamma is the volume-fraction of fluid, Gamma = 1 denotes liquid, and Gamma = 0 denotes air, 0 < Gamma <1 denotes interface between liquid and air.
4.2 Results

Figure 4.6 Simulation of plunging jet at sub-critical conditions corresponding to steady-cusp formation. The 2-D section of the 3-D computational domain shows entrainment of an air film, and not formation of a steady cusp. This result does not reflect expected physics. Gamma is the volume-fraction of fluid, Gamma = 1 denotes liquid, and Gamma = 0 denotes air, 0 < Gamma < 1 denotes interface between liquid and air.
4.2 Results

Figure 4.7 Three meshes used, the finest being twice refined compared to the coarsest mesh. The solution is observed to be highly grid dependent.

into bubbles [Fig. 4.8]. The simulation captures the expected flow physics associated with the entrainment phenomenon in a plunging-jet configuration. In the simulation corresponding to conditions below the entrainment threshold, we still see air being entrained, although to a much lesser extent as compared to the other case [Fig. 4.9]. Even with a resolution of 1 mm, the simulations do not capture the formation of a steady interfacial cusp. This leads us to conclude that we require greater mesh resolutions to capture interface rupture and the subsequent entrainment of air.

In the next section, we list our conclusions from conducting simulations of the plunging-jet configuration.
4.2 Results

Figure 4.8 Axisymmetric simulation carried out at experimentally predicted entrainment conditions; \((Re)_p = 35.18, (We)_p = 108.43\).

Figure 4.9 Axisymmetric simulation carried out at conditions below experimentally predicted entrainment conditions; \((Re)_p = 11.74, (We)_p = 24.33\).
4.3 Conclusions

Simulations of the plunging-jet configuration aimed at capturing interface rupture and the inception of entrainment lead to the following important conclusions:

- Our simulations predict interface rupture and entrainment of air into the receiving pool even when the simulations are carried out at conditions that are below the critical conditions for entrainment to occur. While experimental verisimil-itude is observed for the simulations carried out at the critical entrainment inception conditions, the simulations carried out at sub-critical conditions also show air being entrained, instead of the formation of a steady interfacial cusp.

- Accurate simulations require greater resolutions than 0.1 mm. Increasing mesh resolution leads to two inter-related effects.

  - An increase in mesh resolution leads to a large total number of computational cells for simulating the entire computational domain (even if strategies such as non-uniform cell-size distributions are used, the quality of the solution suffers if the interface passes through regions where cells are of varying sizes). This increases the computational time taken, since at each time step, the flow solution needs to computed on a larger number of cells.

  - With an increase in resolution, the Courant number restriction limits the maximum time step values for which the simulations remain stable (see Section 3.3). Hence, the evolution of the solution in time occurs in smaller steps, thereby increasing total computational time.
4.4 Closure

This chapter presented our simulation results of the plunging-jet configuration. The very high mesh resolution requirement proved to be a challenge in capturing the entrainment phenomenon accurately through the simulations. Within the numerical framework used, increasing mesh resolution beyond 0.1 mm leads to large computational meshes, and prohibitively small time-step values. While this approach could still be used to conduct simulations to capture the entrainment phenomenon, we consider it impractical due to the large overall computational time required. In the next chapter, we propose a new approach that allows for the use of the same numerical framework, but alleviates the aforementioned hurdles.
Chapter 5

Scaling Approach

5.1 An Alternate Approach

In the previous chapter, we described the challenges with simulations of the entrainment phenomenon associated with the plunging-jet configuration using the VOF method. In this chapter, we propose an alternate approach. This approach stems from data presented by Lorenceau et al. (2003) and Lorenceau et al. (2004). We first describe their work. Then, we describe the alternate approach to simulate the entrainment phenomenon, and provide supporting arguments for the approach.

5.1.1 Background

Lorenceau et al. (2003) conducted experimental investigations into conditions at which the interface between a viscous liquid and air, or instead of air, another liquid, would rupture. The schematic of the experimental setup they used is shown in Fig. 5.1. The setup consists of a container, the bottom half of which is filled with a viscous liquid, and the top half is filled with a lighter fluid which is immiscible with the liquid beneath it. A cylinder is placed such that half of it is immersed in the lower
5.1 An Alternate Approach

Figure 5.1 Schematic of experimental setup used by Lorenceau et al. (2003)

liquid. The experiment is designed such that this cylinder can be rotated, in a controlled manner, about its primary axis. Lorenceau et al. (2003) conducted separate experiments, some involving air as the lighter fluid, and some involving other liquids as the lighter fluid. When the cylinder rotates clockwise, it drags along a layer of lower liquid from the left side, over the top, and to the right side. This layer plunges into the lower fluid on the right side, causing an interfacial cusp [see Fig. 5.1]. As the angular rotational speed of the cylinder is increased, the tip of the cusp becomes sharper [Fig. 5.2]. Further increase in the rotational speed of the cylinder causes the interfacial cusp to break, leading to entrainment of a thin film of the upper fluid. We note, at this point, that the physics seen in this experimental setup is very similar to that in a laminar plunging-jet configuration - cusp formation and subsequent entrainment with increasing jet velocity.

Experimental results presented by Lorenceau et al. (2003) compare well with theoretical ideas presented by Eggers (2001) previously. As predicted by Eggers (2001), the tip radius is observed to increase with an increase in the viscosity of the upper fluid. Also, as the upper fluid viscosity increases, there is a decrease in the critical capillary number, $Ca_c = \eta V_c / \sigma$, at which the upper fluid is entrained. The variation
5.1 An Alternate Approach

**Figure 5.2** Observed sharpening of the interfacial cusp with increase in flow velocity. The photograph shows a tip of air in a bath of glycerol. The bar indicates 200 $\mu$m. The flow velocities are 14 cm/s and 22 cm/s (Lorenceau et al., 2003)

of $Ca_c$ with $\eta_0/\eta$ can be seen in Fig. 5.3.

Subsequently, Lorenceau et al. (2004) conducted experiments with a laminar plunging-jet configuration. A schematic of the physics exhibited is shown in Fig. 5.4. $V_c$ is the critical velocity at which inception of entrainment occurs. When the velocity of the jet, $V$, is less than $V_c$, an interfacial cusp is sustained [Fig. 5.4.a]. When $V \geq V_c$, the interfacial cusp fails (interfacial rupture occurs), and entrainment inception is said to have occurred.

Central to their results is their theoretical analysis of the forces that sustain the entrained film. Balancing the surface tension forces around the film and viscous forces within the film yields an expression for the film thickness, $h$, [Eq. (5.1)]. As expected, the film thickness increases with increase in viscosity of the entrained fluid (upper fluid). Figure 5.5 shows that Eq. (5.1) for $h$ holds true when compared with the experimental results of Lorenceau et al. (2004).

$$h \approx k^{-1}(\eta_0 V/\sigma)^{2/3}$$  \hspace{1cm} (5.1)

where $k^{-1}$ is the capillary length $= \sqrt{\sigma/\rho g}$.

In the next section, we present our proposed alternate approach to conduct simu-
5.1 An Alternate Approach

![Graph showing critical capillary number Ca_c vs. viscosity ratio \( \eta_0/\eta \). Solid circles represent water-glycerol mixtures as the lower fluid, with air as the upper fluid. Open circles represent glycerol as the lower fluid, with different lighter liquids above.]

**Figure 5.3** Critical capillary number \( Ca_c \) vs. viscosity ratio \( \eta_0/\eta \). Solid circles represent water-glycerol mixtures as the lower fluid, with air as the upper fluid. Open circles represent glycerol as the lower fluid, with different lighter liquids above.

![Diagram showing cylindrical jet of viscosity \( \eta \) plunges into a bath of the same liquid. The jet is surrounded by a lighter fluid of viscosity \( \eta_0 \). a) shows the interfacial cusp before inception of entrainment. b) shows the lighter fluid being entrained as a film with thickness of \( h \) (Lorenceau et al., 2004).]

**Figure 5.4** Cylindrical jet of viscosity \( \eta \) plunges into a bath of the same liquid. The jet is surrounded by a lighter fluid of viscosity \( \eta_0 \). a) shows the interfacial cusp before inception of entrainment. b) shows the lighter fluid being entrained as a film with thickness of \( h \) (Lorenceau et al., 2004).
5.1 An Alternate Approach

Figure 5.5 Thickness of film entrained by glycerol jet ($\eta = 900mPas$); a) entrained fluid is air ($\eta_0 = 2 \times 10^{-2}mPas$), b) entrained fluid is silicon oils of different viscosities (black - $\eta_0 = 8mPas$, white - $\eta_0 = 20mPas$, grey - $\eta_0 = 32mPas$). The thickness of the film is seen to increase by a factor of 1000 when the entrained fluid is a lighter liquid instead of air. (Lorenceau et al., 2004)

lations of laminar plunging jets with a view to accurately capturing the entrainment phenomenon.

5.1.2 Proposed Alternate Approach and Supporting Arguments

In this section, we propose an alternate approach to conduct simulations of the entrainment phenomenon associated with laminar plunging jets. We then connect key results from Lorenceau et al. (2003) and Lorenceau et al. (2004) to our work, in order to provide support to our claim.

Consider a liquid jet of a certain viscosity for which the critical entrainment velocity in an environment of air needs to be ascertained. The proposed approach is as follows:
5.1 An Alternate Approach

Proposed Approach

The proposed approach involves the scaling of the underlying physics of interfacial rupture/entrainment inception. Subsequent references to the “scaling approach” in this work refer to this proposed approach.

1. Perform simulations of the rotating cylinder problem with the jet liquid as the lower liquid, and three lighter liquids having different viscosities as the upper fluids instead of air.

2. Plot critical values of the capillary number, $Ca_c$, vs. the viscosity ratio, $\eta_0/\eta$, in the same manner as in the work of Lorenceau et al. (2003).

3. Extrapolate to what would be the critical capillary number $Ca_c$ with air as the entrained fluid, and calculate the entrainment velocity from the definition of $Ca_c$.

Supporting Arguments

Here, we list supporting arguments as evidence of the viability of the proposed approach in order to conduct simulations of the entrainment phenomenon seen in laminar plunging jets.

- The effect of the proposed approach on adequate grid resolution is remarkable. Our previous results with air as the entrained fluid suggest that we could not achieve adequate grid resolution to capture inception of entrainment. The inception of entrainment can be captured accurately only if the interfacial cusp is resolved, thus predicting correctly the surface tension forces that hold the interface together. The results of Lorenceau et al. (2003) show that the tip radius is of the order of microns when air is entrained, but increases with increase in
5.2 Closure

the viscosity of the entrained fluid. The flow configuration used by Lorenceau et al. (2003) (rotating cylinder at an interface) exhibits similar physics as the plunging jet. Furthermore, Lorenceau et al. (2004) show that the thickness of film of upper fluid entrained also increases with the viscosity of that fluid. Together, these results show that the resolution required to capture the interfacial cusp and the subsequent entrainment film is 1000 times lesser when the entrained fluid is a liquid of higher viscosity than that of air. Lesser spatial grid resolution requirements for the accurate capture of entrainment inception translates to larger time-step values for stable computations. Hence, capturing entrainment inception using numerical simulations becomes tractable.

- Lorenceau et al. (2003) show that the critical capillary number reduces with an increase in the viscosity ratio between the lighter upper fluid and the lower liquid [Fig. 5.3]. Hence, the entrainment velocity is much smaller in configurations involving liquids as the entrained fluid as their viscosity is much smaller than that of air. This also influences the solution process, in that, stable computations can be carried out at higher time-step values.

5.2 Closure

This chapter provides background information for an alternate approach to numerically predict critical conditions at which entrainment inception occurs for a particular liquid. The approach is based on scaling of the underlying physics. Evidence suggests that the approach will alleviate some of the challenges posed by the physics on our numerical methodology. In the next chapter, we use this scaling approach to investigate the inception of entrainment (interface rupture), and numerically predict the conditions at which surface-tension forces fail to preserve the integrity of the interface.
5.2 Closure

and entrainment inception occurs.
Chapter 6

Spurious Currents

The rationale behind using the scaling approach in the modeling and simulation of interfacial rupture was provided in Chapter 5. The scaling approach involves simulations of interfacial evolution between two liquids instead of a liquid and air. Briefly, the scaling approach circumvents the need for meshes of micron-scale resolution, and as a consequence of reducing the resolution required to the order of millimeters, the maximum time step employable for stable computations is increased (guided by the Courant number, see section 3.3).

Details of the investigation we undertake to elicit the effect of the scaling approach on spurious/parasitic currents are discussed in this chapter. Laplace’s theorem states that the surface tension force must balance the pressure difference across an interface. Depending on how surface tension force is discretized, the numerical (discrete) surface tension force may not exactly balance the pressure difference across the interface. This imbalance leads to artificial velocities that are called spurious or parasitic currents ((Popinet, 2009) (Popinet & Zaleski, 1999)). Spurious currents tend to destroy the integrity of the interface, and lead to unstable computations (since artificially high velocities in the domain affect numerical stability through the Courant num-
ber). The aim here is to show that using the scaling approach decreases the spurious currents, better preserves the integrity of the interface, and improves stability of the computations, in that, much higher time steps can be used without the computations becoming unstable.

6.1 Effect of Scaling Approach on Spurious Currents

The Continuum Surface Force (CSF) formulation is used to model interfacial-tension forces at the interface in a finite-volume framework. The CSF formulation was assessed by Brackbill et al. (1992) using the nonequilibrium rod problem. Since the scaling approach involves using a liquid as the entrained fluid instead of air, we explore the effect of using a liquid on the genesis of spurious currents by simulating the non-equilibrium rod problem with lower density and viscosity ratios.

6.1.1 Problem Definition

To show the effect of the scaling approach on spurious currents, we choose the nonequilibrium rod problem. The CSF formulation is described in Section 3.1.4. The nonequilibrium rod consists of a square drop/bubble in another liquid, and extends to infinity in the third direction [Fig. 6.1]. This set-up is assumed to be in a zero gravity field. The square drop/bubble will deform and ultimately reach a circular shape which is the minimal-energy configuration for the interface.

To elicit the effect of scaling on spurious currents, we conduct the simulations detailed in Table 6.1. Viscosity, density and interfacial tension are denoted by $\eta$, $\rho$ and $\sigma$, respectively. For all the cases listed in Table 6.1, the computational domain
6.1 Effect of Scaling Approach on Spurious Currents

is a two-dimensional square of side 70 mm, and the drop is a square of side 40 mm placed centrally in the domain. The evolution of the interface is driven by surface tension forces. High surface tension forces are seen in high curvature regions - the corners of the square drop. Eventually, the drop/bubble should attain a circular shape when a balance between forces is achieved, i.e., interfacial tension balances the pressure difference between the inside and outside of the drop/bubble.

In the next section, we present the results.

6.1.2 Results

First, we simulate a square air bubble in a surrounding liquid [fluid properties corresponding to Case 1]. The evolution of the interface is shown in Fig. 6.2. Surface tension forces drive the evolution of the interface from a square to a circular shape. Our results exhibit the same characteristics as observed by Brackbill et al. (1992). It is observed that even after considerable time, the interface continues to oscillate about a mean circular shape. While the amplitude of the oscillations decreases due to viscous damping by the surrounding liquid, the frequency remains constant, and
6.1 Effect of Scaling Approach on Spurious Currents

Table 6.1 Simulations conducted to investigate spurious currents

<table>
<thead>
<tr>
<th>Case #</th>
<th>$\eta_{\text{drop}}$</th>
<th>$\rho_{\text{drop}}$</th>
<th>$\eta_{\text{surr. fluid}}$</th>
<th>$\rho_{\text{surr. fluid}}$</th>
<th>$\sigma$</th>
<th>Mesh</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(mPas)</td>
<td>(kg/m$^3$)</td>
<td>(mPas)</td>
<td>(kg/m$^3$)</td>
<td>(mN/m)</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1e-2</td>
<td>1.1768</td>
<td>1.2</td>
<td>797.88</td>
<td>23.61</td>
<td>30x30</td>
</tr>
<tr>
<td>2</td>
<td>1e-2</td>
<td>1.1768</td>
<td>1.2</td>
<td>797.88</td>
<td>23.61</td>
<td>60x60</td>
</tr>
<tr>
<td>3</td>
<td>1e-2</td>
<td>1.1768</td>
<td>1.2</td>
<td>797.88</td>
<td>23.61</td>
<td>120x120</td>
</tr>
</tbody>
</table>

Simulations using Scaling Approach

<table>
<thead>
<tr>
<th></th>
<th>$\eta_{\text{drop}}$</th>
<th>$\rho_{\text{drop}}$</th>
<th>$\eta_{\text{surr. fluid}}$</th>
<th>$\rho_{\text{surr. fluid}}$</th>
<th>$\sigma$</th>
<th>Mesh</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>83</td>
<td>980</td>
<td>900</td>
<td>1120</td>
<td>26</td>
<td>30x30</td>
</tr>
<tr>
<td>5</td>
<td>41.5</td>
<td>980</td>
<td>900</td>
<td>1120</td>
<td>26</td>
<td>30x30</td>
</tr>
<tr>
<td>6</td>
<td>8.3</td>
<td>980</td>
<td>900</td>
<td>1120</td>
<td>26</td>
<td>30x30</td>
</tr>
</tbody>
</table>

the oscillations persist for a long time.

In comparison, a liquid square drop [fluid properties corresponding to Case 4] evolves in time to quickly attain a circular shape, and does not deform further. This indicates a decrease in the imbalance between the pressure difference across the interface and the calculated surface tension forces. Figure 6.3 provides evidence to support the claim that spurious currents are much smaller when the viscosity ratios are smaller (as compared to high viscosity ratios involved when the drop is air). This result is expected, and is similar to what has been observed previously by other investigators (Renardy & Renardy, 2002).

In Table 6.2, the maximum and the mean velocity magnitudes of the interface at various times are recorded for an air bubble. Amongst Cases 1, 2 and 3, the difference is in the mesh resolution used. With higher resolution, the spurious currents increase. This is important insofar as to negate the notion that improved mesh resolution will decrease spurious currents. Also, this confirms that the imbalance of forces which
6.1 Effect of Scaling Approach on Spurious Currents

Figure 6.2 Evolution of square air bubble in surrounding liquid
6.1 Effect of Scaling Approach on Spurious Currents

Figure 6.3 Evolution of square liquid drop in surrounding liquid
### 6.1 Effect of Scaling Approach on Spurious Currents

**Table 6.2** Maximum and mean velocity magnitudes during evolution of interface for an air drop/bubble

<table>
<thead>
<tr>
<th>Case #</th>
<th>time(t)</th>
<th>v_max</th>
<th>v_mean</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(s)</td>
<td>(m/s)</td>
<td>(m/s)</td>
</tr>
<tr>
<td>1</td>
<td>4.0</td>
<td>0.01283</td>
<td>0.01046</td>
</tr>
<tr>
<td></td>
<td>4.2</td>
<td>0.00945</td>
<td>0.00425</td>
</tr>
<tr>
<td></td>
<td>4.4</td>
<td>0.00689</td>
<td>0.00561</td>
</tr>
<tr>
<td></td>
<td>4.6</td>
<td>0.01223</td>
<td>0.00958</td>
</tr>
<tr>
<td></td>
<td>4.8</td>
<td>0.00947</td>
<td>0.00490</td>
</tr>
<tr>
<td></td>
<td>5.0</td>
<td>0.00538</td>
<td>0.00412</td>
</tr>
<tr>
<td>2</td>
<td>4.0</td>
<td>0.00796</td>
<td>0.00468</td>
</tr>
<tr>
<td></td>
<td>4.2</td>
<td>0.01356</td>
<td>0.00938</td>
</tr>
<tr>
<td></td>
<td>4.4</td>
<td>0.01958</td>
<td>0.01602</td>
</tr>
<tr>
<td></td>
<td>4.6</td>
<td>0.00558</td>
<td>0.00371</td>
</tr>
<tr>
<td></td>
<td>4.8</td>
<td>0.00742</td>
<td>0.00522</td>
</tr>
<tr>
<td></td>
<td>5.0</td>
<td>0.02128</td>
<td>0.01590</td>
</tr>
<tr>
<td>3</td>
<td>4.0</td>
<td>0.02808</td>
<td>0.02023</td>
</tr>
<tr>
<td></td>
<td>4.2</td>
<td>0.02169</td>
<td>0.01347</td>
</tr>
<tr>
<td></td>
<td>4.4</td>
<td>0.01704</td>
<td>0.00715</td>
</tr>
<tr>
<td></td>
<td>4.6</td>
<td>0.03580</td>
<td>0.02598</td>
</tr>
<tr>
<td></td>
<td>4.8</td>
<td>0.01091</td>
<td>0.00672</td>
</tr>
<tr>
<td></td>
<td>5.0</td>
<td>0.01876</td>
<td>0.01152</td>
</tr>
</tbody>
</table>
6.1 Effect of Scaling Approach on Spurious Currents

cause spurious currents is inherent to the discretization of the governing dynamics. In the literature, a number of ways to decrease spurious currents have been proposed, two of which are by Renardy & Renardy (2002), and Popinet & Zaleski (1999).

Aligned with the proposed scaling approach, Cases 4, 5 and 6 involve a pair of liquids. In comparison to the air bubble cases, the spurious velocity magnitudes are observed to be smaller by at least two orders of magnitude [Table 6.3]. Cases 4, 5 and 6 differ from one another only in the viscosity of the drop/bubble. Amongst these cases involving an interface between two liquids, the highest spurious velocities are seen in the case with the highest viscosity ratio.

6.1.3 Conclusions

The investigation into the nonequilibrium drop gives further credence to our proposed approach of scaling. The following conclusions can be drawn from the simulation results:

- The numerical framework used in this study is prone to artificial velocities at the interface due to an imbalance in forces;
- Increasing mesh resolution only increases the spurious currents;
- Spurious currents are significantly reduced when the density ratios and viscosity ratios are small;
- Using the proposed scaling approach is advantageous with respect to decreasing spurious currents.
### 6.1 Effect of Scaling Approach on Spurious Currents

**Table 6.3** Maximum and mean velocity magnitudes during evolution of interface for a liquid drop/bubble

| Case # | time\( (t) \) | \( |v_{max}| \) \( (m/s) \) | \( |v_{mean}| \) \( (m/s) \) |
|--------|----------------|--------------------------|--------------------------|
| 4      | 4.0            | 9.3768e-5                | 5.1456e-5                |
|        | 4.2            | 9.1319e-5                | 4.9935e-5                |
|        | 4.4            | 8.7449e-5                | 4.7587e-5                |
|        | 4.6            | 8.4536e-5                | 4.5852e-5                |
|        | 4.8            | 8.2501e-5                | 4.4224e-5                |
|        | 5.0            | 8.0932e-5                | 4.2690e-5                |
| 5      | 4.0            | 9.7548e-5                | 5.3527e-5                |
|        | 4.2            | 9.4602e-5                | 5.1471e-5                |
|        | 4.4            | 9.1677e-5                | 4.9526e-5                |
|        | 4.6            | 8.9473e-5                | 4.7686e-5                |
|        | 4.8            | 8.7296e-5                | 4.5941e-5                |
|        | 5.0            | 8.5144e-5                | 4.4286e-5                |
| 6      | 4.0            | 10.540e-5                | 5.5827e-5                |
|        | 4.2            | 10.280e-5                | 5.3557e-5                |
|        | 4.4            | 10.018e-5                | 5.1403e-5                |
|        | 4.6            | 9.7564e-5                | 4.9366e-5                |
|        | 4.8            | 9.4981e-5                | 4.7427e-5                |
|        | 5.0            | 9.2453e-5                | 4.5580e-5                |
6.1 Effect of Scaling Approach on Spurious Currents

6.1.4 Closure

We have now described how the proposed scaling approach helps reduce spurious currents. In the next section, we describe applying the proposed scaling approach to simulate the canonical problem, i.e., the rotating cylinder at an interface, and present the numerical results obtained.
Chapter 7

Interface Rupture Simulations

In this chapter, we describe the simulation of the canonical configuration of the rotating cylinder placed centrally at the interface between two fluids. As described in Chapter 5, Lorenceau et al. (2003) use the same configuration to identify the scaling of the physics which involved the critical capillary number, $Ca_c$, and the viscosity ratio, $\frac{\rho_0}{\eta}$. Chapter 5 provided a detailed description of the rotating-cylinder configuration and the associated scaling of physics. This chapter describes using the scaling approach to simulate the flow field for the rotating-cylinder configuration, and the results thus obtained. The chapter also discusses the applicability of this approach to the original problem with air as the entrained fluid.

7.1 Canonical Problem: Rotating Cylinder at an Interface

The rotating-cylinder problem [Fig. 7.1] consists of a cylinder placed centrally at an interface between two fluids. The radius of the cylinder is $R = 2 \text{ cm}$. The heavier fluid (Fluid 1) is a liquid with density $\rho$, and dynamic viscosity $\eta$. The lighter fluid
7.1 Canonical Problem: Rotating Cylinder at an Interface

(Fluid 2) is either air, or a lighter liquid, with density $\rho_0$, and dynamic viscosity $\eta_0$. The interfacial tension between the two fluids is denoted by $\sigma$. As the cylinder rotates clockwise, the heavier fluid is dragged by the cylinder on one side, and is plunged into itself on the other side, and the interface develops a cusp-like shape. As the rotational speed of the cylinder increases, the interfacial cusp becomes sharper, and at a critical velocity, the cusp breaks, since the interfacial-tension forces are no longer adequate to keep the interface from rupturing. When interface rupture occurs, a thin film of the lighter fluid is entrained into the heavier fluid. At this critical velocity, denoted by $V_c$, entrainment inception is said to have occurred. The aim of our simulations is to capture the inception of entrainment, and from the simulation results, elicit the critical conditions at which entrainment inception occurs.

![Figure 7.1 Schematic of rotating cylinder at an interface between two fluids](image)

Next, we list the specific objectives to be achieved for establishing the critical entrainment conditions for a particular liquid of interest.
7.1 Canonical Problem: Rotating Cylinder at an Interface

7.1.1 Specific Objectives

1. Create a computational domain, and generate appropriate meshes to simulate interface rupture (inception of entrainment).

2. Select the lower/heavier liquid whose interface rupture characteristics are of interest. In this work, we consider Aqueous Glycerol to be the liquid of interest. Denote the viscosity of this liquid as \( \eta \).

3. Select different viscosity ratios, \( \frac{\eta_0}{\eta} \), and calculate the corresponding viscosities of the entrained lighter fluid. In the present work, Silicon Oil is chosen as the lighter fluid which is entrained. Silicon Oil’s viscosity can be varied without affecting its other fluid properties like density and interfacial tension with Aqueous Glycerol. Table 7.1 shows the viscosity ratios used in the study.

<table>
<thead>
<tr>
<th>Case #</th>
<th>( \eta_0/\eta )</th>
<th>( \eta ) (Aqueous Glycerol)</th>
<th>( \eta_0 ) (Silicon Oil)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.1</td>
<td>900 mPas</td>
<td>90 mPas</td>
</tr>
<tr>
<td>2</td>
<td>0.2</td>
<td>900 mPas</td>
<td>180 mPas</td>
</tr>
<tr>
<td>3</td>
<td>0.4</td>
<td>900 mPas</td>
<td>360 mPas</td>
</tr>
<tr>
<td>4</td>
<td>0.9</td>
<td>900 mPas</td>
<td>810 mPas</td>
</tr>
</tbody>
</table>

4. Perform the simulations and record the conditions at which the interface ruptures for the cases corresponding to the viscosity ratios listed in Table 7.1.

5. Plot the simulation results for critical capillary number, \( Ca_c \) vs. viscosity ratio, \( \frac{\eta_0}{\eta} \), and compare with experimental data of Lorenceau et al. (2003) shown in Fig. 7.2.

The following sections describe the work done to achieve these objectives.
7.1 Canonical Problem: Rotating Cylinder at an Interface

7.1.2 Computational Domain and Mesh Generation

Modeling and simulation involves isolating a pertinent domain of interest, and modeling the physics within this domain. The choice of domain extent depends on the phenomenon of interest. For example, in the case of weather prediction, domain sizes extend to many miles. On the other hand, interface rupture occurs at a much smaller scale: at least microns in the case where air is entrained, and at most millimeters in cases where lighter liquids are entrained. The computational domain constructed to simulate interface rupture is as shown in Fig. 7.3. The radius of the rotating cylinder, \( R \), is 2 cm (as in Lorenceau et al. (2003)’s experimental set up). In Fig. 7.3, regions marked Region 1, Region 2, and Region 3 comprise the total computational domain constructed for this problem. The outer bound of the domain is chosen such that it is far enough from the expected point of interface rupture so as to have minimal effect on the phenomenon.

For a description of the physical domain, consider a container with a cylinder

![Figure 7.2 Scaling of physics using capillary number, \( Ca_c \), and viscosity ratio, \( \frac{\eta_0}{\eta} \) (Lorenceau et al., 2003)
at the center. In the container, the heavier liquid is poured in until it reaches the midplane of the rotating cylinder. The rest of the container is occupied by either air, or is filled with a lighter liquid. The top of the container is open to the atmosphere.

The shape of the outer boundary of the constructed computational domain also requires justification. We initially considered a square domain. This led to some skewed cells due to the transition from a polar, cylinder-aligned grid in the vicinity of the cylinder to a Cartesian mesh in the outer region of the square domain. Skewness affects quality of the numerical solutions and stability of the solution process. Hence, we aimed to limit changes in mesh topography in regions that might include the interface as the flow field evolves. Therefore, the outer boundary is constructed to be circular, except for a 60 degree segment near the top (Region 3 in Fig. 7.3) where interface rupture is not expected to occur. The outer boundary of the 60 degree segment is a straight line since liquid surfaces tend to orient themselves in the least
energy configurations, which, in this case, would be a plane.

The mesh generation process involves decomposing the computational domain into cells or control volumes. As described in Section 2.2.2, this process is needed for discretizing the governing partial differential equations. The mesh generation process is guided by the resolution required, and the resolution required depends on the physics we want to capture. In the present work, the smallest length scale that the meshes need to capture is the radius of curvature of the interfacial cusp [Fig. 7.4 a.]. Lorenceau et al. (2003) have presented the experimentally measured values of the radius of curvature as a function of the capillary number [Fig. 7.4 b.].

$$r = 993e^{-1.91Ca}$$

Equation (7.1) represents the empirical relationship they obtained using an exponential fit. The minimum resolution required for each case listed in Table 7.1 can then be estimated by using the cusp radius of curvature for the expected experimentally determined critical capillary number, $Ca_c$. For a viscosity ratio of 0.1, the experimentally determined $Ca_c$ is approximately 1.14 [from Fig. 7.2]. Higher the capillary number, smaller the radius of curvature. Also, as Fig. 7.2 shows, $Ca_c$ is larger for smaller values of viscosity ratio $\frac{\nu_1}{\eta}$. Hence, we estimate the resolution required for the most restrictive case ($\frac{\nu_1}{\eta} = 0.1$) in Table 7.1, and use the same mesh resolution for the other lesser restrictive cases ($\frac{\nu_1}{\eta} = 0.2$, $\frac{\nu_1}{\eta} = 0.4$, and $\frac{\nu_1}{\eta} = 0.9$). The corresponding smallest radius of curvature calculated using Eq. (7.1) is 150 microns. For the mesh to capture this curvature, the minimum resolution needs to be smaller than 150 microns. All the meshes used in this study are uniform meshes, that is, the whole computational domain has approximately the same resolution. Table 7.2 shows the mesh resolutions used in this study. For Case 1, two finer meshes are also employed to ascertain how the mesh resolution affects the solution. If the solution does not
Figure 7.4 Interfacial cusp; a. photograph of an experimentally observed interfacial cusp (white line denotes 200 microns), b. variation of radius of curvature of interfacial cusp with capillary number; adapted from Lorenceau et al. (2003)
7.1 Canonical Problem: Rotating Cylinder at an Interface

Table 7.2 Resolution of the computational domain for the four cases studied

<table>
<thead>
<tr>
<th>Case #</th>
<th>Viscosity ratio ((\eta_1/\eta_2))</th>
<th>Mesh Resolution</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.1</td>
<td>100 microns</td>
</tr>
<tr>
<td></td>
<td></td>
<td>75 microns</td>
</tr>
<tr>
<td></td>
<td></td>
<td>50 microns</td>
</tr>
<tr>
<td>2</td>
<td>0.2</td>
<td>100 microns</td>
</tr>
<tr>
<td>3</td>
<td>0.4</td>
<td>100 microns</td>
</tr>
<tr>
<td>4</td>
<td>0.9</td>
<td>100 microns</td>
</tr>
</tbody>
</table>

change significantly due to changing mesh resolution for this case, confidence can be placed in using the coarsest mesh resolution of the most restrictive case for the other cases as well.

The meshes constructed are multi-block and structured. Region 1, Region 2 and Region 3 represent the blocks of the mesh [Fig. 7.5]. Region 1 and Region 2 use polar meshes, while Region 3 uses a Cartesian mesh.

The next section describes the boundary conditions and flow-field initialization employed in this study.

7.1.3 Boundary Conditions and Initialization

The governing equations to be solved are partial differential equations. To obtain a unique solution, physically pertinent boundary and initial conditions need to be applied. These are described next.

- Container: The container is a solid-wall boundary. The normal velocity component at the wall is zero since the wall is non-porous. Also, since the fluids are viscous, the tangential component of velocity at the wall is zero. Since there is
7.1 Canonical Problem: Rotating Cylinder at an Interface

![Figure 7.5 Mesh topology employed; Regions 1 and 2: polar meshes, Region 3: Cartesian mesh](image)

Figure 7.5 Mesh topology employed; Regions 1 and 2: polar meshes, Region 3: Cartesian mesh

no flux through the wall, the normal pressure gradient is set to zero. In this study, we ignore the surface-tension effects between the fluids and the wall by assuming a contact angle of 90 degrees. A 90 degree contact angle corresponds to prescribing a zero normal-gradient of volume fraction.

- Cylinder: The cylinder is a rotating wall. The center of rotation and the angular velocity are specified. An internal calculation within the solver provides the Cartesian velocity components at each boundary cell of the rotating cylinder. As with the static wall, the normal pressure gradient is zero, and the normal gradient of volume fraction is also set to zero.

- Atmosphere: The container is open to the atmosphere.

Initialization: In a time-dependent problem, the solution process requires the flow variables to be specified at time \( t = 0 \), everywhere in the computational domain.
The domain is initialized as shown in Fig. 7.6. Fluid 1 occupies the lower half of the container and a small circular region around the cylinder. The remainder of the container is occupied by Fluid 2. The small circular region around the cylinder filled with Fluid 1 is aphysical, but deliberate. This initialization alleviates issues of contact angle at the cylinder surface. For correct interpretation of our results, we remove the effect of the initialization by running the simulation for an appropriate period of time at a constant, low, angular velocity of the cylinder until the interface reaches a steady, physically accurate position. The angular velocity of the cylinder is then increased until the interface ruptures.

In the following section, we describe the results obtained from our simulations.

7.1.4 Simulation Results

Interface rupture and subsequent entrainment occurs when particular conditions persist in the flow. As the rotational velocity of the cylinder is increased, the plunging jet velocity, $V_j$, reaches a critical velocity $V_c$. When $V_j = V_c$, interface rupture occurs.
Subsequently, a thin film of the lighter fluid (air/lighter oils) is entrained into the heavier liquid. The time-varying rotational-velocity profile prescribed at the cylinder wall is shown in Fig. 7.7. From simulations results, we obtain values of \( V_j \) and values for depth of penetration of the interfacial cusp, \( L \). Both \( V_j \) and \( L \) increase with an increase in rotational velocity of the cylinder.

We require a method to determine the exact conditions at which interface rupture occurs. This is done by plotting \( L \) versus \( V_j \). An example plot constructed using simulation results pertaining to one of the cases considered in this study (Case 4) is shown in Fig. 7.8. As the rotational velocity is increased in a linear manner, we observe a fairly linear relationship between \( L \) and \( V_j \) until a particular value of \( V_j \) is reached. Beyond this value, \( L \) increases in a highly non-linear fashion with respect to \( V_j \). In this study, we define the value of \( V_j \) at the point where the transition to non-linearity occurs as the critical entrainment velocity, \( V_c \). The corresponding critical capillary numbers, \( Ca_c \), are calculated based on \( V_c \) values thus obtained.

**Figure 7.7** Time variation for rotational speed of cylinder
Having described the method to identify the point at which the interface ruptures, we now proceed to evaluate dependence of the simulation results on mesh resolution. Following the mesh independence study, we validate our simulation results against experimental data. Mesh independence and validation are crucial to establish confidence in, and accuracy of, our numerical simulations.

**Mesh Dependence**

In this section, we present results for how the different mesh resolutions used affect the solution. We carry out simulations of the case corresponding to $\eta_0/\eta = 0.1$ with different mesh resolutions - Mesh 1 uses a resolution of 100 microns, Mesh 2 corresponds to 75 micron resolution, and Mesh 3 to 50 micron resolution.

Comparing the results obtained using different mesh resolutions [Fig. 7.9, Fig. 7.10, and Fig. 7.11] for the case corresponding to $\eta_0/\eta = 0.1$, we find that, as long as the
7.1 Canonical Problem: Rotating Cylinder at an Interface

![Graph of L vs time](image1)

**Figure 7.9** Depth of penetration, $L$ as a function of time, $t$

![Graph of $V_j$ vs time](image2)

**Figure 7.10** Plunging jet velocity, $V_j$, as a function of time, $t$
7.1 Canonical Problem: Rotating Cylinder at an Interface

Figure 7.11 Depth of penetration, \( L \), as a function of plunging jet velocity, \( V_j \)

Table 7.3 Mean differences in critical entrainment velocity between different meshes

<table>
<thead>
<tr>
<th></th>
<th>Mesh 2 vs. Mesh 1</th>
<th>Mesh 3 vs. Mesh 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean % difference in ( V_c )</td>
<td>1.0202</td>
<td>0.9639</td>
</tr>
</tbody>
</table>

smallest length scale is resolved (the radius of curvature of the interfacial cusp) by the coarsest mesh employed, results deviate in the mean by about 1%.

Validation using available Experimental Data

Experimental data for the critical capillary numbers, \( Ca_c \), for interfacial rupture as observed in the rotating-cylinder configuration has been published by Lorenceau et al. (2003). Liquid properties used in the simulations correspond to Aqueous Glycerol as the heavier liquid and Silicon Oil as the lighter oil (as in the experiments). The simulations correspond to \( \eta_0/\eta = 0.1, 0.2, 0.4, \) and 0.9. Lorenceau et al. (2003) observed
that their experimental data points straddled a semilogarithmic fit, with a slope of -0.22. We extrapolate this semilogarithmic fit to $\eta_0/\eta = 1$, and compare critical capillary numbers, $Ca_c$, from simulation results to those obtained from extrapolation of the experimental correlation.

Table 7.4 $V_c$ and $Ca_c$ from simulation results, and deviation of $Ca_c$ from extrapolated experimental correlation

<table>
<thead>
<tr>
<th>$\frac{\eta_0}{\eta}$</th>
<th>$V_c$ (m/s)</th>
<th>$Ca_c$</th>
<th>%Deviation of $Ca_c$ from exp. correlation</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.03468</td>
<td>1.20060</td>
<td>0.06586</td>
</tr>
<tr>
<td>0.2</td>
<td>0.02971</td>
<td>1.02825</td>
<td>0.58556</td>
</tr>
<tr>
<td>0.4</td>
<td>0.02680</td>
<td>0.92773</td>
<td>6.97776</td>
</tr>
<tr>
<td>0.9</td>
<td>0.01917</td>
<td>0.66351</td>
<td>4.07893</td>
</tr>
</tbody>
</table>

Table 7.4 shows the deviation of $Ca_c$ predicted by our simulations from the extrapolated experimental correlation. We observe a maximum deviation of less than 10%. It is interesting to note that at the lower viscosity ratios ($\eta_0/\eta = 0.1$ and $\eta_0/\eta = 0.2$), the deviations from the experimental correlation are at least ten times smaller than those seen at the higher viscosity ratios ($\eta_0/\eta = 0.4$ and $\eta_0/\eta = 0.9$). The higher deviation may be due to a transition to a different scaling regime where other forces might become pertinent. Indeed, in the following section, we present evidence that suggests buoyancy effects begin to dominate as viscosity ratios, $\eta_0/\eta$, increase.

So far in this section, we established two important aspects of our numerical study - mesh independence and validation using available experimental data. The simulation results provided us with critical capillary numbers, $Ca_c$, for each viscosity ratio, $\eta_0/\eta$. While the viscosities of the two liquids and the interfacial tension between the liquids are incorporated into the scaling ($Ca_c = \eta V_c/\sigma$ vs. $\eta_0/\eta$), densities of the
two liquids are not. In the next section, we investigate the effect of densities of the two liquids on the critical interfacial-rupture/entrainment-inception conditions.

### 7.2 Exploring Effect of Densities

In the scaling of the flow physics, we considered the variation between the critical capillary number, \( Ca_c = \frac{\eta V}{\sigma} \), and the viscosity ratio, \( \frac{\eta_0}{\eta} \). The densities of the two fluids do not feature in the scaling. In order to investigate the effect of densities on the entrainment inception conditions, we performed simulations with different upper liquids at two different viscosity ratios. The role densities play in the physics of entrainment inception is through their difference, \( \Delta \rho \), which accounts for buoyancy force. For a particular depth of immersion, \( L \), of the interfacial cusp [see Fig. 5.1], greater the difference, \( \Delta \rho \), greater the buoyancy force. Buoyancy acts to suppress the immersion of the interfacial cusp, thereby suppressing entrainment inception. In order
7.2 Exploring Effect of Densities

Table 7.5 \( \eta_0 = 0.1; \rho = 1120 kg/m^3; \sigma = 0.026 N/m \)

<table>
<thead>
<tr>
<th>( \rho_0 ) (kg/m(^3))</th>
<th>( \Delta \rho )</th>
<th>( V_c ) (m/s)</th>
<th>( L_c ) (mm)</th>
<th>( Ca_c )</th>
<th>( Bo_c = \frac{\Delta \rho g L_c^2}{\sigma} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>980</td>
<td>140</td>
<td>0.03209</td>
<td>7.5895</td>
<td>1.11081</td>
<td>3.04264</td>
</tr>
<tr>
<td>840</td>
<td>280</td>
<td>0.03076</td>
<td>5.1662</td>
<td>1.06477</td>
<td>2.81966</td>
</tr>
<tr>
<td>560</td>
<td>560</td>
<td>0.02959</td>
<td>3.5142</td>
<td>1.02427</td>
<td>2.60938</td>
</tr>
</tbody>
</table>

Table 7.6 \( \eta_0 = 0.9; \rho = 1120 kg/m^3; \sigma = 0.026 N/m \)

<table>
<thead>
<tr>
<th>( \rho_0 ) (kg/m(^3))</th>
<th>( \Delta \rho )</th>
<th>( V_c ) (m/s)</th>
<th>( L_c ) (mm)</th>
<th>( Ca_c )</th>
<th>( Bo_c = \frac{\Delta \rho g L_c^2}{\sigma} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>980</td>
<td>140</td>
<td>0.01869</td>
<td>11.4632</td>
<td>0.64696</td>
<td>6.94121</td>
</tr>
<tr>
<td>840</td>
<td>280</td>
<td>0.02001</td>
<td>7.9941</td>
<td>0.69265</td>
<td>6.75138</td>
</tr>
<tr>
<td>560</td>
<td>560</td>
<td>0.02084</td>
<td>4.8389</td>
<td>0.72138</td>
<td>4.94740</td>
</tr>
</tbody>
</table>

to ascertain the effect of buoyancy force in relation to other forces, we calculated a Bond number along with the capillary number at conditions of entrainment inception. The Bond number is the ratio of buoyancy force and surface-tension force, and is defined as \( \frac{\Delta \rho g L_c^2}{\sigma} \). Results from our simulations are collated in Table 7.5 and Table 7.6 for the viscosity ratios 0.1 and 0.9, respectively, and the observations inferred from these results are summarized next.

Observations

- Within the results for both viscosity-ratio cases, we observe that, as \( \Delta \rho \) increases, the critical cusp-immersion depth, \( L_c \), decreases.

- Again, for both viscosity-ratio cases, as \( \Delta \rho \) increases, the critical Bond number, \( Bo_c = \frac{\Delta \rho g L_c^2}{\sigma} \), decreases. The decrease in \( L_c \) supersedes the effect of increasing \( \Delta \rho \). This is counter-intuitive.
7.2 Exploring Effect of Densities

Figure 7.13 Effect of density on critical entrainment inception conditions

- Now, comparing between the two viscosity-ratio cases, $Bo_c$ is observed to decrease for each corresponding $\Delta \rho$ as the viscosity-ratio value decreases. Hence, when the viscosity ratio will be decreased to that corresponding to air being the entrained fluid, the effect of buoyancy is expected to decrease. Amongst buoyancy, viscous, and surface-tension forces, the dominant forces affecting inception of entrainment will then be viscous and surface-tension forces.

- We also observe a reversal in the trend of $Ca_c$ with respect to $\Delta \rho$ about $Ca = 1$ [Fig. 7.13]. This might be an indication that, for higher viscosity ratios, e.g., 0.9, where the expected $Ca_c$ is smaller than 1, buoyancy starts to play a role in the balance of forces at the interfacial cusp.

In this section, we expounded the role of densities in the rupture of the interface between the two immiscible fluids. In the next section, we explore the existence of empirical extrapolations of critical interface-rupture conditions from the rotating-cylinder configuration to the plunging-jet configuration.
7.3 From Rotating-Cylinder Configuration to Plunging-Jet Configuration

Both the rotating-cylinder and the plunging-jet configurations involve a plunging jet of liquid impinging upon a pool of the same liquid. The rotating-cylinder configuration is two-dimensional, and the forcing mechanism for entrainment inception is a rotating cylinder placed centrally at an interface between two fluids. In contrast, the plunging-jet configuration is three-dimensional, and the forcing mechanism for entrainment to occur is the core of a liquid jet [Fig. 7.14]. In this section, we explore connections between the two configurations as pertaining to interface rupture and entrainment.

The rotating-cylinder simulations conducted for validation against experimental data were for a liquid with a viscosity of 0.9 Pas. Lin & Donnelly (1966)’s plunging-jet results did not include a liquid with a viscosity of 0.9 Pas. Hence, additional rotating-cylinder simulations (see Table 7.7) were conducted using liquids having viscosities of 0.4 Pas, 0.2 Pas, and 0.1 Pas, so that a comparison can be made between the
7.3 From Rotating-Cylinder Configuration to Plunging-Jet Configuration

Table 7.7 Additional simulation cases: for liquids with $\eta = 0.4, 0.2, 0.1\text{Pas}$

<table>
<thead>
<tr>
<th>Case #</th>
<th>$\eta_0/\eta$</th>
<th>$\eta$ (Aqueous Glycerol)</th>
<th>$\eta_0$ (Silicon Oil)</th>
<th>$Ca_c$ from simulations</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.1</td>
<td>400 mPas</td>
<td>40 mPas</td>
<td>0.907112</td>
</tr>
<tr>
<td>2</td>
<td>0.4</td>
<td>400 mPas</td>
<td>160 mPas</td>
<td>0.775898</td>
</tr>
<tr>
<td>3</td>
<td>0.9</td>
<td>400 mPas</td>
<td>360 mPas</td>
<td>0.71739</td>
</tr>
<tr>
<td>4</td>
<td>0.1</td>
<td>200 mPas</td>
<td>20 mPas</td>
<td>0.660851</td>
</tr>
<tr>
<td>5</td>
<td>0.4</td>
<td>200 mPas</td>
<td>80 mPas</td>
<td>0.561227</td>
</tr>
<tr>
<td>6</td>
<td>0.9</td>
<td>200 mPas</td>
<td>180 mPas</td>
<td>0.458983</td>
</tr>
<tr>
<td>7</td>
<td>0.1</td>
<td>100 mPas</td>
<td>10 mPas</td>
<td>0.400736</td>
</tr>
<tr>
<td>8</td>
<td>0.4</td>
<td>100 mPas</td>
<td>40 mPas</td>
<td>0.37459</td>
</tr>
<tr>
<td>9</td>
<td>0.9</td>
<td>100 mPas</td>
<td>90 mPas</td>
<td>0.354217</td>
</tr>
</tbody>
</table>

entrainment inception seen in the rotating-cylinder configuration and the plunging-jet configuration. Critical capillary numbers determined from our simulation results for each viscosity ratio are listed in Table 7.7. Inferences drawn from our results are discussed next.

Observations

- The critical capillary number is different for different liquids at the same viscosity ratio. Plotting the simulation results, and extrapolating to Lin & Donnelly (1966)'s plunging-jet data, we find a power-law correlation between the critical Capillary number, $Ca_c$ and viscosity ratio, $\eta_0/\eta$ for each liquid [Fig. 7.15].

- The correlation is of the following form:

$$Ca_c = m\left(\frac{\eta_0}{\eta}\right)^{-n},$$

where $m$ and $n$ for each liquid are given in the following in Table 7.8.

(7.2)
7.3 From Rotating-Cylinder Configuration to Plunging-Jet Configuration

Figure 7.15 Comparison of entrainment inception conditions for present rotating-cylinder configuration simulations with Lin & Donnelly (1966)’s plunging-jet data

Table 7.8 Values of regression parameters - m and n for each liquid

<table>
<thead>
<tr>
<th>η</th>
<th>m</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>0.6388</td>
<td>0.207</td>
</tr>
<tr>
<td>0.2</td>
<td>0.4359</td>
<td>0.222</td>
</tr>
<tr>
<td>0.1</td>
<td>0.2862</td>
<td>0.268</td>
</tr>
</tbody>
</table>
7.4 Conclusions

- As the viscosity ratio, $\eta_0/\eta$, decreases, we believe that inertial effects start to play a role in the force balance at the inception of entrainment. The curves seem like they would collapse onto one curve given the right scaling parameters, although an exact scaling has eluded us until now.

We have shown that we can extrapolate entrainment inception conditions from the rotating-cylinder configuration to the plunging-jet configuration using a power law of the form, $Ca_c = m(\frac{\eta}{\eta_0})^{-n}$.

In the following sections, we present our conclusions and provide closure to the present chapter.

7.4 Conclusions

In this Chapter, we presented details of our numerical investigation of interface rupture and subsequent entrainment using the canonical problem of a rotating cylinder placed centrally at the interface of two fluids. A mesh-independence study was conducted using three different mesh resolutions, followed by validation using available experimental data. Since densities of the two fluids do not explicitly feature in the scaling ($Ca_c$ vs. $\eta_0/\eta$), we conducted simulations to elicit the role that densities play on interfacial rupture. Finally, used results from the scaling approach to extrapolate the results from the two-dimensional rotating-cylinder configuration with a liquid as the entrained fluid to the three-dimensional plunging-jet configuration with air as the entrained fluid. Following are the highlights:

- Rotating-cylinder configuration
  - We established a method to identify the exact conditions at which interface rupture occurs by plotting the depth of immersion, $L$, as a function of
7.4 Conclusions

plunging-jet velocity, $V_j$ (see Fig. 7.8). The point at which the curve of $L$ vs. $V_j$ departs from linearity is considered as the point at which the interface ruptures. The corresponding velocity is the critical velocity, $V_c$. The critical capillary number, $Ca_c$ is calculated as $Ca_c = \frac{\eta V_c}{\sigma}$.

- The mesh-independence study indicated that, as long as the radius of curvature of the interfacial cusp is resolved, the difference in mean results across the three mesh resolutions employed was about 1%, and decreased with increased mesh resolution. This was encouraging, particularly considering the complexity of the problem - a time-dependent two-fluid system with a rotating wall.

- Validation: the simulation results compared well with experimental data. We simulated interfacial rupture for four different values of $\eta_0/\eta$, and recorded the critical $Ca_c$ values. At $\eta_0/\eta = 0.1$ (this corresponds to an experimental data point) the deviation of the simulation result from the experimental value was 0.066%. At $\eta_0/\eta = 0.2, 0.4, 0.9$, we compared simulation results to values arrived at by extrapolation using the experimental correlation provided by Lorenceau *et al.* (2003). While the simulation results were within 7% of the extrapolated values, we found evidence to suggest that, at higher viscosity ratios, buoyancy forces start to play a major role in the force balance. Hence, at higher viscosity ratios, we believe the physics scales differently. The effect of buoyancy on interfacial rupture was brought to light by studying the effect of densities of the two fluids was studied.

- Effect of densities on interface rupture

  - The effect of densities of the two fluids that form an interface manifests
itself as buoyancy force. Buoyancy is proportional to the difference in densities, $\Delta \rho$, and serves as an additional force, along with interfacial tension, to preserve the integrity of the interface, and delays rupture.

- From our simulations, we found that increasing $\Delta \rho$ led to a decrease in $L_c$, the critical depth of cusp-immersion at which rupture occurs, $L_c$ (see Tables 7.5 and 7.6).

- The calculated critical Bond numbers, $Bo_c = \frac{\Delta \rho g L_c^2}{\sigma}$, gave us an idea of the relative strength of the buoyancy force compared to interfacial-tension force. It is interesting to note that as $\Delta \rho$ increased, $Bo$ decreased. This fact was counter-intuitive prior to recording our simulation results for $L_c$. The decrease in $L_c$ causes $Bo$ to decrease, despite an increase in $\Delta \rho$. Hence, when increasingly lighter fluids were being entrained, the effect of buoyancy force was seen to decrease.

- At higher values of $\eta_0/\eta$, we found an increase in $Bo$ (comparing $Bo$ values across Tables 7.5 and 7.6). The increase in $Bo$ suggests that buoyancy starts to play a greater role in the force balance at the point of interface rupture. We believe this is evidence of a different scaling regime at higher viscosity ratios.

- From rotating-cylinder configuration to plunging-jet configuration

  - Using a power-law relation of the form, $Ca_c = m\left(\frac{\eta_0}{\eta}\right)^{-n}$, we have shown that we can extrapolate entrainment inception conditions from the rotating-cylinder configuration to the plunging-jet configuration.
7.5 Closure

In this chapter, we have demonstrated the feasibility of using the scaling approach to capture interface rupture and entrainment inception. The effect of mesh resolution on the solution is studied first, and we have shown that, for the case corresponding to a viscosity ratio of 0.1 (which is the most restrictive case with respect to mesh resolution required), the results compare well, with a mean deviation of about 1% across the meshes. Further, results obtained are within 7% of experimental data. We then proceeded to study the effect of densities of the two fluids on interface rupture and entrainment inception. Following this, we explored extrapolating our results to predict critical entrainment inception conditions for the plunging-jet configuration.

In the next chapter, we summarize the present study, and discuss avenues for future work.
Chapter 8

Summary and Future Direction

In this chapter, we summarize our work, and present avenues for future investigation.

8.1 Summary

• In the present study, we aimed to accurately ascertain critical interfacial-rupture and entrainment conditions for laminar plunging jets, and capture the inception of entrainment using numerical simulations. We use a Volume-Of-Fluid method (VOF) to carry out the two-fluid computations.

• The direct approach is fraught with numerical challenges arising from the physics of the problem. We identify the challenges from the results of our simulations. A key challenge is the range of length scales involved that is required to be resolved. Typically, the length scales range from microns to a few hundred millimeters. Resolution of these length scales in the numerical simulations led to large computational meshes, and in addition, since the maximum resolution is of order of microns, led to prohibitively small time-step values while computing the time-evolving flow field.
A new approach that addresses the challenges identified is then proposed. The approach relies on scaling of the underlying physics. Specifically, the approach involved considering liquids as entrained fluids instead of air. Using liquids as the entrained fluids significantly reduced the range of length scales, and hence, the mesh resolution required to capture interface rupture and entrainment. This reduction in required mesh resolution resulted in higher minimum time-step values for stable computations. Further, this approach was tested using a two-dimensional geometry - a rotating cylinder placed centrally at the interface between two liquids. Hence, using the scaling approach, capturing interface rupture and subsequent entrainment using numerical simulations was now tractable.

A key limiting property of VOF methods is the propensity of these methods to produce spurious/parasitic currents. Spurious currents are numerical artifacts that destroy the integrity of the interface, and lead to unstable computations. We have shown that, as a consequence of using the scaling approach, spurious currents were reduced by two orders of magnitude, which further helped with stability of our computations at higher time-step values.

Simulation results (mesh independence and validation with experimental data) for the rotating-cylinder configuration demonstrated the viability of using the proposed scaling approach.

We also undertook an investigation into the effect of the densities of the two fluids in contact on interface rupture. The effect of densities on the flow field was through buoyancy. Buoyancy is a function of the difference of densities of the two fluids. In the case of the plunging jet, buoyancy, like interfacial tension, is a force that helps impede interface rupture and entrainment. We
8.2 Future Direction

found that the effect of buoyancy (and in turn, the effect of densities) reduces (in comparison to viscous and interfacial tension) as the fluid being entrained becomes lighter and less viscous.

• Finally, we used the critical conditions predicted for the rotating-cylinder configuration (two-dimensional geometry with liquids being entrained) to extrapolate to the critical conditions for a plunging-jet configuration (three-dimensional geometry with air being entrained) with the same liquids for the jet. For each liquid that formed the jet, we found a power-law correlation that fit the critical entrainment conditions across geometrical configurations and across the fluids (lighter liquids/air) being entrained.

8.2 Future Direction

• In the industry, a number of products (shampoo, conditioner, liquid detergent, etc.) involve Non-Newtonian liquids. Understanding filling properties and conditions at which these liquids entrain surrounding fluid is of critical importance. The present work sets the stage for future numerical simulations to predict entrainment conditions for Non-Newtonian liquid plunging jets.

• A similar scaling approach could be potentially beneficial in simulating other flow configurations that present similar ranges of physical length scales. A case in point is the crown splash problem, where a drop of liquid falls onto a thin layer of the same liquid causing a splash. The splash is associated with thin sheets being ejected radially, and forming secondary droplets [Fig. 8.1]. In the literature, researchers have suggested different mechanisms including the Rayleigh-Plateau instability, non-linear amplification, and Richtmyer-Meshkov instability as being responsible for the secondary-droplet formation (Zhang et al., 2010). Sim-
8.2 Future Direction

Simulations using a similar scaling approach as presented in our work may provide further insight into the process.

Figure 8.1 Experimental photograph of a silicon oil crown splash; the 1 mm bar at the bottom right of the picture puts the length scales involved into perspective. (Zhang et al., 2010)

- We have shown that it is possible to simulate complex flow fields using OpenFOAM. OpenFOAM is open-source, and hence, the user has complete access to the source code. The development of OpenFOAM has mirrored the development of Linux operating systems, in that, a number of people from across the world contribute to continuous enhancements. In addition to being open-source, OpenFOAM is free to download and use (no license fees). Further, OpenFOAM is massively parallelizable. These properties make OpenFOAM a very useful tool for research.

In order to utilize OpenFOAM to its full potential, but by using only open-
source software, a CAD software capable of generating STL (stereo lithography) files is required. We strongly believe Blender is one such software which is open source, free to download, and can create STL files. Blender is used by graphic design artists for animations, etc. Dr. Andrew King from Curtin University, Australia, has written a python code for Blender, so the user can export an STL file having given names to boundary faces which OpenFOAM will then recognize. Thus, one can use Blender for pre-processing → OpenFOAM for volume meshing (snappyHexMesh), and solution capability → Paraview for post-processing. This work flow is free and completely open-source, and the only costs involved are for hardware.

8.3 Final Remarks

A number of physical phenomena exhibit characteristics that challenge the prediction capability of state-of-the-art numerical methods. Interfacial rupture is one such phenomenon. Accurate numerical simulations of such phenomena are presently intractable, even with the massive increase in computational power over the last decade. With the present work, we have shown that elegant, novel approaches can be devised to study such problems using modeling and simulation by leveraging the prevailing physics of the problem.
Bibliography


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