ANALYTICAL, NUMERICAL, AND COMPUTATIONAL METHODS TO
ANALYZE THE TIME TO EMPTY OPEN, CLOSED, AND
VARIABLE-TOPPED INVERTED BOTTLES

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ABSTRACT

Analytical, Numerical, and Computational Methods to Analyze the Time to Empty Open, Closed, and Variable-Topped Inverted Bottles

Callen Schwefler

Recent unexpected experimental observations of the emptying of inverted bottles with perforations has generated interest in modeling and simulation of this phenomenon. It was observed that as a perforation, i.e., a small hole at the “top” of the inverted bottle, is added and enlarged, the overall emptying time first increases to a maximum value and then decreases until it reaches a lower limit. The change in emptying time is associated with a transition from jetting, where only water exits the neck, to glugging, a competition between air and water flows at the neck of the bottle.

This paper develops analytical and numerical models to predict emptying time and liquid height as a function of time which capture the jetting-to-glugging transition. When qualitatively compared to experimental data using a bottle with neck diameters of 12.7 mm, 25.4 mm, and 38.1 mm and bottle diameter of approximately 355 mm (equating to several hundred to several thousand seconds to drain) a favorable agreement is observed. These models attempt to explain the transition in terms of a competition between liquid and bubble velocities at the bottle neck and build on an existing model of glugging available in the literature.

The paper also explores the first steps taken toward simulation of bottle emptying using a commercial CFD package (Fluent) to simulate draining for a smaller bottle of neck diameter 21.6 mm and bottle diameter of 62.2 mm. The Fluent simulations are used to further elucidate the jetting-to-glugging transition mechanism by simulating emptying with and without perforations. CFD results reported are limited to a few select large perforation diameters. Specifically, a 4 mm perforation taking 15
hours to simulate and 6 mm perforation taking 5 hours to simulate. Despite the lengthy simulation times, both capture only the approximate 2 seconds required to drain the bottle, but demonstrate the effect of the perforation on emptying time. Smaller perforations on the order of 1 mm, which would align with the experimentally determined maximum emptying time would require unfeasibly long simulations for present resources as dictated by required low Courant numbers. Future work with greater computational capability will further expand upon the simulations conducted in this work.
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Chapter 1

INTRODUCTION

1.1 The Inverted Bottle

Fluid flow from an inverted bottle has long been a subject of interest in the field of fluid dynamics. The emptying of an inverted bottle, see Figure 1.1, is a noteworthy example of two-phase flow where the flows of air and water in the bottle system simultaneously interact with each other, often generating bubbles.

![Figure 1.1: Photographs of water emptying. (a) A sequence of images from the emptying event of an unmodified bottle (closed-topped when inverted as shown). (c) A sequence of images from the emptying event of a bottle with the bottom removed (open-topped when inverted as shown). Superpositions of the emptying events are visible in panels (b) and (d) for the respective emptying [1].](image)

The interaction of air and water at the outlet (i.e., the neck) of an inverted bottle as it drains presents interesting fluid phenomena for analysis. With something as simple as a bottle, and with basic modifications to the bottle, one can produce a surprising...
array of flow scenarios ranging from single-phase draining of a liquid to the remark-
able complexities of two-phase flows. With the appropriate bottle modifications as
will be explored in this work, this range of scenarios can be captured in a single em-
ptying event. As such, the study of emptying inverted bottles can provide novel and
fundamental observations of fluid flow that yield thought-provoking results.
1.2 Time to Empty

A commonly studied feature of fluid flow in an inverted bottle is the time for the liquid to empty from the bottle investigated by authors such as Clanet [2] and Whalley [3]. The time to empty can vary with properties of the liquid as well as geometry of the bottle. Height of the liquid within the bottle is typically the dominant geometry when considering the time to empty from a bottle, and furthermore, the height of the liquid is the time-varying quantity of interest during the emptying of a bottle of fixed dimensions. As such, it is appropriate to develop models of the time to empty with a focus on the height of the fluid within the bottle, see Figure 1.2.

![Diagram of a bottle with varying heights](image)

**Figure 1.2:** Varying height over time in an inverted open-topped bottle with translation to plot of time to empty. A similar sequence of heights is seen in photographs in Figure 1.1c.

Research and simulation of the time to empty an inverted bottle presents the opportunity to embrace the full slate of analysis challenges offered by the draining of the bottle. The viscous effects of the fluids as well as the glugging generated by two phases flowing counter to each other must be fully understood to generate a valid result. Much of the work presented here will explore how to simulate these effects to best represent the true behavior of the system.
1.3 Research Scope

The basis of this work was spawned by unexpected experimental results found when measuring the emptying time of an inverted bottle with a perforation in the top. It was observed by Morrisset that the time to empty an inverted bottle changed noticeably as a perforation was introduced into the top of the bottle with an increase and then decrease of time to empty as the perforation was incrementally enlarged [4]. Follow-up experiments by Mayer [5] confirmed these original findings; see Figure 1.3 for an example of recorded data.

![Figure 1.3: Mayer data showing the trend of time to empty changing as different sized perforations are used [5]. The bottle used had a volume of 0.063 m$^3$, bottle height of 635 mm, and neck diameter of 38.1 mm.](image)

A perforation generates a transition between the jetting regime, where only liquid exits the neck of the bottle, and the glugging regime, where a competition between liquid outflow and air inflow exists at the neck, see Figure 1.4. As the perforation size increases, the bottle approaches the behavior of an open-topped bottle. This
observation lays the foundation for this modeling research and the conclusions that are drawn from it.

![Flow regimes of inverted bottles](image)

**Figure 1.4:** Flow regimes of inverted bottles from the glugging, where liquid smoothly exits the bottle without bubble, of closed-topped bottles to the jetting, where liquid smoothly exits the bottle without bubble, of open-topped bottles.

This project develops analytical (single equation solution), numerical (equations solved at each simulation time step), and computational (numerical simulation using Navier-Stokes equations) methods to model how bottle emptying time will vary as a perforation is introduced at the top of the bottle and then increased in size. The goal of this project is to provide solutions of time to empty a bottle for various perforation diameters and to explain what we observe across different perforation diameters and the mechanism associated with the jetting-to-glugging transition. The time to empty an inverted bottle with a perforation has not yet been rigorously studied on a modeling level creating an opportunity to learn more about this phenomenon. The analytical work will use derived MATLAB models while the numerical work will use ANSYS Fluent to delve into the transient behavior of variable-topped inverted bottles.
Previous work pertaining to two-phase flow in inverted bottles and bubbles in tubes presents foundational ideas on the behavior of inverted bottle fluid flow. The following presents a comprehensive look at the work that most applies to the simulation and modeling efforts of this paper:

- Foundational Work on Bubble Rise and Bubble Initiation
  Single bubble rise behavior in tubes and inverted bottles is useful when considering the glugging regime. Particularly, once the bubble velocity is defined it will be explored as a metric to differentiate between glugging and jetting. The bubble velocity is found to noticeably change depending on the relevancy of surface tension and viscous effects [6].

- Observations on the Time to Empty
  Considerations for the time to empty single-outlet vessels along with height versus time data and the influence of shape are documented. The rate at which a glugging vessel empties is acknowledged to be constant by Clanet [2]. Recent work from Kumar who studied the drainage of tubes suggests that perforations will influence emptying time [7]. Kumar’s work reinforces the validity of experimental results that there is an interesting effect created by perforations in inverted bottles.

- CFD Research on Inverted Bottles
  Computational Fluid Dynamics (CFD) research has been used with bubble generation within the past 10 years to better capture the formation and mechanics
of multiple bubbles in water [8, 9]. Approaches for dealing with a complex two-phase flow interface and the proper modeling of bubble generation have been pursued as computational power expands and CFD codes develop in complexity.
2.1 Foundational Work on Bubble Rise and Bubble Initiation

Bubble rise is a useful metric for bottle emptying that can be used to determine if an emptying bottle is exhibiting glugging or jetting behavior. It is thought that the velocity of a rising bubble can be compared to the velocity of liquid outflow from a bottle, and if the bubble velocity is greater than outflow velocity the flow will exhibit glugging behavior. If the bubble velocity is smaller than the outflow velocity is thought that the flow will exhibit jetting behavior.

Early work completed by Davies and Taylor examined air bubbles as they rose through a vertical tube filled with liquid to understand the rise velocity of large bubbles [10]. With these sized bubbles, surface tension and viscous effects are minimal. In their work they developed an experimentally-validated theoretical relation for bubble rise speed in a tube, $U$, based upon the diameter of the tube, $d_1$, and gravity, $g$. When transformed into a dimensionless ratio, the value of this ratio was found to be 0.328 by theory; see Equation (2.1).

$$\frac{U}{\sqrt{gd_1}} = 0.328$$  \hspace{1cm} (2.1)

The dimensionless ratio also defines the bubble velocity coefficient, $k_1$. Notably, Davies and Taylor found that the bubble velocity coefficient was $\approx 0.28$ for a tube of diameter 12.3 mm (in contrast to 0.328 for larger tube diameters, e.g., 79 mm) indicating smaller sized tube diameters can generate different bubble velocities. The bubbles investigated by Davies and Taylor are similar to the first “glug” of an inverted bottle as compared in Figure 2.1(a) and Figure 2.1(b).
In comparison to the Davies and Taylor bubble velocity coefficient of 0.328, Du-
mitrescu found a coefficient of 0.351 and White and Beardmore found a coefficient of
0.345 [6]. However, as the tube or bubble diameter decrease (on the order of 20 mm
and below), viscous and surface tension effects can decrease the bubble velocity. The
bubble velocity coefficient can be approximated with all viscous and surface tension
considerations using the Eötvös, \(N_{\text{Eö}}\), number and dimensionless inverse viscosity,
\(N_f\), which are dependent on neck diameter, \(d_1\) [6]:

\[
k_1 = 0.345 \left( 1 - e^{-0.01N_f/0.345} \right) \left( 1 - e^{(3.37-N_{\text{Eö}})/m} \right).
\] (2.2)

The Eötvös number, \(N_{\text{Eö}}\), is a dimensionless number that relates the significance of
gravity, or buoyancy for bubbles, to surface tension forces:

\[
N_{\text{Eö}} = \frac{gd_1^2 (\rho_f - \rho_g)}{\sigma}.
\] (2.3)

The liquid and gas phase densities are given by \(\rho_f\) and \(\rho_g\) respectively. Liquid-gas
surface tension is denoted by \(\sigma\). The dimensionless inverse viscosity, \(N_f\), is found
by combining the Morton number, and relates the significance of viscous to surface
tension forces, with the Eötvös number to eliminate surface tension. Thus, the di-

\[
N_f = \frac{g \rho_f d_1^2 (\rho_f - \rho_g)}{\sigma}.
\]
mensionless inverse viscosity measures the significance of gravity, or buoyancy for bubbles, to viscous effects,

\[ N_f = \frac{[d_i^2 g (\rho_f - \rho_g) \rho_f]^\frac{1}{2}}{\mu_f}, \quad (2.4) \]

where \( \mu_f \) represents liquid viscosity. Values of \( m \) within Equation (2.2) are found for different ranges of dimensionless inverse viscosity, \( N_f \), to be:

- \( N_f > 250 \) \( m = 10 \)
- \( 18 < N_f < 250 \) \( m = 69 N_f^{-0.35} \)
- \( N_f < 18 \) \( m = 25 \)

Figure 2.2 displays the bubble velocity coefficient, \( k_1 \), over a range of outlet diameters for water and air as the liquid and gas phases. A neck diameter of 5 mm results in a bubble velocity coefficient of zero suggesting that surface tension would prevent emptying. As neck diameter is increased beyond 5 mm, the bubble velocity coefficient is influenced by surface tension and viscous effects until a diameter of around 20 mm. Beyond 20 mm, the bubble velocity coefficient asymptotically approaches the constant value of 0.345 where surface tension and viscous effects no longer play a role.

**Figure 2.2:** Bubble velocity coefficient, \( k_1 \), plotted against outlet diameter for air and water as the gas and liquid phases. The following values are used: \( \rho_f = 997 \text{ kg} \cdot \text{m}^{-3} \), \( \rho_g = 1.27 \text{ kg} \cdot \text{m}^{-3} \), \( \mu_f = 0.001 \text{ N} \cdot \text{s} \cdot \text{m}^{-2} \), and \( \sigma = 0.0729 \text{ N} \cdot \text{m}^{-1} \).
2.2 Observations on the Time to Empty

Analysis of the time to empty an inverted bottle or tube was a novel expansion of research on bubbles. Whalley examined bubble initiation and used bottles instead of tubes in his research [11]. Whalley focused on the flooding, where the bubble phase is moving upward and the liquid phase downward, and slugging, the creation of air bubbles in the liquid, of the liquid in the bottle as it was emptying. When looking at the bubble movement in these glugs, Whalley used several different types of bottles and examined the emptying times of these bottles. He noted four core results: hot water has significant effect on emptying time, extension of the bottle neck with tubes of varying diameters does not increase emptying time, the length of neck extension has small effect on emptying time, and the inclination of the bottle does effect emptying time with minimum emptying time occurring around an inclination of 30 to 45 degrees from the vertical [11]. However, it is worth noting that the bottles Whalley used all had a neck of some distance as he was using conventional bottles, see Figure 2.3(a), instead of ideal bottles, bottles with square edges and orifice outlets instead of necks which were manufactured specifically for experimentation.

![Figure 2.3](image)

**Figure 2.3:** (a) The four bottle types used by Whalley in his experiments. Note all bottle types have a significant length of neck, granted some necks are longer and some are shorter [11]. (b) An example of the extension tubes used by Whaley for his research on the effect longer necks have on time to empty [3].
Whalley followed up on his prior work and determined that the flooding of the bottle instead of the slugging accounts for the major features in the bottle emptying phenomena [3]. Whalley also further developed his analysis of the effect length of neck had on the time to empty a given bottle. Whalley determined that a greatly extended neck had little effect on the time to empty the given bottle or bubble mechanics, see Figure 2.3(b), but notably did not conduct an analysis of bottles without a neck (having an orifice outlet). In other words, extending an already long neck has little impact. This is in contrast, as we will see later, to the variation in bubble fraction as seen between orifices and short necks.

The time for a bottle to empty was also found to vary with bottle geometry and fluid properties. Hanin studied the emptying speed, and by extension emptying time, of a variety of tank shapes [12]. Hanin found that tank shape dramatically impacts the time to empty. Hanin developed “emptying efficiencies”, $k$, for several types of tank shapes; see Table 2.1. The emptying efficiencies are normalized to a large ideal tank emptying through a small hole ($k = 1$) and higher efficiencies correlate to a faster time to empty.

**Table 2.1:** Emptying efficiencies for different tank geometries (higher emptying efficiency implies more efficient emptying) [12].

<table>
<thead>
<tr>
<th>Tank Shape</th>
<th>Cone</th>
<th>Hemisphere</th>
<th>Sphere</th>
<th>Cylinder</th>
<th>Inverse Cone</th>
</tr>
</thead>
<tbody>
<tr>
<td>Emptying Efficiency</td>
<td>1.2</td>
<td>1.4</td>
<td>1.6</td>
<td>2</td>
<td>3.2</td>
</tr>
</tbody>
</table>

The tank bodies that smoothly transitioned to the outlet of the tank (Inverse Cone (funnel shaped) or Cylinder) had the best emptying efficiencies and fastest emptying times. For example, a tank with the shape of a point-upward cone had an emptying efficiency of 1.2 compared to a tank with the shape of a point-downward inverse cone (funnel shaped) with an emptying efficiency of 3.2. The outcomes of this model are indicative of what values can be expected for time to empty when using different
bottle geometries as well as capturing how geometry can impact the time to empty. For this work, all models and experimental data will use cylinder geometries avoiding the bias that may be introduced by different geometries.

Idealized analytical models which are inviscid and use a cylindrical bottle geometry to predict the time for a single outlet inverted bottle to empty have been previously constructed. These often incorporate the neck diameter and average bottle diameter as key parameters for predicting time to empty. Schmidt observed the emptying time of bottles and characterized the liquid discharge velocity through the outlet, \( u \), in terms of the average bottle diameter, \( D_v \), and the outlet diameter, \( D \) [13]:

\[
   u = 0.47 g \left( \frac{D_v D}{D} \right)^{0.25} .
\]  

(2.5)

Schmidt noted that the discharge velocity increased with increase in vessel diameter as well as increase in diameter of the outlet. This increased discharge velocity can be seen as a steeper height versus time curve where height is the height of the liquid in the bottle.

Schmidt also experimented with profiled outlets to determine that the outlet profile can have an effect on the time to empty with different profiles having different magnitudes of losses imposed upon the exiting flow, see Figure 2.4. Similar to Hanin, Schmidt found that vessels with profiles (similar to the point-downward inverse cone) emptied more efficiently, or had higher rates of outflow [13, 12].
Schmidt’s work on discharge analysis was continued by his coauthor Kubie who modeled outflow from closed-topped single-outlet vessels and provided data on the change in height over time for a given bottle; see Appendix A [14]. Kubie found that the rate of discharge during glugging was constant and generates a linear relationship between height of liquid and time.

Independent of Schmidt and Kubie, Clanet focused on the time to empty a glugging idealized bottle looking at the oscillatory glugging effect on the bottle as it emptied [2]. Clanet also recognized that during glugging, there is a linear relationship between height of liquid and time, or a constant discharge rate existed. Clanet developed a time to empty, \( T_e \), equation for an ideal bottle using liquid height, \( L \), bottle diameter, \( D_0 \), and neck diameter, \( d \), see Equation (2.6). Notably, Clanet recognized that a steady flow could be achieved by considering the bubble fraction and bubble velocity. Clanet used the Davies and Taylor bubble velocity model when applying Equation (2.6) to his own data.

\[
T_e = \frac{L}{\alpha \sqrt{g D_0}} \left( \frac{D_0}{d} \right)^{\frac{3}{2}}
\]  

(2.6)

Equation (2.6) is derived and explored in Appendix B where a focus on bubble fraction and how it may be interpreted by considering neck geometry is examined. The bubble fraction is the amount of air entering a vessel for a single glug and a core component
of Equation (2.6) as it determines the discharge rate of the liquid. Bubble fraction is also further explored in Section 3 Methods and Approaches.

Equation (2.6) is critical to the work of this paper and interpreted as the best equation to model the long time scale, on the scale of the bottle emptying, effects of glugging in inverted bottles. Features used by Clanet to develop this relation including bubble fraction and bubble velocity are critical to the analytical and numerical modeling effort. Clanet also provided data on the change in height over time for an ideal bottle with an orifice-like outlet using outlets ranging from 10 mm to 77.5 mm; see Appendix A.

Kumar has completed research closest to the scope of this project by examining draining tubes with small pierced holes in the top [7]. Kumar studied draining with Taylor fingering growth where a tube is closed on the top as well as draining when a hole is added in the top of the tube. Kumar found that the introduction of a hole in the top of the tube changes how the time to empty varies with fraction of volume (synonymous to height); see Figure 2.5. This observation matches our expectations and observations from experimental data; see Section 1.3.
Figure 2.5: The typical draining curves generated by Kumar for (a) draining due to Taylor fingering, (b) draining due to air entry from top (pierced hole in top), and (c) coupled mechanisms of (a) and (b) [7]. Inspection of where the curves intersect the horizontal axis shows the increase in emptying time due to the perforation.
2.3 CFD Research on Inverted Bottles

With the advent of more computational power and better CFD codes bubbles have become continually easier to explore. Within the past 10 years, approaches to proper modeling of bubbles have been completed by Geiger and Mer [8, 9]. Notably, modeling the formation of bubbles as well as tracking the interface and movements of a two-phase flow have been areas of focus. These CFD models often use the full extent of fluid properties attached to each fluid in the two-phase flow to solve the conditions of a given system. As such, these models provide comprehensive information on the behavior of fluid systems over time with a detailed view of all components of the system.

Figure 2.6: (a) Simulated bubble formations from the base of an ideal bottle (see (b)) by Geiger for different diameter outlets: 10 mm (black), 20 mm (dark grey), and 30 mm (light grey). (b) Variation of outlet diameters used: 10 mm, 20 mm, and 30 mm [8]. The entirety of the bottle simulated is not fully shown.

Geiger utilized viscous effects and fluid parameters such as surface tension to create a CFD model for an inverted bottle with two-phase flow [8]. Geiger looked at the differences in flow over several types of neck diameters and how these different diameters influence bubble formation with the onset of glugging, see Figure 2.6. It was
noted that for a closed top bottle the type of exit flow changed as the neck diameter was modified with larger bubbles being associated with larger neck diameters.

Most recently, Mer explored CFD modeling of two-phase flow in a glugging closed-topped tube by examining how to model the gas-liquid interface [9]. This involved examination of momentum exchange models in the NEPTUNE_CFD software (Large Interface Model (LIM), Generalized Large Interface Model (GLIM), and Large Bubble Model (LBM)) when modeling glugging effects in comparison with experimental results. Figure 2.7 displays the models in comparison to experimental results 4.2 seconds after introducing a bubble swarm to the system.

![Figure 2.7: Simulated bubble formations and experimental data compared at 4.2 seconds after introduction of bubble swarm using NEPTUNE_CFD [9]. Image modified to show initial states of air and water.](image-url)

Mer notes that the distribution of the gas volume fraction for the various simulations differ extensively and found air compressibility to play a critical role in the modeling as it generated the pressure oscillations in the upper air gap of the tube [9].
Overall, two-phase flow is challenging to model and computationally expensive to complete. Due to this computation expense, often only a few seconds of draining is observed in simulation. Geiger notes that for detailed simulation information involving small turbulent eddies and fluctuations, fine meshes and small time steps are required which can potentially take several months of computation time, perhaps even on a parallel system [8]. As a result of these complexities and computation limitations, simulations as a part of this thesis will be conducted with coarse meshes looking at bulk fluid movement and coarse simulations showing first bubble formation.
Inverted bottle emptying models will be constructed to help build a model that matches experimental data for variable-topped bottles by capturing the transition from jetting to glugging. Analytical, numerical, and CFD models will be built with complexity added at each level in the following order:

1. Inviscid Open-Topped Analytical
2. Viscous Open-Topped Analytical
3. Viscous Variable-Topped Analytical
4. Viscous Variable-Topped Numerical with Glugging
5. Viscous Variable-Topped CFD (ANSYS Fluent)

**Analytical Methods**

To ensure the validity of finalized models, idealized analytical models will be used to build toward a CFD solution with growing complexity. An inviscid approach with an open-topped bottle will first be modeled and evaluated in MATLAB as a baseline. Next an open-topped bottle will be modeled with viscous effects. Building upon this, the model will then grow to incorporate a variable-topped bottle. None of these models will have air moving through the neck of the bottle and as such remain single-phase flow.
**Numerical Methods**

The numerical model will be simulated in MATLAB and allows the flow of the inverted bottle to switch from jetting to glugging as determined by the hypothesized bubble velocity metric that transition occurs as the velocity of the liquid in the neck becomes smaller than the bubble rise velocity based upon the neck diameter. This code steps numerically through time checking for the transition and modeling fluid properties at each step. For jetting the variable-topped analytical model is used and for glugging the Clanet glugging model is used.

**CFD Methods**

The CFD codes developed by ANSYS in their Fluent package will be used to model the flow from a bottle. Several cases will be examined using the Fluent codes and the analytical and numerical models will serve to capture the details of the two-phase flow that are not modeled in the numerical model (bubble rise in neck) and attempt to observe the jetting-to-glugging transition to confirm the transitionary bubble velocity hypothesis that transition occurs as the velocity of the liquid in the neck becomes smaller than the bubble rise velocity based upon the neck diameter.

**Modeled Bottle Geometry**

This work will use two types of bottles. These will be the Type A bottle and Type B bottle, see Figure 3.1 [5]. The Type A bottle has a single neck diameter of 21.6 mm and small internal volume. The Type A bottle will be used when simulating bottle emptying in Fluent. The Type A bottle was chosen to be used with the CFD work in Fluent as the time to empty is within 2 seconds for many cases of Type A bottle emptying making simulations easier to complete.
The Type B bottle is used for three neck diameters which will be specified when referenced: 12.7 mm, 25.4 mm, and 38.1 mm. The Type B bottle has a large internal volume and was chosen so that crude measurement for liquid height versus time could be collected. Experimental data from these bottles will be used to compare against model and simulation results. Furthermore, future experimental work including high resolution imaging and high speed imaging is planned for both the Type A bottle and Type B bottle.

![Figure 3.1](image)

**Figure 3.1:** (a) Type A bottle with dimensions. (b) Type B bottle with dimensions. A neck diameter of 25.4 mm is shown, but neck diameters of 12.7 mm and 38.1 mm are also used for the Type B bottle.

Select experimental emptying data from the Type A bottle and Type B bottle is provided in Appendix A.
3.1 Critical Modeling Considerations

Critical modeling considerations are model attributes in the analytical and numerical models that help determine the time to empty and act as variables to tune the accuracy of the model based on comparison to existing experimental data. Examples of the models in their final state are included to show why a given assumption was made and how this decision is implemented.

The considerations discussed include:

1. Bubble Fraction

   The bubble fraction is the fraction of the glugging period in which air is entering the inverted bottle and critical to determining the rate at which a liquid exits a vessel. It is explored how neck geometry may impact this value and how it may be approximated.

2. Glugging versus Jetting Regimes

   The outlet flow of liquid from an inverted bottle varies depending upon whether the liquid is glugging or jetting. As such, determination of the time at which the transition occurs impacts the time to empty the bottle. It is hypothesized that when the neck velocity becomes equal to the bubble velocity the flow will transition from jetting to glugging. Experimental observation that liquid exit velocity decreases up to the point of transition seems to suggest the validity of the bubble velocity metric.
3. Bubble Velocity

The bubble velocity is the metric by which we distinguish the glugging and jetting regimes. The bubble velocity is simple to capture for larger outlet diameters, but requires more complexity when considering smaller outlets where surface tension and viscous effects are present.

4. Orifice Efficiency Coefficient

The orifice efficiency coefficient is the loss coefficient term related to the flow of air from the atmosphere to inside the perforated diameter. The coefficient impacts the modeled time to empty and is a result of the added perforation.
3.1.1 Bubble Fraction

Of particular interest to this report is the bubble fraction, or fraction of the glugging period, where liquid chaotically exits the bottle with bubbles, in which air enters the bottle, $\alpha$. The bubble fraction is discussed in depth by Clanet [2] in his work looking at ideal bottles. Clanet derives his equations for the time to empty glugging bottles using a bubble fraction of $\frac{1}{3}$. While this value matches his data exceptionally well, an analysis of several bottle emptying experiments suggests that the bubble fraction value can vary dramatically thereby changing estimates for the time to empty a glugging bottle; see Appendix B.

![Figure 3.2: Clanet illustration of the bubble fraction, $\alpha$, that occurs on the short time scale, the time scale looking at individual “glugs”, of the bottle emptying [2].](image)

Figure 3.2 was produced by Clanet to help explain the bubble fraction phenomena. As seen in Figure 3.2, the bubble fraction is the fraction of the glugging period in which air is entering the inverted bottle. When large frequent slugs are entering the bottle the bubble fraction will be larger and when smaller bubbles are slowly
entering the bottle, the bubble fraction will be smaller. For a bubble fraction of 0 there is no bubble entry and therefore no draining, whereas a bubble fraction of 1 is a long slug that always sits in the neck. The establishment of Clanet’s time to empty glugging equation is replicated with emphasis on the bubble velocity in Appendix B.1. Where available in the literature with quantitative data, the bubble fraction has been extracted. The approximate bubble fraction value was found for Kubie’s work in [14] in Appendix B.2. Bubble fraction values were also found for the experimental data provided by Mayer in Appendix B.3; see Table 3.1 [5].

<table>
<thead>
<tr>
<th>Clanet</th>
<th>Kubie</th>
<th>Type B Bottle</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bubble Fraction</td>
<td>0.33</td>
<td>0.49</td>
</tr>
<tr>
<td>Outlet Length (mm)</td>
<td>Thin (≈ 0)</td>
<td>6 to 17</td>
</tr>
</tbody>
</table>

It is suspected that the broad difference in bubble fraction is linked to the exit geometry for a given bottle, however, more analysis of this phenomena is required. The outlet for the Clanet model was a thin orifice. The outlet for the Kubie model was a thicker orifice. The outlet for the Mayer data was a 25.4 mm neck. While more data is required to make assertions on the matter, it seems that a larger outlet pathway may allow for a larger bubble fraction, or a realized neck instead of an orifice allows for the development of larger slugs of bubbles which generates a faster exchange of mass flow; see Appendix B.4.

Due to the assumption that neck geometry influences bubble fraction, we use best engineering judgment when choosing a bubble fraction for a bottle. The Type A bottle is assumed to have a bubble fraction of 0.6, chosen as a rough value between the Kubie and Type B bottle bubble fractions, when being simulated as it has an outlet length of 17.3 mm which is just above the largest outlet length used by Kubie who has an experimental bubble fraction of 0.49.
3.1.2 Glugging versus Jetting Regimes

While a closed-topped bottle presents glugging behavior and the open-topped bottle presents jetting behavior, it is the variable-topped bottle that presents the interesting phenomena of experiencing both glugging and jetting regimes at the outlet during separate intervals. The pressure drop in the air gap is the dominant reason glugging effects are generated, see Figure 3.3.

![Figure 3.3: The air gap in the closed-topped model is of lower pressure than atmospheric whereas the open-topped model is at atmospheric pressure.](image)

For a closed-topped bottle, there is no air to fill the expanding air gap at the top of the inverted bottle as the water level begins to lower. As such, the outlet flow slows and glugging immediately occurs to alleviate the drop in pressure. The pressure drop still occurs as a perforation is introduced into the top of the inverted bottle, however, the pressure stabilizes below atmospheric pressure as the perforation helps to alleviate the magnitude of the pressure and thus velocity drop.
Using the variable-topped numerical with glugging model from Section 5 it can be seen that with a perforation in an inverted bottle the pressure in the air gap is initially below atmospheric with jetting behavior. As draining occurs, the pressure of the air gap slowly approaches atmospheric pressure until conditions are met to transition to fully glugging upon which the pressure within the air gap is unknown for this simulation, see Figure 3.4. Kubie suggests that as glugging occurs the pressure of the air gap increases in an oscillatory manner, from glugging bubbles, to atmospheric pressure [15].

![Figure 3.4: Difference in pressure from atmospheric for a Type B bottle of 25.4 mm neck and 1.18 mm perforation where glugging occurs.](image)

A transition from jetting to glugging can also be viewed directly in the Mayer experimental data, see Figure 3.5 where the rate of emptying follows different trendlines. Thus, separate models for the glugging and jetting regimes will be required to fully model the variable-topped system. The bubble velocity will be used to determine this transition.
3.1.3 Bubble Velocity

The bubble velocity is used in this report as a metric to differentiate glugging from jetting flow, see Equation (3.1). This is particularly important in regard to the transitionary stages presented by the perforation diameter in the top of an inverted bottle. With a closed-topped bottle, the flow is dominated entirely by glugging, however, for an open-topped bottle the flow is dominated by jetting. The introduction of a perforation in the top of the bottle generates cases where there is jetting that transitions to glugging at a given intermediate height. The analytical models that will be developed focus on the jetting regime whereas the work of Clanet [2] focuses on the glugging regime. As such, determining the point of transition between these regimes is critical to modeling bottle emptying. Wallis presents Equation (2.2) as a bubble velocity coefficient solution that accounts for surface tension and viscous effects using the dimensionless inverse viscosity, $N_f$, and the Eötvös number, $N_{E\ddot{o}}$ [6].

$$\frac{U}{\sqrt{gd_1}} = k_1$$  \hspace{1cm} (3.1)
We hypothesize that the bubble velocity can be used to predict the transition from jetting to glugging. The core concept is that there is a competition between the outlet liquid velocity (velocity of liquid moving downward) and the bubble rise velocity (velocity of gas moving upward). As a bottle drains through jetting, the outlet liquid velocity decreases. Under certain conditions, the outlet liquid velocity can drop below the bubble rise velocity. Once the outlet liquid velocity slows beyond the theoretical bubble rise velocity, this should allow the entrance of a bubble into the inverted bottle neck leading to the transition from jetting to glugging.

Several instances of the flow changing from jetting to glugging can be viewed in Figures 3.6 through 3.9 with the neck velocity and bubble velocity displayed using the Type B bottle data (note the bubble velocity is a constant and the liquid height and neck velocity data are experimental). Neck velocity is inferred from liquid height data using conservation of mass and the bubble velocity curve is not a measured quantity but provided for reference. The change in slope of the bottle height on these plots indicates a regime change from jetting to glugging. We would expect the neck and bubble velocity to intersect or be similar in value when a regime change occurs based on our assumption that when bubble velocity equals outlet velocity, jetting will transition to glugging.

Figure 3.6 is an instance where using the bubble velocity metric provides a fair interpretation of when the flow will transition, granted in this case it predicts a regime change earlier.
Figure 3.6: Experimental data provided by Mayer showing the transition from jetting to glugging for a Type B bottle with 25.4 mm diameter neck and 1.18 mm perforation diameter.

Figure 3.7 is an instance where using the bubble velocity metric lines up nicely with the experimental data. The neck velocity approaches the bubble velocity metric within 10 seconds of transition.

Figure 3.7: Experimental data provided by Mayer showing the transition from jetting to glugging for a Type B bottle with 38.1 mm diameter neck and 2.08 mm perforation diameter.
Figure 3.8 is an instance where the bubble metric is not explicitly achieved in the experimental data, but the neck velocity is within 20% of the bubble velocity when transition occurs.

![Graph showing transition from jetting to glugging](image)

**Figure 3.8:** Experimental data provided by Mayer showing the transition from jetting to glugging for a Type B bottle with 38.1 mm diameter neck and 2.26 mm perforation diameter.

Figure 3.9 is an instance where using the bubble velocity metric begins to break down. With the 12.7 mm neck diameter the bubble velocity metric does not seem to capture the transitioning regime change.
From inspection of Type B bottle data, e.g. as shown in Figures 3.6 through 3.9, the transition between jetting and glugging reasonably matches the bubble velocity hypothesis for neck diameters of 25.4 mm and 38.1 mm. The bubble velocity hypothesis fails to account for the transition for the 12.7 mm neck. At first glance, this might not be unexpected, as around a 12 mm neck diameter the bubble velocity coefficient begins to change significantly, see Figure 3.10. However, the plot of Figure 3.10 and the predicted transition velocity already accounts for the small neck diameter. At present this discrepancy is not explained. Despite this, the bubble velocity hypothesis is an adequate starting point for our modeling because it will be shown to capture the broader time to empty versus perforation diameter trends observed. Further evidence to support or refute the bubble velocity hypothesis is expected to come from future CFD simulations.
Figure 3.10: Bubble velocity coefficient as a function of neck diameter including experimental coefficients from a Type B bottle. Note the large difference between experimental and theoretical coefficients at 12.7 mm.

3.1.4 Orifice Efficiency Coefficient

The orifice efficiency coefficient is the loss coefficient term arising from air entering the perforation of the inverted bottle. A suitable value from theory was not found and an experimental coefficient is used. An orifice efficiency coefficient of 1.2 was found to produce model results closely matching the experimental results of Mayer [5]; see Figures 3.11, 3.12, and 3.13. While it is suspected this value may change with perforation diameter, it was chosen to use an orifice efficiency coefficient of 1.2 for all simulations.
**Figure 3.11:** Example height versus time plot for different orifice coefficients on an inverted bottle using a Type B bottle with 38.1 mm outlet and 1.93 mm perforation diameter.

Figures 3.11 and 3.12 display the orifice coefficient of 1.2 best modeling the bottle emptying when compared to the Mayer data.

**Figure 3.12:** Example height versus time plot for different orifice coefficients on an inverted bottle using a Type B bottle with 38.1 mm outlet and 2.87 mm perforation diameter.
Figure 3.13 displays the orifice coefficient of 1.2 still giving a fair approximation of the experimental data.

**Figure 3.13:** Example height versus time plot for different orifice coefficients on an inverted bottle using a Type B bottle with 25.4 mm outlet and 1.70 mm perforation diameter.

The orifice coefficient will be approximated as 1.2 using best engineering judgment from the jetting Type B bottle data.
3.2 Methods Summary

This section outlines the models that will be developed as well as the four major controlling variables used in the MATLAB modeling and how they are best approximated.

The bubble fraction value is used to determine the rate at which liquid exits the inverted bottle and thereby the time to empty the bottle. The bubble fraction is inferred using best engineering judgment by considering the outlet geometry.

The transition from jetting to glugging when a perforation is present is a key feature necessary to properly model bottle emptying. This capability is essential when modeling variable-topped bottles that fall between the jetting open-topped bottle regime and the glugging closed-topped bottle regime.

The hypothesized bubble velocity is a key metric by which we initiate the transition from jetting to glugging. When the neck velocity is greater than the bubble velocity it is assumed jetting is occurring. When the bubble velocity is greater than the neck velocity it is assumed glugging is occurring.

The orifice efficiency coefficient is used to best approximate the loss coefficient as air enters the perforation. A value of 1.2 was found to be optimal for the Mayer data and is expanded to other such bottle geometries using best engineering judgment.
There are three analytical solutions built to model the emptying time of inverted bottles. These include an inviscid solution for an open-topped bottle, a viscous solution for an open-topped bottle, and a viscous solution for a variable-topped bottle. Each of these models adds another layer of physics to the previous model building complexity to fully model an inverted bottle. A figure comparison of the three scenarios is included in Figure 4.1.

Figure 4.1: Progression of models constructed to simulate the emptying bottle: inviscid open-topped, viscous open-topped, and viscous variable-topped.

These models are evaluated in MATLAB and experimental data from the Type B bottle provided by Mayer is used as a comparison for these models [5].
4.1 Derivation of Time to Empty Inviscid Open-Topped Bottle

The following derives the analytical equation that may be used to evaluate the time to empty an inviscid-flow open-topped bottle. The derivation utilizes a model which neglects the viscous effects, the losses associated with contraction, of the bottle. The following assumptions are used in this calculation:

- Inviscid
- Incompressible

To find an analytical time to empty for the open-topped inviscid case, we will first develop continuity relations, then build a relationship between the velocity at state 1 and state 2 in Figure 4.2.

**Figure 4.2:** Diagram of open-topped bottle model.
4.1.1 Conservation of Mass for Inviscid and Viscous Solutions

We will begin the analysis by first developing Conservation of Mass for this system between indicated states 1 and 2 in Figure 4.2, see Equation (4.1).

\[
\left( \frac{dM}{dt} \right)_{sys} = \frac{\partial}{\partial t} \int_{CV} \rho dV + \int_{CS_1} \rho \vec{v} \cdot d\vec{A} + \int_{CS_2} \rho \vec{v} \cdot d\vec{A} \tag{4.1}
\]

With a constant system mass, Equation (4.1) will simplify to mass flow rates and the time-dependent change of the liquid in the control volume:

\[
\frac{\partial}{\partial t} \int_{CV} \rho dV = (\rho v A)_1 - (\rho v A)_2
\]

As we are interested in the liquid that exits the neck, we will modify our control volume to move with surface 2, the upper level of water, as the water level lowers. With this modification, the velocity at surface 2 is now zero and the mass flow rate for surface 2 is zero. Thus, we know that the time-dependent change of the liquid in the control volume is equal to the mass flow rate at surface 1, the neck of the bottle. The new relation formed can be interpreted as the equality of the mass flow rate at surface 1 to the change in mass of the system over time:

\[
\frac{\partial}{\partial t} \int_{CV} \rho dV = (\rho v A)_1
\]

This relation may be further rearranged by rewriting areas in terms of diameter and refactoring the time-dependent term into a relationship between liquid height and time. This allows for a function that can compute how the height of the liquid in the system changes over time depending upon the outlet velocity, neck diameter, and body diameter:

\[
\frac{\partial h}{\partial t} \frac{\rho \pi d_2^2}{4} = \frac{\rho v_1 \pi d_1^2}{4}
\]
\[
\frac{\partial h}{\partial t} = v_1 \left( \frac{d_1}{d_2} \right)^2
\]  
(4.2)

The relation in Equation (4.2) is relevant for all three analytical solutions. Equation (4.2) coupled with the neck velocity in terms of height and constants may be used to explicitly solve for the time it takes for the level of liquid in a bottle to descend a given height. Critical to the development of Equation (4.2) is that it is applicable for viscous solutions as well.
4.1.2 Developing Neck Velocity using Bernoulli’s Equation

The neck velocity is the remaining component required to generate an analytical solution. We will use Bernoulli’s equation to begin relating the neck velocity to the height of the liquid in the bottle, referenced to a datum at state 1:

\[
\left( \frac{P}{\rho} + \frac{v^2}{2} \right)_1 = \left( \frac{P}{\rho} + \frac{v^2}{2} + gh \right)_2
\]  \hspace{1cm} (4.3)

This will properly model the time to empty the liquid from the main body of the bottle. The neck volume is typically small so the influence of neck time based on drainage will not significantly impact emptying time.

We may further reduce Equation (4.3) by considering the pressure terms as equivalent at states 1 and 2 as they are both subject to atmospheric pressure:

\[
v_1^2 = v_2^2 + 2gh
\]

We may next relate the velocity at state 1 to state 2 using continuity principles to simplify this equation. The mass flow rates at states 1 and 2 are equivalent so we may develop a solution for the velocity of the bottle, state 2, in terms of the velocity of the neck, state 1:

\[
v_1 A_1 = v_2 A_2
\]

\[
v_2 = v_1 \left( \frac{d_1}{d_2} \right)^2
\]

Using the continuity relation, we may further simplify the Bernoulli interpretation of our system to be comprised of the neck velocity, the height, and constants, see Equation (4.4):

\[
v_1^2 = v_1^2 \left( \frac{d_1}{d_2} \right)^4 + 2gh
\]
\[ v_1 = \sqrt{\frac{2gh}{1 - \left(\frac{a_1}{a_2}\right)^4}} \] (4.4)
4.1.3 Explicit Solution for Emptying Time as a Function of Height

Equation (4.4) holds true when the height term is greater than the height of the neck, or when there is still liquid in the body of the bottle. We may now combine Equation (4.4) with Equation (4.2) to relate height and time solely as a function of diameters. Through several steps involving integration and adjusting variable placement, we will find our desired solution displayed in Equation (4.5):

\[
\frac{\partial h}{\partial t} = \sqrt{\frac{2gh}{1 - \left(\frac{d_1}{d_2}\right)^4}} \left(\frac{d_1}{d_2}\right)^2
\]

\[
\int_0^h \frac{\partial h}{\sqrt{h}} = \int_0^t \sqrt{\frac{2g}{1 - \left(\frac{d_1}{d_2}\right)^4}} \left(\frac{d_1}{d_2}\right)^2 \partial t
\]

\[
2h^{\frac{1}{2}} = \sqrt{\frac{2g}{1 - \left(\frac{d_1}{d_2}\right)^4}} \left(\frac{d_1}{d_2}\right)^2 t
\]

\[
t = 2h^{\frac{1}{2}} \left(\frac{d_2}{d_1}\right)^2 \sqrt{\frac{1 - \left(\frac{d_1}{d_2}\right)^4}{2g}}
\]

Equation (4.5) is the inviscid solution for the relationship between time, \(t\), and liquid height, \(h\). If the total time to empty is desired, then \(h\) should be set to \(H\) in which case \(t\) becomes \(T_{\text{empty}}\). Note, if there is a neck on the bottle, the height of the neck must be included in the liquid height term. Because of this, one must remove the emptying time attributed to the neck as seen in Equation (4.6). This will hold true for the following analytical solutions as well.

\[
T_{\text{empty}} = T_{\text{empty}}(H + L) - T_{\text{empty}}(L)
\]
4.1.4 Inviscid Model Results

The open-topped inviscid model given by Equation (4.5) is the most simplistic model formed as we build toward an inverted bottle model. The case most similar to this model is the 25.4 mm outlet Type B bottle with a 6.4 mm perforation diameter (approximately open-topped), see Figure 4.3.

![Figure 4.3: Plot of inviscid open-topped analytical model against an approximately open-topped Type B bottle of neck diameter 25.4 mm.](image)

As a reference, it is also useful to visualize the inviscid open-topped case with experimental data from an inverted bottle with a perforation that transitions from jetting to glugging as it is the ultimate goal to model this; see Figure 4.4.
Figure 4.4: Plot of inviscid open-topped analytical model against a variable-topped Type B bottle of neck diameter 25.4 mm and perforation diameter of 1.18 mm.

As expected, the inviscid open-topped model does a poor job of modeling the fully realized variable-topped inverted bottle case and the observed trend with changing perforation diameter, see Figure 4.5, but begins the process of incrementally building confidence in model results. Notably, this model was constructed before the computational models at which point an inviscid computational model was deemed unnecessary. To improve the model, we will add viscous effects.
Figure 4.5: The trend of time to empty changing as different sized perforations are used with predictions of the inviscid open-topped analytical model for a Type B bottle with neck 25.4 mm.
4.2 Derivation of Time to Empty Viscous Open-Topped Bottle

The following derives the analytical equation that may be used to evaluate the time to empty a viscous-flow open-topped bottle. The derivation utilizes a model that accounts for the viscous effects, the losses associated with contraction, of the bottle. The following assumptions are used in this calculation:

- Incompressible
- Uniform Velocity Profile in the Bottle Body \((\alpha = 1)\)
- Uniform Velocity Profile in the Bottle Neck \((\alpha = 1)\)

We assume the flow in the neck and body are not fully-developed flows and have profiles that are nearly uniform. For this derivation \(\alpha\) will refer to kinetic energy coefficients instead of bubble fraction.

To find an analytical time to empty for the open-topped viscous case, we will first develop a relationship between the velocity at state 1 and state 2 (refer back to Figure 4.2) to be used with the continuity relation, Equation (4.2).
4.2.1 Solving for Neck Velocity using Pipeflow Equations

As the continuity relations developed in Section 4.1 Equation (4.2) are still valid, we may move to directly solve for the neck velocity. We will use pipeflow relations to begin relating the neck velocity to the height of the liquid in the bottle:

\[ \left( \frac{P_2}{\rho} + \alpha_2 \frac{v_2^2}{2} + gz_2 \right) - \left( \frac{P_1}{\rho} + \alpha_1 \frac{v_1^2}{2} + gz_1 \right) + \frac{\dot{W}_{in}}{m} = H_l + h_l \]  

(4.7)

The work term, \( \dot{W}_{in} \) is eliminated as there is no shaft work. Major losses, \( H_l \), are considered negligible for flow within the bottle as diameter is large and average velocity small in comparison to the neck velocity. Major losses in the bottle neck are neglected due to short length of the neck. The only loss to consider is the minor loss associated with the contraction from the body of the bottle to the neck:

\[ \left( \frac{P_2}{\rho} + \alpha_2 \frac{v_2^2}{2} + gz_2 \right) - \left( \frac{P_1}{\rho} + \alpha_1 \frac{v_1^2}{2} + gz_1 \right) = K_{2\rightarrow1} \frac{v_2^2}{2} \]

Note that from continuity we may also relate the bottle and neck velocity:

\[ v_2 = v_1 \left( \frac{d_1}{d_2} \right)^2 \]

The pipeflow relation may be further reduced by adjusting variable placement and substituting in continuity relations:

\[ \frac{v_2^2}{2} \alpha_2 - \frac{v_1^2}{2} (K_{2\rightarrow1} + \alpha_1) = \frac{P_1 - P_2}{\rho} - gh \]

\[ v_2^2 \alpha_2 - v_1^2 (K_{2\rightarrow1} + \alpha_1) = \frac{2(P_1 - P_2)}{\rho} - 2gh \]

\[ v_1^2 \left( \frac{d_1}{d_2} \right)^4 \alpha_2 - v_1^2 (K_{2\rightarrow1} + \alpha_1) = \frac{2(P_1 - P_2)}{\rho} - 2gh \]
\[ v_1^2 \left( \left( \frac{d_1}{d_2} \right)^4 \alpha_2 - (K_{2 \rightarrow 1} + \alpha_1) \right) = \frac{2(P_1 - P_2)}{\rho} - 2gh \]

\[ v_1 = \sqrt{\frac{2(P_1 - P_2)}{\rho} - 2gh} \]

\[ \frac{\alpha_2 \left( \frac{d_1}{d_2} \right)^4 - (K_{2 \rightarrow 1} + \alpha_1)}{\frac{d_1}{d_2}} \]

Lastly, we may neglect the pressure terms as both states 1 and 2 are subject to atmospheric pressure. This simplifies the neck velocity equation for a viscous open-topped bottle to Equation (4.8).

\[ v_1 = \sqrt{\frac{-2gh}{\alpha_2 \left( \frac{d_1}{d_2} \right)^4 - (K_{2 \rightarrow 1} + \alpha_1)}} \quad (4.8) \]

As a note of interest, the inviscid velocity relation can be retrieved out of this solution. To return the inviscid solution, the contraction loss would become zero and the kinetic energy coefficients, \( \alpha \), will be allotted values of one implying uniform velocity profiles:

\[ v_1 = \sqrt{\frac{-2gh}{\left( \frac{d_1}{d_2} \right)^4 - 1}} \]

With some adjustment we achieve the exact inviscid solution for neck velocity previously derived out of the viscous solution:

\[ v_1 = \sqrt{\frac{2gh}{1 - \left( \frac{d_1}{d_2} \right)^4}} \]
4.2.2 Explicit Solution for Emptying Time as a Function of Height

Similar to the inviscid solution, we may now use conservation of mass, see Equation (4.2), to relate height and time to a function of diameters:

\[
\frac{\partial h}{\partial t} = \sqrt{-\frac{-2gh}{\alpha_2 \left( \frac{d_1}{d_2} \right)^4 - (K_{2\rightarrow1} + \alpha_1)} \left( \frac{d_2}{d_1} \right)^2}
\]

\[
\int_0^t \partial t = \int_0^h \left( \sqrt{\frac{\alpha_2 \left( \frac{d_1}{d_2} \right)^4 - (K_{2\rightarrow1} + \alpha_1)}{-2g}} \right) h^{-\frac{1}{2}} \left( \frac{d_2}{d_1} \right)^2 \partial h
\]

\[
t = 2h^{\frac{1}{2}} \left( \frac{d_2}{d_1} \right)^2 \left( \sqrt{\frac{\alpha_2 \left( \frac{d_1}{d_2} \right)^4 - (K_{2\rightarrow1} + \alpha_1)}{-2g}} \right)
\]  (4.9)

Equation (4.9) is the viscous solution for the time it will take for a liquid of a given height in a bottle to drain. The same time adjustment from Equation (4.6) is relevant for this solution. If the total time to empty is desired, then \( h \) should be set to \( H \) in which case \( t \) becomes \( T_{\text{empty}} \).
4.2.3 Viscous Open-Topped Model Results

The viscous model for an open-topped bottle results in the analytical solution of Equation (4.9).

The open-topped viscous model is the second step toward forming an inverted bottle model. Same as the inviscid open-topped model, the case most similar to this model is from the Mayer data where there is a 6.35 mm perforation in the top of the bottle (approximately open-topped), see Figure 4.6.

![Figure 4.6: Plot of viscous open-topped analytical model against an approximately open-topped Type B bottle of neck diameter 25.4 mm.](image)

It is still useful to visualize the viscous open-topped case with experimental data from an inverted bottle with a perforation, see Figure 4.7. The viscous open-topped model shows improvement in matching the experimental data compared to the inviscid open-topped model.
Figure 4.7: Plot of viscous open-topped analytical model against a variable-topped Type B bottle of neck diameter 25.4 mm and perforation diameter of 1.18 mm.

As the viscous open-topped model is not taking into account a transition from jetting to glugging, the model continues to do a poor job of modeling the fully realized variable-topped inverted bottle case as well as the observed trend with changing perforation diameter, see Figure 4.8. The viscous open-topped model also neglects the pressure of the air gap. To improve the model, we will consider the variable top.
Figure 4.8: The trend of time to empty changing as different sized perforations are used with predictions of the viscous open-topped analytical model for a Type B bottle with neck 25.4 mm.
4.3 Derivation of Time to Empty Viscous Variable-Topped Bottle

The following derives the analytical equation that may be used to evaluate the time to empty a viscous-flow variable-topped bottle. The derivation utilizes a model that accounts for the viscous effects, the losses associated with contraction, of the bottle as well as a variable-topped condition. The following assumptions are used in this calculation:

- Incompressible
- Uniform Velocity Profile in the Bottle Body ($\alpha = 1$)
- Uniform Velocity Profile in the Bottle Neck ($\alpha = 1$)

To find an analytical time to empty for the variable-topped viscous case, we will develop several relationships between the indicated reference states in Figure 4.9.

Figure 4.9: Diagram of variable-topped bottle model.
4.3.1 Relate States of the Model

Our solution process will involve using continuity and pipe flow equations to relate each state to each state to ultimately relate neck velocity to the height of the liquid in the bottle.

Known Parameters

- $v_1 = 0$
- $v_{2,\text{water}} = v_{2,\text{air}}$ or the air and water interface is moving at the same velocity
- $z_4 - z_3 \approx 0$
- There are no major losses ($H_l$)
- $P_1 = P_4 = P_{\text{atm}}$

There are currently 5 unknowns that need to be explored: $P_2, P_3, v_1, v_2, v_3$.

As such, we need to develop five relations to connect these variables such that our system may be solvable.
Continuity State 1 to State 2

We may apply conservation of mass to relate the velocities of states 1 and 2 in Equation (4.10). Note that we are tracking the liquid in this equation.

\[ \dot{m}_1 = \dot{m}_2 \]
\[ v_1 A_1 = v_2 A_2 \]
\[ v_1 = v_2 \left( \frac{d_2}{d_1} \right)^2 \]
\[ v_2 = v_1 \left( \frac{d_1}{d_2} \right)^2 \]

(4.10)

Continuity State 2 to State 3

We may apply conservation of mass to relate the velocities of states 2 and 3 in Equation (4.11). Note that we are tracking the gas in this equation.

\[ \dot{m}_2 = \dot{m}_3 \]
\[ v_2 A_2 = v_3 A_3 \]
\[ v_2 = v_3 \left( \frac{d_3}{d_2} \right)^2 \]
\[ v_3 = v_2 \left( \frac{d_2}{d_3} \right)^2 \]

(4.11)
Pipe Flow State 1 to State 2

We may apply pipe flow relations from state 1 to state 2 in Equation (4.12).

\[
\left( \frac{P_2}{\rho_{water}} + \alpha_2 \frac{v_2^2}{2} + gh \right) - \left( \frac{P_1}{\rho_{water}} + \alpha_1 \frac{v_1^2}{2} \right) = \frac{v_1^2}{2} K_{2\rightarrow 1} \tag{4.12}
\]

We will now work to write \( v_1 \) in terms of constants and \( P_2 \):

\[
\left( \frac{P_2 - P_1}{\rho_{water}} \right) + gh + \alpha_2 \frac{v_2^2}{2} - \alpha_1 \frac{v_1^2}{2} = \frac{v_1^2}{2} K_{2\rightarrow 1}
\]

From Continuity between State 1 and State 2, Equation (4.10), we will rewrite the equation to be in terms of \( v_1 \):

\[
\left( \frac{P_2 - P_1}{\rho_{water}} \right) + gh = \frac{v_1^2}{2} \left[ K_{2\rightarrow 1} - \alpha_2 \left( \frac{d_1}{d_2} \right)^4 + \alpha_1 \right]
\]

\[
v_1 = \sqrt{\frac{2 \left( \frac{P_2 - P_1}{\rho_{water}} \right) + 2gh}{K_{2\rightarrow 1} + \alpha_1 - \alpha_2 \left( \frac{d_1}{d_2} \right)^4}} \tag{4.13}
\]

Equation (4.13) allows for solving neck velocity when the pressure of state 2 is known.

Pipe Flow State 2 to State 3

We may apply pipe flow relations from state 2 to state 3 in Equation (4.14).

\[
\left( \frac{P_3}{\rho_{air}} + \alpha_3 \frac{v_3^2}{2} \right) - \left( \frac{P_2}{\rho_{air}} + \alpha_2 \frac{v_2^2}{2} \right) = \frac{v_2^2}{2} K_{3\rightarrow 2} \tag{4.14}
\]
Note, as this phase deals with air we will neglect the potential energy terms. We assume the bottom fluid in the bottle, typically water, is much more dense than the other fluid, air.

We will work to write $v_1$ in terms of constants, $P_2$, and $P_3$:

$$\left( \frac{P_3 - P_2}{\rho_{\text{air}}} \right) + \alpha_3 \frac{v_3^2}{2} - \alpha_2 \frac{v_2^2}{2} = \frac{v_3^2}{2} K_{3\rightarrow2}$$

From Continuity between states 1, 2, and 3, Equations (4.10) and (4.11), we will rewrite the equation to be in terms of $v_1$:

$$\left( \frac{P_3 - P_2}{\rho_{\text{air}}} \right) + \alpha_3 \frac{v_1^2}{2} \left( \frac{d_1}{d_2} \right)^4 - \alpha_2 \frac{v_1^2}{2} \left( \frac{d_1}{d_2} \right)^4 = \frac{v_1^2}{2} \left( \frac{d_1}{d_2} \right)^4 K_{3\rightarrow2}$$

$$v_1^2 \left[ K_{3\rightarrow2} \left( \frac{d_1}{d_2} \right)^4 - \alpha_3 \left( \frac{d_1}{d_3} \right)^4 + \alpha_2 \left( \frac{d_1}{d_2} \right)^4 \right] = 2 \left( \frac{P_3 - P_2}{\rho_{\text{air}}} \right)$$

$$v_1 = \sqrt{\frac{2 \left( \frac{P_3 - P_2}{\rho_{\text{air}}} \right)}{K_{3\rightarrow2} \left( \frac{d_1}{d_2} \right)^4 - \alpha_3 \left( \frac{d_1}{d_3} \right)^4 + \alpha_2 \left( \frac{d_1}{d_2} \right)^4}} \tag{4.15}$$

Equation (4.15) allows for solving neck velocity when the pressure of state 2 and state 3 are known.

**Pipe Flow State 3 to State 4**

We may apply pipe flow relations from state 2 to state 3 in Equation (4.16).

$$\left( \frac{P_4}{\rho_{\text{air}}} \right) - \left( \frac{P_3}{\rho_{\text{air}}} + \alpha_3 \frac{v_3^2}{2} \right) = \frac{v_3^2}{2} K_{4\rightarrow3} \tag{4.16}$$
We will now work to write \( v_1 \) in terms of constants and \( P_2 \) and use continuity between states 1, 2, and 3, Equations (4.10) and (4.11):

\[
\left( \frac{P_4}{\rho_{air}} \right) - \left( \frac{P_3}{\rho_{air}} + \alpha_3 \frac{v_1^2}{2} \left( \frac{d_1}{d_2} \frac{d_2}{d_3} \right)^4 \right) = \frac{v_1^2}{2} \left( \frac{d_1}{d_2} \frac{d_2}{d_3} \right)^4 K_{4\rightarrow3}
\]

\[
v_1^2 \left( \frac{d_1}{d_3} \right)^4 (K_{4\rightarrow3} + \alpha_3) = 2 \left( \frac{P_4 - P_3}{\rho_{air}} \right)
\]

\[
v_1 = \sqrt{\frac{2 \left( \frac{P_4 - P_3}{\rho_{air}} \right)}{\left( \frac{d_1}{d_3} \right)^4 (K_{4\rightarrow3} + \alpha_3)}} \quad (4.17)
\]

Equation (4.17) allows for solving neck velocity when the pressure of State 3 is known.
4.3.2 Analyze Current Equations

We now have three equations (Equations (4.13), (4.15), and (4.17)) from the pipe flow analysis that solve for neck velocity, \( v_1 \), as functions of the pressure at state 2, \( P_2 \), and the pressure at state 3, \( P_3 \):

Pipeflow from State 1 to State 2: \( v_1 = f(P_2) \)

Pipeflow from State 2 to State 3: \( v_1 = f(P_2, P_3) \)

Pipeflow from State 3 to State 4: \( v_1 = f(P_3) \)

This generates three equations with three unknowns and is thus solvable. For simplicity we shall rewrite our equations with constants:

Equation (4.13) (State 1 to 2)

\[
v_1 = \sqrt{\frac{2 \left( \frac{P_2 - P_1}{\rho_{\text{water}}} \right)}{C_1}} + 2gh\]

where \( C_1 = K_{2\rightarrow1} + \alpha_1 - \alpha_2 \left( \frac{d_1}{d_2} \right)^4 \)

Equation (4.15) (State 2 to 3)

\[
v_1 = \sqrt{\frac{2 \left( \frac{P_3 - P_2}{\rho_{\text{air}}} \right)}{C_2}}\]

where \( C_2 = K_{3\rightarrow2} \left( \frac{d_1}{d_2} \right)^4 - \alpha_3 \left( \frac{d_1}{d_3} \right)^4 + \alpha_2 \left( \frac{d_1}{d_2} \right)^4 \)

Equation (4.17) (State 3 to 4)

\[
v_1 = \sqrt{\frac{2 \left( \frac{P_3 - P_2}{\rho_{\text{air}}} \right)}{C_3}}\]

where \( C_3 = \left( \frac{d_1}{d_3} \right)^4 (K_{4\rightarrow3} + \alpha_3) \)

We desire an explicit solution for the neck velocity so that we may use continuity to solve for time to empty. We will use our simplified equations above to solve for \( P_2 \),
Equation (4.13), and $P_3$, Equation (4.17), in terms of the neck velocity, $v_1$, so that we may plug these into Equation (4.15) for an explicit solution.

Solve for $P_2$ in terms of $v_1$ using Equation (4.13)

Equation (4.13) (State 1 to 2)

$$v_1 = \sqrt{\frac{2 (P_2 - P_1)}{\rho_{\text{water}}} + 2gh}$$

$$P_2 = \frac{\rho_{\text{water}} (v_1^2 C_1 - 2gh)}{2} + P_1$$ (4.18)

Equation (4.18) yields pressure in State 2 given neck velocity.

Solve for $P_3$ in terms of $v_1$ using Equation 3

Equation (4.17) (State 3 to 4)

$$v_1 = \sqrt{\frac{2 (P_3 - P_4)}{\rho_{\text{air}}} C_3}$$

$$P_3 = P_4 - \frac{\rho_{\text{air}} (v_1^2 C_3)}{2}$$ (4.19)

Equation (4.19) yields pressure in State 3 given neck velocity.

Solve for neck velocity, $v_1$, in constants using Equation (4.15) with pressure equations (4.18) and (4.19)

Equation (4.15) (State 2 to 3)

$$v_1 = \sqrt{\frac{2 (P_3 - P_2)}{\rho_{\text{air}}} C_2}$$
\[ v_1 = \sqrt{\frac{-\rho_\text{air} (v_1^2 C_3) - \rho_\text{water} (v_1^2 C_1 - 2gh)}{\rho_\text{air} C_2}} \]

Note that \( P_1 \) and \( P_4 \) are both atmospheric pressure and cancel yielding neck velocity as a function of constants in Equation (4.20):

\[ v_1 = \sqrt{\frac{-\rho_\text{air} (v_1^2 C_3) - \rho_\text{water} (v_1^2 C_1 - 2gh)}{\rho_\text{air} C_2}} \]

\[ v_1^2 C_2 = -v_1^2 C_3 - \frac{\rho_\text{water}}{\rho_\text{air}} v_1^2 C_1 + 2gh \frac{\rho_\text{water}}{\rho_\text{air}} \]

\[ v_1^2 \left( C_2 + C_3 + \frac{\rho_\text{water}}{\rho_\text{air}} \right) = 2gh \frac{\rho_\text{water}}{\rho_\text{air}} \]

\[ v_1 = \sqrt{\frac{2gh \frac{\rho_\text{water}}{\rho_\text{air}}}{C_2 + C_3 + \frac{\rho_\text{water}}{\rho_\text{air}} C_1}} \quad (4.20) \]

As before, the original, inviscid open-topped solution may be retrieved by neglecting loss coefficients:

\[ v_1 = \sqrt{\frac{2gh \frac{\rho_\text{water}}{\rho_\text{air}}}{-\alpha_3 \left( \frac{d_1}{d_3} \right)^4 + \alpha_2 \frac{d_1}{d_2} \frac{d_2}{d_3} \frac{d_3}{d_4} \frac{d_4}{d_5} + \alpha_1 \frac{d_1}{d_2} \frac{d_2}{d_3} \frac{d_3}{d_4} \left( \alpha_1 - \alpha_2 \left( \frac{d_1}{d_2} \right)^4 \right)}} \]

\[ v_1 = \sqrt{\frac{2gh \frac{\rho_\text{water}}{\rho_\text{air}}}{\alpha_2 \frac{d_1}{d_2} \frac{d_2}{d_3} \frac{d_3}{d_4} \left( \alpha_1 - \alpha_2 \left( \frac{d_1}{d_2} \right)^4 \right)}} \]

We will also neglect the kinetic energy of the air, \( \alpha_2 \frac{d_1}{d_2} \frac{d_2}{d_3} \frac{d_3}{d_4} \frac{d_4}{d_5} \) when solving back out the inviscid open-topped case. For the inviscid case we did not consider the kinetic energy of the air and this is a minor effect when doing an analysis of the orders of magnitude of these values. The kinetic energy coefficients will also be set to uniform velocity profile values of one:
\[ v_1 = \sqrt{\frac{2gh \rho_{\text{water}}}{\rho_{\text{air}}} \left( 1 - \left( \frac{d_1}{d_2} \right)^4 \right)} \]

\[ v_1 = \sqrt{\frac{2gh}{1 - \left( \frac{d_1}{d_2} \right)^4}} \]

The inviscid solution may be correctly extracted from the viscous variable-topped solution providing a check that these equations are accurately derived.
4.3.3 Explicit Solution for Emptying Time as a Function of Height

The neck velocity, see Equation (4.20), has been solved as a function of known constants and we may use Conservation of Mass, see Equation (4.2), to solve for the time to empty at a given height using integration same as for the viscous and inviscid open-topped solutions:

\[
\frac{\partial h}{\partial t} = \sqrt{\frac{2gh \frac{\rho_{\text{water}}}{\rho_{\text{air}}}}{C_2 + C_3 + \frac{\rho_{\text{water}}}{\rho_{\text{air}}} C_1}} \left( \frac{d_1}{d_2} \right)^2
\]

\[
\int_0^h \frac{\partial h}{h^{\frac{3}{2}}} = \int_0^t \sqrt{\frac{2g \frac{\rho_{\text{water}}}{\rho_{\text{air}}}}{C_2 + C_3 + \frac{\rho_{\text{water}}}{\rho_{\text{air}}} C_1}} \left( \frac{d_1}{d_2} \right)^2 \, dt
\]

\[
2h^{\frac{1}{2}} = \sqrt{\frac{2g \frac{\rho_{\text{water}}}{\rho_{\text{air}}}}{C_2 + C_3 + \frac{\rho_{\text{water}}}{\rho_{\text{air}}} C_1}} \left( \frac{d_1}{d_2} \right)^2 t
\]

\[
t = 2h^{\frac{1}{2}} \sqrt{\frac{C_2 + C_3 + \frac{\rho_{\text{water}}}{\rho_{\text{air}}} C_1}{2g \frac{\rho_{\text{water}}}{\rho_{\text{air}}}}} \left( \frac{d_2}{d_1} \right)^2
\]

Equation (4.21) is the final solution for the time it will take for a liquid of given height in a variable-topped bottle to drain (with adjustment from Equation (4.6)). If the

\[
C_1 = K_{2 \rightarrow 1} + \alpha_1 - \alpha_2 \left( \frac{d_1}{d_2} \right)^4
\]

\[
C_2 = K_{3 \rightarrow 2} \left( \frac{d_1}{d_2} \right)^4 - \alpha_3 \left( \frac{d_1}{d_3} \right)^4 + \alpha_2 \left( \frac{d_1}{d_2} \right)^4
\]

\[
C_3 = \left( \frac{d_1}{d_3} \right)^4 \left( K_{4 \rightarrow 3} + \alpha_3 \right)
\]
total time to empty is desired, then $h$ should be set to $H$ in which case $t$ becomes $T_{empty}$. Note that $K_{4\rightarrow3}$ is considered the orifice efficiency coefficient.
4.3.4 Viscous Variable-Topped Model Results

The viscous model for a variable-topped bottle results in the analytical solution of Equation (4.21).

The variable-topped viscous model is the third step toward forming an inverted bottle model. An example case for this model from the Mayer data is displayed in Figure 4.10 where there is a 1.18 mm perforation in the top of the bottle. The good fit is partially driven by the fitted orifice efficiency coefficient.

![Figure 4.10: Plot of viscous-variable analytical model against a variable-topped Type B bottle of neck diameter 25.4 mm and perforation diameter of 1.18 mm.](image)

As expected, the viscous variable-topped model does a good job modeling the jetting component of the inverted bottle. However, this model cannot recognize when the flow shifts from jetting to glugging nor model the glugging time to empty. Without glugging considerations the trends in time to empty with varying perforation diameter disappear, see Figure 4.11. To improve the model, we will enable a change in flow regime from jetting to glugging, however, this will need to be done numerically.
Figure 4.11: The trend of time to empty changing as different sized perforations are used with predictions of the viscous variable-topped analytical model for a Type B bottle with neck 25.4 mm.
Chapter 5

NUMERICAL SOLUTIONS

5.1 Viscous Variable-Topped Model with Glugging Effect Results

Adding the ability to transition from jetting to glugging flow is the final step to fully model an inverted bottle. To check the flow regime, the numerical model will step through time to calculate fluid properties and use the bubble velocity to check against the neck velocity at each given time step. When the neck velocity is lower than the bubble velocity, the model will know to transition from jetting to glugging. Upon transitioning, the established time to empty equation generated by Clanet with specified bubble fraction, neck diameter, and bottle diameter will take effect assigning linear height versus time behavior for the remaining of the emptying, see Equation (5.1) and Appendix B [2]. Here $h(t = t_{trans})$ indicates the height of the liquid in the bottle at transition and $t_{glug}$ represents the total time associated with glugging after transition occurs. Notably, there is no single analytical equation that captures both glugging and jetting behavior. As such the previous variable-topped solution model and the Clanet model are used with a logic check dictating the transition between the two.

$$t_{glug} = \frac{h(t = t_{trans})}{\alpha \sqrt{gd_2}} \left( \frac{d_2}{d_1} \right)^{\frac{5}{2}}$$  \hspace{1cm} (5.1)

As expected, the viscous variable-topped model with glugging does a fair job modeling the jetting and glugging components of the inverted bottle, however the point of transition does not line up with the experimental data, see Figure 5.1. This could be
attributed to either a failure of the bubble velocity transition hypothesis or the previously identified discrepancy between the bubble velocity coefficient and the observed velocity at transition.

Figure 5.1: Plot of viscous variable-topped with glugging effects numerical model against a variable-topped Type B bottle of neck diameter 25.4 mm and perforation diameter of 1.18 mm.

Despite the discrepancy between the transition velocity, the viscous variable-topped model with glugging effects provides a servicable model of the inverted bottle that can predict the time to empty inverted bottles and produce trends similar to experimental results when considering time to empty across varying perforation diameters, see Figure 7.3.
Figure 5.2: Plot of time to empty against upper diameter for a Type B bottle with 25.4 mm neck.
CFD simulations were completed to help validate and improve the models developed. This presented several computational challenges that resulted in simulations being confined to the modeling of simple open-topped bottles, the first bubble of closed-topped bottles, and select variable-topped bottles.

For a Type A bottle, simulations for an open-topped case, a closed-topped case, and a variable-topped case with perforations of 4 mm and 6 mm were completed. Each Fluent solution will use these dimensions and be axisymmetric.
6.1 CFD Model Mechanics

The Volume of Fluid (VOF) model will be used for this analysis of the inverted bottle. The VOF model can model two fluids by solving a set of momentum equations and tracking the volume fraction for each of the fluids [16].

The VOF model is typically used to compute time-dependent solutions and relies on the two fluids being simulated not interpenetrating, or not having significant mixing of the phases. For each phase introduced there exists a volume fraction of the phase within a computational cell. The properties of the cell are dependent upon the volume-averaged parameters of each phase. A cell can be empty of a fluid, entirely full of a fluid, or contain an interface between multiple fluids.

6.1.1 Volume of Fluid Model Overview

In a multiphase flow, the tracking of the interface between phases can be achieved by using continuity on the volume fraction of a phase [16]. A single momentum equation is solved and dependent on the volume fraction of the phases and their properties for density and viscosity. Similarly, the energy equation is solved using properties determined by the phases in a cell. The VOF model can also account for the effects of surface tension between phases.

When modeling the interface between fluids using the VOF model, either the Geometric Reconstruction Scheme or the Donor-Acceptor Scheme can be employed to generate an interface shape (see Figure 6.1). The Geometric Reconstruction Scheme is more accurate and applicable for general unstructured meshes while the Donor-Acceptor Scheme is used to limit numerical diffusion at the interface. For this project, the Geometric Reconstruction Scheme is implemented as no issues with numerical dif-
fusion arose. If numerical diffusion had become a problem with the simulations, the Donor-Acceptor Scheme would have been used or the mesh would have been further refined.

![Figure 6.1: ANSYS Fluent figure displaying how the interface calculations differ for the Geometric Reconstruction Scheme and the Donor-Acceptor Scheme [16].](image)

### 6.1.2 Volume of Fluid Model Limitations

For the ANSYS Fluent application of the VOF model there are several limitations. These limitations are outlined along with how they may affect simulation. The limitations include: the VOF model can only be used with the pressure-based solver, the VOF model does not allow for void regions, and the VOF model does not allow for the modeling of streamwise periodic flow.
The VOF model only works with the pressure-based solver and also dictates that only one of the phases can be defined as a compressible ideal gas. The simulation of inverted bottles does not use compressible flows that will require a density-based solver but instead uses incompressible flows well below 0.3M for both phases. As such, the pressure-based solver is ideal for simulation and the incompressible flow modeled fits within the constraints of the VOF model.

Void regions where no fluid is present are not allowed when using the VOF model. Each individual region must be filled with a single fluid phase or combination of phases. The simulations are run with two regions (water and air) with each region indicating the fluid present in the initial state. Under this constraint, the bottle walls will not be included as a region.

Periodic flows occur when the geometry of the stream is replicated multiple times preventing a single fully developed solution, but instead presenting a pattern of solutions. For example, multiple rods added in a pipe flow at uniform steps can prevent the pipe flow from becoming fully developed presenting a periodic flow. The geometry of the inverted bottle is in no way periodic and should not trouble the VOF model.

### 6.1.3 Inverted Bottle CFD Model

The properties of the two phases (air and water) are assumed to be constant for these simulations. The simulation is transient and axisymmetric as well as explicitly solved.

Data is collected using an adaptive time advancement. This method allows for the maximum timestep to occur while still producing valid results. Validity of results is checked using the Global Courant Number which is dependent upon mesh size and time step. The time to empty as well as the fluid height over time are the desired outputs. Liquid height can be found by checking the volume of fluid in the system.
Wall boundary conditions are applied to the edges of the bottle, pressure outlet to the outlet of the bottle, and pressure inlet to the inlet of the bottle. As a note, the wall adhesion angle needs to be specified for air and water for each wall surface (90 degrees for the non-wet wall and 175 degrees for the wet wall).

The mesh is generated to capture the full geometry of an inverted bottle using a replay script. As such, the replay script allows for the ability to change the dimensions of the perforation diameter on the top of the bottle as well as the neck and bottle diameters, see Figure 6.2. The mesh is built along the x-axis with “ground” being in the positive x-direction.

![Axisymmetric, open-topped inverted bottle mesh along the x-axis.](image)

**Figure 6.2:** Axisymmetric, open-topped inverted bottle mesh along the x-axis.

Notably, the mesh of Figure 6.2 is composed of 2 phases with the lighter orange symbolic of water and the darker purple symbolic of air. See Appendix C for the replay script to generate an inverted bottle mesh. With the inverted bottle mesh simulations can be run with data extracted from Fluent.

For each simulation, volume of water within the bottle was used to track the height of water in the bottle. As such, when the water approached the outlet, at a given point it would “punch through” the outlet with the neck no longer being full of water. To remove neck effects from comparisons, we consider the Fluent bottle to be empty with respect to the body of the bottle when it is calculated by volume that there is 10 mm of water height left in the main bottle. Below this height, the draining models used are no longer valid due to neck effects and water resting on the edge of the internal lip connecting the body of the bottle to the neck.
6.1.4 The Courant number

Before delving into CFD results it is relevant to discuss the Courant number. The Courant number is a convergence condition used when solving numerical equations for explicit time integration schemes. If exceeded, a simulation will provide incorrect results.

The Courant number is simply a combination of simulation velocity $u$, time step $\Delta t$, and mesh size $\Delta x$, see Equation (6.1). For too small of a mesh or too large of a time step the simulation will not converge and produce inaccurate results. The Fluent default target for Courant number is 2 with the Courant limit of 250 being used to determine if a simulation is too inaccurate.

\[
\text{Courant Number} = \frac{u\Delta t}{\Delta x} \tag{6.1}
\]

It was found that for the VOF simulations, when small mesh sizes were used, the Courant number would grow beyond the required limit for accuracy and the simulation diverge. To avoid these issues and use the resources allowed for this document, it was found that a more coarse mesh resulted in convergence with reasonable times to model. About 1.5 seconds of simulation for a 5 mm mesh size open-topped bottle took about 15 minutes and about 2 seconds of simulation time for a 5 mm mesh size variable-topped bottle took about 5 to 15 hours.

6.2 Open-Topped Simulation

The open-topped mesh is the simplest case to model effectively. It consists of a pressure inlet and pressure outlet, both set to atmospheric, enclosed by walls. Several
meshes were used to find the best combination resulting in valid and reasonable results.

6.2.1 Diverging Open-Topped Solutions

Initial modeling attempts for an open-topped solution used the Fluent default target Courant value of 2. This was ultimately found to be too high when using an adaptive time step, however, three mesh sizes were simulated using the Courant value of 2 with the diverging results discussed.

The first open-topped solution that diverged was an open-topped inverted bottle using a 1 mm mesh size, see Figure 6.3.

![Figure 6.3: 1 mm mesh of an open-topped bottle.](image)

Upon running the 1 mm mesh open-topped bottle using Fluent codes, the solution quickly diverged by the Courant number metric. Reversed flow occurred across the inlet and outlet of the mesh due to the refined nature of the mesh being associated with too large of a time step. A plot of the position of phases upon divergence of the 1 mm open-topped simulation is included in Figure 6.4. In an attempt to alleviate this issue, the mesh size was increased to reduce the Courant number.
Figure 6.4: Phases (light red is air, dark blue is water) of a 1 mm mesh of an open-topped bottle upon divergence from Courant number target of 2 at 0.05 seconds.

The second open-topped solution that diverged was an inverted bottle using a larger 2 mm mesh size to reduce the Courant number, see Figure 6.5.

Figure 6.5: 2 mm mesh of an open-topped bottle.

Upon running the 2 mm mesh using Fluent codes, the solution was found to not diverge by the Courant number metric, but behaved unexpectedly with a high pressure point being generated at the air/water interface on the axisymmetric line, see Figure 6.6.

Figure 6.6: Pressure anomaly in 2 mm open-topped mesh where light spike in pressure vacuum reduced outlet flow.
The high pressure found in the 2 mm mesh size open-topped simulation resulted in the height of the liquid in the bottle moving very slowly compared to what would be expected. In this case, the simulation is experiencing a mesh size that is still too refined for the given time step used. As a result odd conditions occurred that did not reflect reality, see Figure 6.7. A notable takeaway from the failure of this simulation is to always check the validity of simulations beyond the metrics provided by Fluent. Similar to the 1mm mesh, in an attempt to resolve this the mesh size was further increased to 5 mm.

![Figure 6.7: Phases (light red is air, dark blue is water) of a 2mm mesh of an open-topped bottle after reaching a semi-steady state. Notably, images of the phases appear as expected but the simulated result is incorrect.](image)

The third open-topped solution that diverged was an inverted bottle using a larger 5 mm mesh size to reduce the Courant number further, see Figure 6.8.

![Figure 6.8: 5 mm mesh of an open-topped bottle.](image)

Upon running the 5 mm open-topped mesh using Fluent codes, the mesh was found to be within the Courant number metric and exhibit draining behavior, however, from
observation the fluid phases the simulation was performing in ways nonreflective of reality, see Figure 6.9.

![Figure 6.9: Phases (light red is air, dark blue is water) from the 5 mm mesh of an open-topped bottle due to too large of a time step with a coarse mesh.](image)

The important metric to fix these simulation inaccuracies lies in the Courant number. In these cases, the time step was simply too large and increasing the mesh size was not enough to allow for proper convergence of the simulation. The adaptive time step feature in Fluent uses the Courant number to choose each time step and the time steps being chosen were too large and led to divergence. To avoid divergence and attain reasonable results, the target Courant number should be reduced. This reduction leads to attainable and reliable results.

### 6.2.2 Open-Topped Solutions

The target Courant number was modified from 2 to 0.1 to take a slower simulation approach so that less calculation and movement between the fluid phases would occur for each time step. With this implementation, a model was reached that presents a reasonable simulation of an open-topped inverted bottle. The 2 mm open-topped mesh was revisited upon successfully running a 5 mm open-topped mesh and run
with the lower time step conditions (about 1 hour for 2 seconds of simulation of a 2 mm mesh size open-topped bottle). A 3.5 mm mesh was also simulated and all three open-topped simulations with different mesh sizes are visually compared in Figure 6.10.

![Figure 6.10](image)

**Figure 6.10**: Modeled results from a 2.0 mm, 3.5 mm, and 5.0 mm mesh of an open-topped bottle shown over the time to empty (light red is air, dark blue is water).

### 6.2.3 Model Convergence

A convergence plot was also developed in comparison with the analytical results, see Figure 6.11.
Figure 6.11: Convergence plot for open-topped bottle showing different mesh sizes used. Note the 3.5 mm and 2 mm mesh size simulations are very close and overlap when plotted.

A key takeaway from Figures 6.10 and 6.11 is that the three mesh sizes of 5 mm, 3.5 mm, and 2 mm converge to the same time to empty results. As such, the 5 mm coarse mesh will be used for the closed-topped and variable-topped cases considered to minimize computation time.

A Richardson extrapolation technique is used to estimate the error of the open-topped solution. The first step of the technique is to define a representative cell size, $h$ for each of the mesh sizes, see Equation (6.2). For the 2 mm (2343 cells), 3.5 mm (1007 cells), and 5 mm (551 cells) meshes the respective representative cell sizes are 2.2, 3.3, and 4.5.

$$h = \left[ \frac{1}{N} \sum_{i=1}^{N} (\Delta A_i) \right]^{\frac{1}{2}} \quad (6.2)$$
The next step of the technique is to choose a critical simulation value, $\phi$. For the open-topped solution the value will be the time to empty which for the 2 mm, 3.5 mm, and 5 mm meshes is $1.496$ s, $1.478$ s, and $1.446$ s respectively, see Figure 6.12.

For the next step we will calculate the apparent order, $p$, of the solution by assuming extrapolated values, $\phi^{21}_{ext}$ and $\phi^{32}_{ext}$, are equivalent, see Equations (6.3) and (6.4).

Let $h_1 < h_2 < h_3$ where $r_{21} = \frac{h_2}{h_1}$ and $r_{32} = \frac{h_3}{h_2}$

$$\phi^{21}_{ext} = \frac{(r^{p}_{21} \phi_1 - \phi_2)}{(r^{p}_{21} - 1)} \quad (6.3)$$

$$\phi^{32}_{ext} = \frac{(r^{p}_{32} \phi_2 - \phi_3)}{(r^{p}_{32} - 1)} \quad (6.4)$$

This yields an apparent order, $p$, of 2.56 for the solution.

With the developed values several error estimates may be made that will be totaled into our estimated CFD error.
An approximate relative error of 0.0121 is found, see Equation (6.5).

\[ e_{a}^{21} = \frac{\phi_{1} - \phi_{2}}{\phi_{1}} \]  

(6.5)

An extrapolated relative error of 6.53e - 4 is found, see Equation (6.6).

\[ e_{ext}^{21} = \frac{\phi_{ext}^{21} - \phi_{1}}{\phi_{ext}^{21}} \]  

(6.6)

A fine-grid convergence index of 3.71e - 41 is found, see Equation (6.7).

\[ GCI_{fine}^{21} = \frac{1.25e_{a}^{21}}{r_{21}^{p} - 1} \]  

(6.7)

Combining these error estimates yields a CFD error tolerance of 0.0128 seconds. This level of error is acceptable for the given conditions of the simulation and yields a 0.9% error in the time to empty. Notably, the closed-topped and variable-topped meshes are simulated with a 5 mm mesh instead of a 2 mm or 3.5 mm mesh size to develop a usable result for the given resources available.
6.3 Closed-Topped Simulation

The ability of Fluent to model the first bubble pulled into an inverted bottle was examined. It was found that Fluent could simulate the entry of the first bubble into the bottle, notably the entry behavior expected is axisymmetric, see Figure 6.13. While the bottle geometry of Figure 6.13(a) and 6.13(b) are different the images suggest Fluent can simulate the entry of a bubble. However, more work is required to tune the first bubble simulation to be realistic.

![Figure 6.13](image)

**Figure 6.13:** (a) Fluent simulation of bubble entry for a 2mm mesh closed-topped Type A bottle after simulation start (light red is air, dark blue is water). (b) Mayer images of bubble entry after experiment start [5]. (a) and (b) use different bottle geometries, but are compared to show the similarities in bubble entry.

The axisymmetric Fluent model does not fully match the experimental first bubble movements, see Figure 6.13. The Fluent bubble acts chaotically after detaching and
does not retract from the neck of the bottle to the same extent of the Mayer bubble. It is expected that because of these discrepancies, a simulation of emptying time for a glugging bottle would be unreliable. However, there is value in simulating the conditions allowing for bubble rise in the variable-topped case as it will allow for verification or rejection of the bubble velocity metric for transitioning from jetting to glugging.
6.4 Variable-Topped Simulation

Variable-topped bottles with 6 mm and 4 mm perforation diameters were simulated within Fluent using a 5 mm mesh. The 5 mm mesh size was chosen both for most efficient simulation time as well as because the 5 mm, 3.5 mm, and 2 mm meshes for the open-topped solution presented approximately the same time to empty within 0.05 seconds. From the analytical models, it is expected that the variable-topped bottle would take longer to empty and glugging behavior is avoided to maintain validity of the simulation.

6.4.1 6 mm Perforation

The 6 mm perforation mesh, see Figure 6.14, was constructed to have a longer time to empty than the open-topped solution. The mesh took approximately 5 hours to fully simulate from full to empty.

Figure 6.14: 5 mm mesh of a variable-topped bottle with 6 mm perforation.

Figure 6.15 displays height over time for the 6 mm perforation mesh with the analytical model included for comparison.
Figure 6.15: Height versus time plot using the analytical MATLAB model and Fluent simulation for a 6 mm perforation inverted bottle.

Figure 6.16 displays the pressure over time for the 6 mm perforation mesh with the analytical model included for comparison.

Figure 6.16: Pressure versus time plot using the analytical MATLAB model and Fluent simulation for a 6 mm perforation inverted bottle.
### 6.4.2 4 mm Perforation

The 4 mm perforation mesh, see Figure 6.17, was constructed to have a longer time to empty than the 6 mm perforation solution. The mesh took approximately 15 hours to fully simulate from full to empty.

**Figure 6.17:** 5 mm mesh of a variable-topped bottle with 4 mm perforation.

Figure 6.18 displays height over time for the 4 mm perforation mesh with the analytical model included for comparison.

**Figure 6.18:** Height versus time plot using the analytical MATLAB model and Fluent simulation for an emptying 4 mm perforation inverted bottle.

Figure 6.19 displays the pressure over time for the 4 mm perforation mesh with the analytical model included for comparison.
6.4.3 Variable-Topped Simulation Comparison

Figures 6.20 and 6.21 show full pressure and time to empty comparisons for the perforation and open-topped simulations.

**Figure 6.19:** Pressure versus time plot using the analytical MATLAB model and Fluent simulation for a 4 mm perforation inverted bottle.

**Figure 6.20:** Height versus time plot using the analytical MATLAB model and Fluent simulations for an emptying 4 mm and 6 mm perforation inverted bottle.
Figure 6.21: Pressure versus time plot using the analytical MATLAB model and Fluent simulations for an emptying 4 mm and 6 mm perforation inverted bottle.

The analytical models for height versus time and pressure versus time match the trends present in the Fluent simulation with the exception of the “startup and shutdown” behavior. The analytical models operate under the assumption of instantly fully operational, where the acceleration of the fluid from rest is neglected, whereas the Fluent simulation presents the more realistic startup and shutdown conditions. Fluent presents startup behavior with the system accelerating to the fully operational state over $\approx 0.2$ seconds. Fluent also presents shutdown behavior with neck effects when the water pushes through the outlet and then slowly drains under different conditions.

The air gap pressure plot of Figure 6.21 shows the analytical and Fluent models matching with the exception of the startup and shutdown conditions. This similarity places confidence in the Fluent model even when the predicted time to empty is different for the analytical and Fluent models.
6.5 Variable-Topped Solutions with Transition to Glugging

Challenges were experienced when developing a variable-topped mesh that transitions from jetting to glugging and satisfies the Courant number for the Volume of Fluid transient simulation. It was found that for a refined mesh, very small time steps are necessary to capture the two-phase flow behavior. The time step required to achieve useful data for a variable-topped bottle that transitions to glugging is discussed further in Section 7.2.3. The unreliability of bubble simulation brings into question whether a full simulation of the transition from jetting to glugging would be reliable or useful, however, the simulation of a variable-topped bottle transitioning from jetting to glugging would be useful to better explore the conditions under which transition occurs.
Chapter 7

DISCUSSION AND CONCLUSIONS

This project set out to ultimately understand why the time to empty an inverted bottle changed as a perforation is added and how this effect may be modeled.

It was found that the time to empty an inverted bottle required four notable considerations: bubble fraction, glugging versus jetting, bubble velocity, and orifice efficiency coefficient. With these considerations the fluid flow may be modeled whether jetting or glugging from a numerical algorithm.

The CFD work in Fluent further explored the effect perforations had on time to empty and the capability presented by the software to model glugging. The Fluent simulations were found to present reliable results with jetting and the capability to capture a first bubble formation, but unreliable results with glugging.

The culmination of the modeling effort is summarized in Figure 7.1 for the Type A bottle. Importantly the trend of the time to empty increasing and then decreasing as perforation diameter increases matches the data. The points at which the transition from jetting to glugging occur is also well captured by the model.
Figure 7.1: Plot of time to empty against upper diameter for the Type A bottle with results from the analytical, numerical, and CFD models displayed.
7.1 Analytical, Numerical, and CFD Model Comparisons and Discussion

Utilizing the numerical variable-topped viscous model with glugging we can generate figures comparing perforation diameter to time to empty which served as the initial interest for this project.

Using the Mayer data as reference, we can plot time to empty against perforation diameter for a Type B bottle with 12.7 mm outlet diameter, see Figure 7.2. Notably, the increase in time to empty is viewable, however, it does not approach the peak values set by the experimental data. The peak time to empty occurs at a perforation diameter of 0.54 mm and 0.41 mm for the model and experiment respectively.

![Figure 7.2: Plot of time to empty against upper diameter for a Type B bottle with 12.7 mm neck.](image)

Using the Mayer data again as reference, we can plot time to empty against top diameter for a Type B bottle with 25.4 mm outlet diameter, see Figure 7.3. The developed model matches the experimental data fairly well as we would expect. The peak time to empty occurs at a perforation diameter of 1.38 mm and 1.40 mm for the model and experiment respectively.
Using the Mayer data again as reference, we can plot time to empty against top diameter for a Type B bottle with 38.1 mm outlet diameter, see Figure 7.3. The developed model again matches the experimental data fairly well as we would expect. The peak time to empty occurs at a perforation diameter of 2.28 mm and 2.51 mm for the model and experiment respectively.

**Figure 7.3:** Plot of time to empty against upper diameter for a Type B bottle with 25.4 mm neck.

**Figure 7.4:** Plot of time to empty against upper diameter for 38.1 mm neck.
Notable for all figures plotting time to empty against the perforation diameter is that the time to empty increases and then decreases as the perforation is introduced and then expanded. This effect is due to the pressure in the air gap.

For a closed-topped inverted bottle, the pressure in the air gap is immediately below atmospheric. To alleviate this pressure differential, air is drawn into the bottle. This generates glugging with bottle emptying dominated by the expulsion of water for air.

For a variable-topped inverted bottle, the pressure of the air gap is not constant and creates a "pressure drag" that slows the flow. This helps generate the peak in time to empty visible in the plots of time to empty against perforation diameter, see Figure 7.5.

![Figure 7.5: Plot of pressure in the air gap for a variable-topped bottle with critical states called out.](image)

For an open-topped inverted bottle, the pressure of the air gap is always atmospheric and the bottle will empty without any "pressure drag" slowing the flow.
From Figure 7.5 we may step through the emptying process for a variable-topped bottle to see why the peak in time to empty occurs when the modeling is switching from jetting to glugging.

**State 1:**

The pressure drop immediately takes effect in the air gap as the potential energy of the water forces itself out the outlet. The more potential energy the water has, the faster it will exit the outlet and the higher the pressure in the air gap. Glugging does not immediately occur as the top diameter allows flow of air to partially balance the pressure in the air gap. The flow maintains jetting behavior and begins to empty, however, the negative air pressure is applying a “pressure drag” upon the liquid making it drain slower in the jetting regime than if it were simply an open-topped bottle. Notably, only the variable-topped models account for changes in pressure to the air gap.

**State 2:**

The bottle continues to drain in the jetting regime at a slower pace from the “pressure drag”, however, the negative pressure in the air gap slowly decreases. This negative pressure decrease is due to the flow at the outlet slowing. As the bottle drains, there is less potential energy to force liquid out the outlet, so the rate at which liquid exits decreases lessening the pressure in the air gap, however, the pressure differential in the air gap is still balanced at a value that is low enough to not slow the outlet velocity below the bubble velocity initiating glugging.

**State 3:**

The pressure differential in the air gap combined with the declining potential energy of the water in the bottle from draining slows the neck velocity of the liquid past the
bubble velocity. Once the bubble velocity is greater than the neck velocity, bubbles form at the outlet and glugging is initiated. The pressure in the air gap is now impacted by both the air flow through the perforation as well as the air flow from rising bubbles. The numerical variable-topped model can capture this transition whereas the analytical models cannot.

**State 4:**

Glugging continues to be the dominant mode in which the bottle is emptied. The numerical variable-topped model uses Clanet’s equation for glugging to determine the time to empty from when glugging occurs [2].

Of significance to this result is that we are observing a different mechanism by which glugging is initiated, see Figure 7.6.

![Figure 7.6](image)

**Figure 7.6:** Plot of time to empty against perforation diameter for a Type B bottle with 38.1 mm neck. Emphasis is placed on glugging (method 1 or method 2) and jetting behaviors.

**Method 1 by which glugging occurs (closed-topped):**
The pressure in the air gap drops as water begins to exit. The pressure drop becomes so extreme that the outlet velocity instantly is less than the bubble velocity and air begins to enter the bottle to alleviate the negative pressure.

**Method 2 by which glugging occurs (variable-topped):**

The flow slows from a combination of lack of potential energy and flow resistant pressure drag until the outlet velocity approaches the bubble velocity. Once the bubble velocity is greater than the outlet velocity, bubbles begin to travel upward within the bottle initiating glugging.
7.2 Limitations

The three limitations of this work that could be improved upon are the understanding of the bubble fraction, the understanding of the bubble velocity, and CFD simulation of the inverted bottle as it transitions from jetting to glugging.

7.2.1 Bubble Fraction Limitations

The bubble fraction determines the rate at which liquid exits the bottle and for this work, neck geometry and best engineering judgment is used to best approximate the bubble fraction, see Appendix B. Exploration of a theory based model beyond best judgment would benefit this work and is a notable consideration for future work.

7.2.2 Bubble Velocity Limitations

The bubble velocity determines when the flow transitions from jetting to glugging. Depending on when this transition occurs, the flow will experience a combination of quicker glugging or slower pressure dragged jetting. A lower bubble velocity generates a higher peak in the time to empty versus perforation diameter plot. The Wallis equation used for this work to determine the bubble velocity coefficient is comprehensive, but struggles to match our results for diameters under 25 mm. It is thought that the bubble fraction coefficient changes quickly for small diameters so small deviations in measurement can change the bubble velocity substantially or the outlet diameter for different neck geometries is perhaps an imperfect value to use with this equation.
7.2.3 CFD limitations

Challenges with efficiently simulating a variable-topped bottle with small perforations to observe a transition to glugging (on the order of 1.5 mm for the Type A bottle) were encountered. It was found that very small time steps on the order of 1e-7 seconds were required to generate a converging solution. Simulating these perforations and observing a first bubble entry after jetting was deemed too computationally expensive for this work.

A summary of findings trying to simulate the variable-topped bottle are discussed in the following. A 2 mm mesh in the body of the bottle and 0.7 mm mesh in the air inlet was created for these attempts. These mesh sizes were chosen from experience with the open-topped bottle and ensuring that there was more than one cell in a given axis direction for the inlet, see Figure 7.7. For considerations on simulation time, the resources for this project could complete \( \approx 100 \) time steps per minute using 3 parallel Fluent licenses.

![Variable 2 mm bottle and 0.7 mm inlet mesh.](image)

**Figure 7.7:** Variable 2 mm bottle and 0.7 mm inlet mesh.

7.2.3.1 1e-7s Time Step (Constant Time Step)

The 1e-7 second time step was run for about 0.0006 simulation seconds (one hour) and found to not diverge during this time period. Notably, the velocity and pressure gradients of the bottle used were well defined and of reasonable values, see Figures 7.8 and 7.9. However, it cannot be confirmed using the resources available if this implementation will be able to complete without divergence.
Figure 7.8: Pressure plot from the variable-topped mesh at 0.0002 seconds for 1e-7s time step showing convergence for the given time.

Figure 7.9: Velocity plot at air inlet from the variable-topped mesh at 0.0002 seconds for 1e-7s time step showing convergence for the given time.

These smooth gradients and lack of divergence suggest that the 1e-7 time step may effectively model the variable-topped bottle. The adaptive approach, which evaluates the Courant number each time step to choose a suitable next time step, was explored next to see if a more efficient simulation method could be implemented.
7.2.3.2 0.1 Courant Number (Adaptive Time Step)

A starting point of 0.1 was used for evaluating the optimal target Courant number. The adaptive time step for this simulation was on the order of 1e-4s and 1e-5s which resulted in divergence at 0.007 simulation seconds, see Figure 7.10. This indicates that a smaller time step is required for convergence of the model.

Figure 7.10: Phases (light red is air, dark blue is water) from the variable-topped mesh at 0.007 seconds for Courant number target value of 0.1 showing divergence.

7.2.3.3 0.05 Courant Number (Adaptive Time Step)

Next a Courant number of 0.05 was used which maintained a simulation time step on the order of 1e-5s. The simulation diverged at 0.030 simulation seconds which is about four times further than the model using a courant number of 0.1 indicating that the model is being brought closer to convergence, but still requires a smaller time step, see Figure 7.11.
7.2.3.4 0.01 Courant Number (Adaptive Time Step)

Next a Courant number of 0.01 was used which maintained a simulation time step on the order of $1e^{-6}$s. The simulation did not diverge and reached a simulation time of 0.063 and continued to converge (2.5 hours to reach 0.063 seconds simulation time), see Figure 7.12. More extensive computational processing would be required to verify that convergence will continue with this given time step.

**Figure 7.12:** Velocity plot at air inlet from the variable-topped mesh at 0.040 seconds for Courant number target value of 0.01 showing continued convergence for the given time.
7.2.3.5 0.001 Courant Number (Adaptive Time Step)

Next a Courant number of 0.001 was used which maintained a simulation time step on the order of 1e-6 and 1e-7. The simulation was allowed to run for 0.0135 simulation seconds (1.5 hours) with no signs of divergence. Notably, the pressure contour is again well defined, see Figure 7.13. If the 0.01 Courant number simulation were to diverge, this would be the next time step to look at implementing for the model.

Figure 7.13: Pressure plot at air inlet from the variable-topped mesh at 0.0045 seconds for Courant number target value of 0.001 showing convergence for the given time.

7.2.3.6 Future Solutions

The most notable future solution is to gain access to more computation power for running simulations. With higher computation power, smaller meshes can be run with small timesteps that would allow accurate modeling of the transition from jetting to glugging for the inverted bottle in a CFD format.


APPENDICES

Appendix A

EXPERIMENTAL DATA

The following is experimental data on the time to empty inverted bottles by Mayer, Kubie, and Clanet [5, 14, 2]. The data for Kubie and Clanet was extracted by hand from graphs provided by these authors. The Mayer data for the Type B bottle has indications where the flow transitioned from a jetting to glugging regime using grey cells.
Table A.1: Experimental data provided by Hans Mayer for the Type B bottle with a neck diameter of 12.7 mm [5].

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Table A.3: Experimental data provided by Hans Mayer for the Type B bottle with a neck diameter of 38.1 mm [5].

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Table A.4: Continued experimental data provided by Hans Mayer for the Type B bottle with a neck diameter of 38.1 mm

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[5]
Table A.5: Experimental time to empty data provided by Hans Mayer for the Type A bottle for various perforation diameters.

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<th>Avg. Time to Empty (seconds)</th>
<th>Std Dev on Time to Empty (seconds)</th>
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Table A.6: Kubie data extracted for an inverted bottle with bottle diameter 190 mm [14].

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<th>The time (seconds) at which the water was at a given height for a closed-topped bottle of outlet diameter (mm):</th>
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Table A.7: Clanet data extracted for an inverted, closed-topped bottle with bottle diameter 174 mm [2].

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Appendix B

BBBLE FRACTION ANALYSIS

Appendix B will explore the bubble fraction by first examining the role it plays in glugging, then finding the bubble fraction from multiple sources of experimental data and comparing them. These will appear in the order:

- B.1: Derivation and Explanation of Clanet’s Time to Empty Equation
- B.2: Bubble Fraction of Kubie Data
- B.3: Bubble Fraction of Mayer Data
- B.4: Bubble Fraction Comparison
B.1 Derivation and Explanation of Clanet’s Time to Empty Equation

The following is a rederivation of the emptying time of a bottle as shown by Clanet in [2] with an emphasis on the bubble fraction, see Figure B.1.

To introduce the bubble fraction, Clanet uses a closed-topped model and notes that the outlet flow is constrained by conservation of mass. Thus, when glugging occurs the mass flow rate of the water out is dependent upon how much air is allowed to enter the bottle. The bubble fraction is the fraction of air that enters the bottle in a glugging period and determines how much water exits the bottle, see Equation (B.1).

\[ U_i D_0^2 = \alpha U_b d^2 \]  

Equation (B.1) relates the velocity of the bottle water level, \( U_i \), the bottle diameter, \( D_0 \), the bubble velocity, \( U_b \), the outlet diameter, \( d \), and the bubble fraction, \( \alpha \). Equa-
tion (B.1) uses the bubble fraction to establish conservation of mass for the fluid flow and connect the overall rate of bottle emptying to the glugging of the bottle.

Clanet uses this relation while noting that the bubble velocity is proportional to the square root of gravity and outlet diameter, see Equation (B.2), and that the time to empty a given cylinder is simply the length of the cylinder over the bottle water level velocity, see Equation (B.3).

\[ U_b \propto \sqrt{gd} \quad \text{(B.2)} \]

And:

\[ T_e = \frac{L}{U_i} \quad \text{(B.3)} \]

Through several steps outlined below we can reach Clanet’s final equation starting with Equation (B.1) and deriving Equation (B.4).

\[ U_i D_0^2 = \alpha d^2 \sqrt{gd} \]

\[ U_i = \alpha \sqrt{g} \frac{d^{\frac{5}{2}}}{D_0^2} \]

\[ T_e = \frac{L}{\alpha \sqrt{g} \frac{D_0^2}{d^{\frac{5}{2}}}} \]

Or:

\[ T_e = \frac{L}{\alpha \sqrt{g} D_0} \left( \frac{D_0}{d} \right)^{\frac{5}{2}} \quad \text{(B.4)} \]

From Clanet’s approximation of the emptying time of an unrestricted cylinder, \( T_{e0} \), we can see within a few steps that he chose a bubble fraction of \( \frac{1}{3} \) for his work, see Equation (B.5).

\[ T_{e0} \approx \frac{3L}{\sqrt{g} D_0} \quad \text{(B.5)} \]
The relation between emptying time of a bottle and emptying time of an unrestricted cylinder is given by Clanet in Equation (B.6).

\[
\frac{T_e}{T_{e0}} = \left( \frac{D_0}{d} \right)^{\frac{5}{2}} \quad \text{(B.6)}
\]

Equations (B.5) and (B.6) together yields Equation (B.7) which matches the Clanet interpretation that is used throughout his paper and matches his data with a given bubble fraction of \(\frac{1}{3}\).

\[
T_e = \frac{3L}{\sqrt{gD_0}} \left( \frac{D_0}{d} \right)^{\frac{5}{2}} \quad \text{(B.7)}
\]

Equation (B.7) specifies the time for a glugging bottle with bubble fraction of \(\frac{1}{3}\) to empty. It is important to note, that the bubble fraction may be between 0 (there is no bubble movement) and 1 (there is significant bubble movement in the form of slugs). By conservation principles, the bubble fraction must be locked between 0 and 1.

Another note is that for this derivation, we ignore any constants presented by the bubble velocity proportionality, see Equation (B.2). We believe that the bubble velocity coefficient is ultimately connected to the bubble fraction and that we still gain insight into the bubble fraction by setting this value to one.
B.2 Bubble Fraction of Kubie Data [14]

We may apply Clanet’s Equation, see Equation (B.8), to the Kubie data which used a 190 mm bottle height, see Equation (B.9).

\[ T_e = \frac{L}{\alpha \sqrt{g D_0}} \left( \frac{D_0}{d} \right)^{\frac{3}{2}} \]  

(B.8)

\[ T_e = \frac{1.0}{\alpha \sqrt{9.81 \times 0.19}} \left( \frac{0.19}{0.19} \right)^{\frac{3}{2}} \]  

(B.9)

For the three cases presented by Kubie simple relations between the time to empty and bubble fraction may be developed, see Equations (B.10), (B.11), (B.12).

For outlet of 12 mm:

\[ T_e = \frac{1}{\alpha \sqrt{9.81 \times 0.19}} \left( \frac{0.19}{0.012} \right)^{\frac{3}{2}} \]  

\[ T_e = \frac{731}{\alpha} \]  

(B.10)

For outlet of 25 mm:

\[ T_e = \frac{1}{\alpha \sqrt{9.81 \times 0.19}} \left( \frac{0.19}{0.025} \right)^{\frac{3}{2}} \]  

\[ T_e = \frac{117}{\alpha} \]  

(B.11)

For outlet of 40 mm:

\[ T_e = \frac{1}{\alpha \sqrt{9.81 \times 0.19}} \left( \frac{0.19}{0.040} \right)^{\frac{3}{2}} \]  

\[ T_e = \frac{36}{\alpha} \]  

(B.12)
The Kubie data with respective time to empties of 1405, 223, and 88 for the 12 mm, 25 mm, and 40 mm outlet diameters correlate to bubble fraction values of those seen in Table B.1. This yields an approximate bubble fraction, $\alpha$, for the Kubie data of $\approx 0.49$.

**Table B.1:** Bubble fraction values for Kubie data.

<table>
<thead>
<tr>
<th>Outlet Diameter</th>
<th>Bubble Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>12 mm</td>
<td>0.520</td>
</tr>
<tr>
<td>25 mm</td>
<td>0.524</td>
</tr>
<tr>
<td>40 mm</td>
<td>0.409</td>
</tr>
<tr>
<td>Average</td>
<td>0.485</td>
</tr>
</tbody>
</table>
B.3 Bubble Fraction of Mayer Data [5]

We may further apply Clanet’s time to empty equation to the Mayer data for Type B bottles with a bottle height of 355 mm, see Equation (B.13). Note that only the closed topped cases that are exclusively glugging are used to find the bubble fractions.

\[
T_e = \frac{1.0}{\alpha \sqrt{9.81 \times 0.355}} \left( \frac{0.355}{d} \right)^{\frac{5}{2}}
\]  

(B.13)

For the three outlets presented by Mayer simple relations between time to empty and bubble fraction may be developed, see Equations (B.14), (B.15), and (B.16).

For outlet of 12.7 mm:

\[
T_e = \frac{0.635}{\alpha \sqrt{9.81 \times 0.355}} \left( \frac{0.355}{0.0127} \right)^{\frac{5}{2}}
\]

\[
T_e = 1406 / \alpha
\]  

(B.14)

For outlet of 25.4 mm:

\[
T_e = \frac{0.635}{\alpha \sqrt{9.81 \times 0.355}} \left( \frac{0.355}{0.0254} \right)^{\frac{5}{2}}
\]

\[
T_e = 248 / \alpha
\]  

(B.15)

For outlet of 38.1 mm:

\[
T_e = \frac{0.635}{\alpha \sqrt{9.81 \times 0.355}} \left( \frac{0.355}{0.0381} \right)^{\frac{5}{2}}
\]

\[
T_e = 90 / \alpha
\]  

(B.16)
The Mayer data with respective time to empties of 1695, 252, and 118 for the 12.7 mm, 25.4 mm, and 38.1 mm outlet diameters correlate to bubble fraction values of those seen in Table B.2. This yields an approximate bubble fraction, $\alpha$, for the Mayer data of $\approx 0.86$.

**Table B.2**: Bubble fraction values for Mayer data.

<table>
<thead>
<tr>
<th>Outlet Diameter</th>
<th>Bubble Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>12.7 mm</td>
<td>0.829</td>
</tr>
<tr>
<td>25.4 mm</td>
<td>0.984</td>
</tr>
<tr>
<td>38.1 mm</td>
<td>0.763</td>
</tr>
<tr>
<td>Average</td>
<td>0.859</td>
</tr>
</tbody>
</table>
B.4 Bubble Fraction Comparison

Table B.3: Bubble fraction values and outlet lengths for Experimental datasets.

<table>
<thead>
<tr>
<th></th>
<th>Clanet</th>
<th>Kubie</th>
<th>Mayer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bubble Fraction</td>
<td>0.33</td>
<td>0.49</td>
<td>0.86</td>
</tr>
<tr>
<td>Outlet Length (mm)</td>
<td>Thin (~0)</td>
<td>6 to 17</td>
<td>25.4</td>
</tr>
</tbody>
</table>

The bubble fractions from collected experimental data are displayed in Table B.3. From the data, there is a wide variety of possible bubble fractions from the different experiments. A potential source of this discrepancy may come from the geometry of the outlet, see Figure B.2.

Figure B.2: Different experimental outputs used when measuring time to empty [2, 13, 5].

The Clanet data with the lowest bubble fraction has a thin orifice as an outlet. The Kubie data has a mid-range bubble fraction and has a thicker orifice (on the scale of 6 to 17 mm) used as an outlet. The Mayer data has a high bubble fraction and has a long neck used as an outlet (on the scale of 25.4 mm). It is thought that the longer outlets may better allow for the realization of slugs of air to translate into the bottle and generate a higher bubble fraction and therefore, quicker time to empty. More analysis is required in this area to determine if this is the true cause of the discrepancy in bubble fraction, but this trend will be used to best estimate a given bottles bubble fraction.
Appendix C

CFD SETUP: ANSYS ICEM AND ANSYS FLUENT

Appendix C will delve into the setup used for the CFD work of this paper. This will be split between inputs for ANSYS ICEM, where the meshes are generated, and ANSYS Fluent, where the CFD codes are applied:

- C.1: Mesh Generation (ANSYS ICEM)
- C.2: CFD Setup (ANSYS Fluent)
C.1 Mesh Generation (ANSYS ICEM)

ANSYS ICEM is the tool used in this report to generate meshes for simulation. Replay scripts are used to generate the meshes and an example of the 5 mm mesh size Type A bottle with a 6 mm perforation diameter is included in Listing C.1. This may be easily implemented by using replay control in ANSYS ICEM to load and run the script (*File* → *ReplayScripts* → *ReplayControl*).

The mesh generated by the replay file in Listing C.1 may be viewed in Figure C.1.

**Figure C.1**: ICEM ANSYS generated axisymmetric mesh with water (darker color) and air (lighter color).
Listing C.1: Replay script used to generate a Type A bottle in ANSYS ICEM.

# Replay script for inverted bottle
#
# define parameters
set L 17.3
set H 174.5
set d1 21.6
set d2 62.2
set d3 6
set botthick 5
set airgap 20
set maxht 5
#
# define points
ic_geo_new_family PNT
ic_empty_tetin
ic_point {} PNT pnt.00 0,0,0
ic_point {} PNT pnt.01 0,d3/2,0
ic_point {} PNT pnt.02 0,d1/2,0
ic_point {} PNT pnt.03 =L,0,0
ic_point {} PNT pnt.04 =L,d3/2,0
ic_point {} PNT pnt.05 =L,d1/2,0
ic_point {} PNT pnt.06 =L,d2/2,0
ic_point {} PNT pnt.07 =L+H,0,0
ic_point {} PNT pnt.08 =L+H,d3/2,0
ic_point {} PNT pnt.09 =L+H,d1/2,0
ic_point {} PNT pnt.10 =L+H,d2/2,0
ic_point {} PNT pnt.11 =L+H+airgap,0,0
ic_point {} PNT pnt.12 =L+H+airgap,d3/2,0
ic_point {} PNT pnt.13 =L+H+airgap,d1/2,0
ic_point {} PNT pnt.14 =L+H+airgap,d2/2,0
ic_point {} PNT pnt.15 =L+H+airgap+botthick,0,0
ic_point {} PNT pnt.16 =L+H+airgap+botthick,d3/2,0
#
# define curves with boundary names
ic_geo_new_family WALL
ic_curve point WALL crv.00 {pnt.02 pnt.05}
ic_curve point WALL crv.01 {pnt.05 pnt.06}
ic_curve point WALL crv.02 {pnt.06 pnt.10}
ic_curve point WALL crv.03 {pnt.10 pnt.14}
ic_curve point WALL crv.04 {pnt.14 pnt.13}
ic_curve point WALL crv.05 {pnt.13 pnt.12}
ic_curve point WALL crv.06 {pnt.12 pnt.16}
ic_geo_new_family INLET
ic_curve point INLET crv.07 {pnt.15 pnt.16}
ic_geo_new_family OUTLET
ic_curve point OUTLET crv.08 {pnt.00 pnt.01}
ic_curve point OUTLET crv.09 {pnt.01 pnt.02}
ic_geo_new_family SYMMETRY
ic_curve point SYMMETRY crv.10 {pnt.00 pnt.03}
ic_curve point SYMMETRY crv.11 {pnt.03 pnt.07}
ic_curve point SYMMETRY crv.12 {pnt.07 pnt.11}
ic_curve point SYMMETRY crv.13 {pnt.11 pnt.15}
# define surfaces with zone name
ic_geo_new_family INTERIOR
ic_curve point INTERIOR crv.14 {pnt.01 pnt.04}
ic_curve point INTERIOR crv.15 {pnt.03 pnt.04}
ic_curve point INTERIOR crv.16 {pnt.04 pnt.05}
ic_curve point INTERIOR crv.17 {pnt.04 pnt.08}
ic_curve point INTERIOR crv.18 {pnt.05 pnt.09}
ic_curve point INTERIOR crv.19 {pnt.07 pnt.08}
ic_curve point INTERIOR crv.20 {pnt.08 pnt.09}
ic_curve point INTERIOR crv.21 {pnt.09 pnt.10}
ic_curve point INTERIOR crv.22 {pnt.12 pnt.08}
ic_curve point INTERIOR crv.23 {pnt.13 pnt.09}
ic_curve point INTERIOR crv.24 {pnt.11 pnt.12}

# define surfaces with zone name
ic_geo_new_family FLUID1
ic_surface 2=4crvs FLUID1 srf.00 {0.01 {crv.08 crv.10 crv.15 crv.14}}
ic_surface 2=4crvs FLUID1 srf.01 {0.01 {crv.00 crv.09 crv.14 crv.16}}
ic_surface 2=4crvs FLUID1 srf.02 {0.01 {crv.11 crv.15 crv.17 crv.19}}
ic_surface 2=4crvs FLUID1 srf.03 {0.01 {crv.16 crv.17 crv.20 crv.18}}
ic_surface 2=4crvs FLUID1 srf.04 {0.01 {crv.18 crv.21 crv.02 crv.01}}
ic_geo_new_family FLUID2
ic_surface 2=4crvs FLUID2 srf.05 {0.01 {crv.12 crv.19 crv.22 crv.24}}
ic_surface 2=4crvs FLUID2 srf.06 {0.01 {crv.22 crv.20 crv.23 crv.05}}
ic_surface 2=4crvs FLUID2 srf.07 {0.01 {crv.23 crv.21 crv.03 crv.04}}
ic_surface 2=4crvs FLUID2 srf.08 {0.01 {crv.13 crv.24 crv.06 crv.07}}

# set meshing params surface {srf.01 srf.02 srf.03 srf.04 srf.05 srf.06 srf.07 srf.08} emax $maxht emin 0 ehgt 0 edev 0 erat 0 ewid 0 nlay 0 hrat 0 prism_height_limit 0 law -1 etyp 2 emethod -1
ic_set_meshing_params surface {srf.01 srf.02 srf.03 srf.04 srf.05 srf.06 srf.07 srf.08} etyp 2 ic_quad2 what surfaces entities {} element 4 proj 1 conver 0.025 geo_tol 0 ele_tol 0.1 dev 0.0 improvement 1 block 0.2 bunch 0 debug 0 adjust_nodes 0 adjust_nodes_max 0 try_harder 1 error_subset Failed_surfaces pattern 150 big 1 board 0 remove_old -1 inner 0 simple_offset 0 enn 0 b_smooth 0 time_max 0 ele_max 0 four 0 merge_dormant 1 max_length 0.0 max_area 0.0 min_angle 0.0 max_nodes 0 max_elements 0 smooth_dormant 0 breakpoint 0 freeb 0 n_threads 0 snorm 1 shape 0

# set boundary conditions
ic_boco_set INTERIOR {{{1 INTER 0}}}
ic_boco_set WALL {{{1 WALL 0}}}
ic_boco_set INLET {{{1 PRESI 0}}}
ic_boco_set OUTLET {{{1 PRESO 0}}}
ic_boco_set SYMMETRY {{{1 SYM 0}}}
C.2 CFD Setup (ANSYS Fluent)

ANSYS Fluent is used as the CFD solver for the solutions provided. The following provides a step-by-step approach to generating the solutions given the bottle mesh. Note that the model is axisymmetric about the x-axis and “down” is simulated as the positive x-direction.

**Step 1: Reading the Mesh and Initialization**

The ANSYS Fluent solution for the mesh provided uses the 2D dimension and Double Precision initial selections. The Pressure-Based solver is used with transient and axisymmetric conditions. Gravity is enabled and set to $9.81 \frac{m}{s^2}$ in the positive x-direction based on the geometry of the mesh. As an aside, it is good practice to use the Check feature to check the mesh and Display to view the mesh with the symmetry enabled (view → views → apply mirrored planes). Ensure the units are in the proper scale for the simulation (change length to mm and surface tension to dyn/cm). Lastly, the mesh needs to be scaled to mm (Scale → mesh was created in mm → scale).

**Step 2: Add Fluids and Implement Models**

To add water: Materials → Fluid → Fluent Database → waterliquid → copy. Now that we have water and air as materials for the system, we will enable multiphase and our energy model. Under Models, enable the energy equation and enable Multiphase using the Volume of Fluid model and use explicit solver. Go to phases and rename the air phase ‘air’ and the water phase ‘water’. Under Phase Interaction, set the surface tension coefficient as a constant 73.5 dyn/cm. Select Surface Tension Force Modeling and Wall Adhesion.

**Step 3: Alter Boundary Conditions**
All boundary conditions are set in ICEM, however, the symmetry boundary conditions must be changed to axis for the axisymmetric capability to be used in Fluent. There will be two walls of which one will be wet, from provided replay script this would be wall, and one will be non-wet, from provided replay script this would be wall:002. The contact angle for the wet wall should be 175 degrees and for the non-wet wall should be 90 degrees.

**Step 4: Methods Used**

In the Methods tab, enable Non-Iterative Time Advancement, select a Fractional Step scheme and ensure the Volume Fraction is set to Geo-Reconstruct (this setting is better for coarse meshes).

**Step 5: Initialize and Patch in Fluid**

In initialization, use the default settings and select Initialize. Now select the Patch option which should be newly available on the screen. On the pop-up screen, change the Phase selection to water, select Volume Fraction as the variable, change Value to 1 and choose the desired water region as the zone to patch, from the provided replay script, fluid1 is the water region which would be selected and fluid2 is the air region. Patch the air region, from provided script this would be fluid2, with a value of 0 for water as well. To verify that this was done correctly, go to Graphics → Contours and select contours of Phases, then Compute and Save/Display to visualize the phases in the graphic tab. Verify that the phases are correctly displayed as seen in Figure C.2.
Figure C.2: Initial phase output from Fluent. Red (lighter color) indicates air and blue (darker color) indicates water.

Step 6: Setup Calculation

Go to Calculation Activities and indicate how often the simulation should autosave. A new report definition for volume should be created to track the fluid within the bottle and pull out height for given times. In Run Calculation, choose an adaptive type time advancement for a total time duration specification. The global Courant number should be adjusted accordingly for simulation. A good order to test for convergence with Courant numbers is 2.0, 0.5, 0.1, and 0.01. If required the settings tab within Run Calculation can be used to lower the minimum time step.

Step 7: Run Calculation

Select calculate within the Run Calculation tab and track the data as desired for the indicated time period. When complete be sure to write the case and data of the simulation to a file. A saved simulation remembers the time step it is currently at and can continue forward in time, but not backwards to a previous state.