SIMULATION OF HIGH SPEED FILLING

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ABSTRACT

Computational fluid dynamics (CFD) software is used to simulate the filling process in two case studies. The method tracks the shape of the liquid-air interface in the bottle as it is filled and indicates the appearance of splashing or a disturbed liquid surface which generates foam. Use of simulation allows the design engineer to conduct a number of "virtual experiments" before changes are made to the filling line or bottle geometry. This allows a wide range of conditions to be tested and provides a tool to optimize the filling process in a way which cannot be practically done using empirical methods.

INTRODUCTION

Design or modification of a high-speed filling system is typically accomplished through experience and testing. This has been the state of most equipment design. Recently, however, powerful computational tools have become available to the design engineer which allow designs and design modifications to be evaluated prior to implementation. In the structural engineering field these methods have taken the form of Finite Element Analysis (FEA), while in the fluid flow and heat transfer arena Computational Fluid Dynamics (CFD) software has revolutionized the design process. This paper deals with the application of CFD modeling to the simulation of high-speed liquid filling. Liquid filling is among the most challenging applications of CFD due to the need to track not only fluid motion but to also simulate the evolution of the air-liquid interface. Two case studies will be described, one dealing with optimization of a filling line and the other dealing with evaluating a bottle design from a filling standpoint prior to construction of bottle molds or filling equipment.

ANALYSIS METHODS

The computational methods on which CFD analysis is based are described in numerous texts. Especially, useful are those of Patankar (1980) and Minkowycz, et al (1988). Many CFD programs are available commercially, though not all are capable of solving "free surface" problems which include air-liquid interfaces. The most robust commercial code for these types of problems is FLOW-3D (Flow Science, Inc. (1996)) and this program is used to conduct the analysis of the case study problems described in the next two sections. Other programs which offer this capability are FLUENT (Fluent, Inc. (1996)) and PHOENICS (CHAM, Ltd. (1997)).

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FLOW-3D uses a variant on the VOF method (Hirt and Nichols (1981)) to calculate the location and shape of the liquid-air interface. The model is divided by a grid into small rectangular regions or “computational cells.” Each of these cells is assigned a velocity and pressure which evolve as the solution progresses. This is standard for all CFD programs. The VOF method differs in that in addition to velocities and pressures, an new variable F, the fluid fraction, is tracked. When $F = 0$ in a computational cell there is no fluid in that cell. When $F = 1$ the computational cell is filled with fluid. Cells in which $0 < F < 1$ are partially full and thus have a liquid-air interface running through them; this situation is shown in Figure 1 below. Therefore, by tracking F the VOF method allows the identification of the location and shape of the free surface in the model. This surface can be extremely complex and can include multiple regions such as bubbles.

From the engineer’s point of view, setting up a CFD analysis requires four steps:

1. Setup of the problem geometry.
2. Establishment of a computational grid.
3. Setting problem-specific values such as the viscosity and density of the fluid.
4. Establishment of boundary conditions such as pressures and flow rates.

The program then solves the flow problem for a given length of simulated time. Results are provided in the form of numerical tables and plots. The plots can be animated to provide a real-time view of the results.

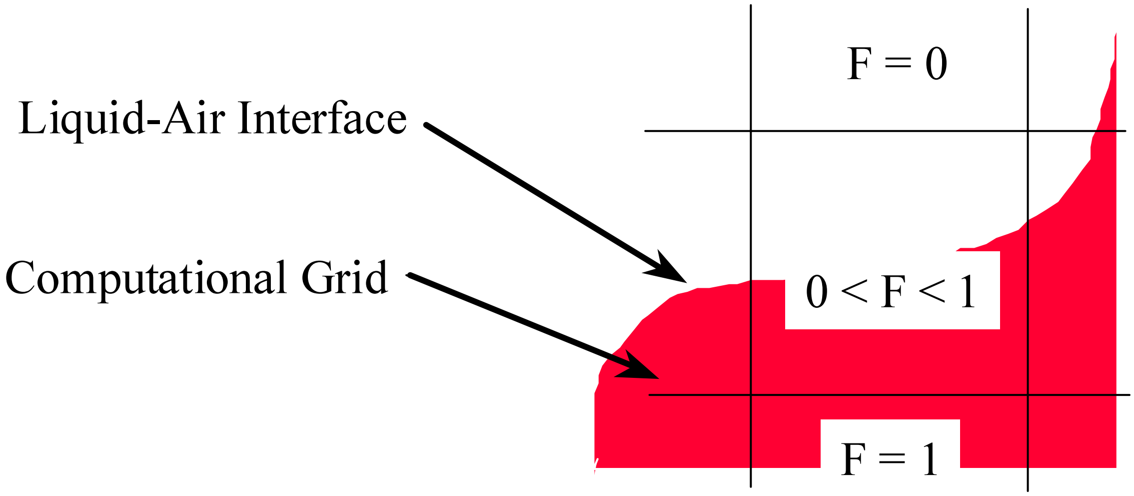


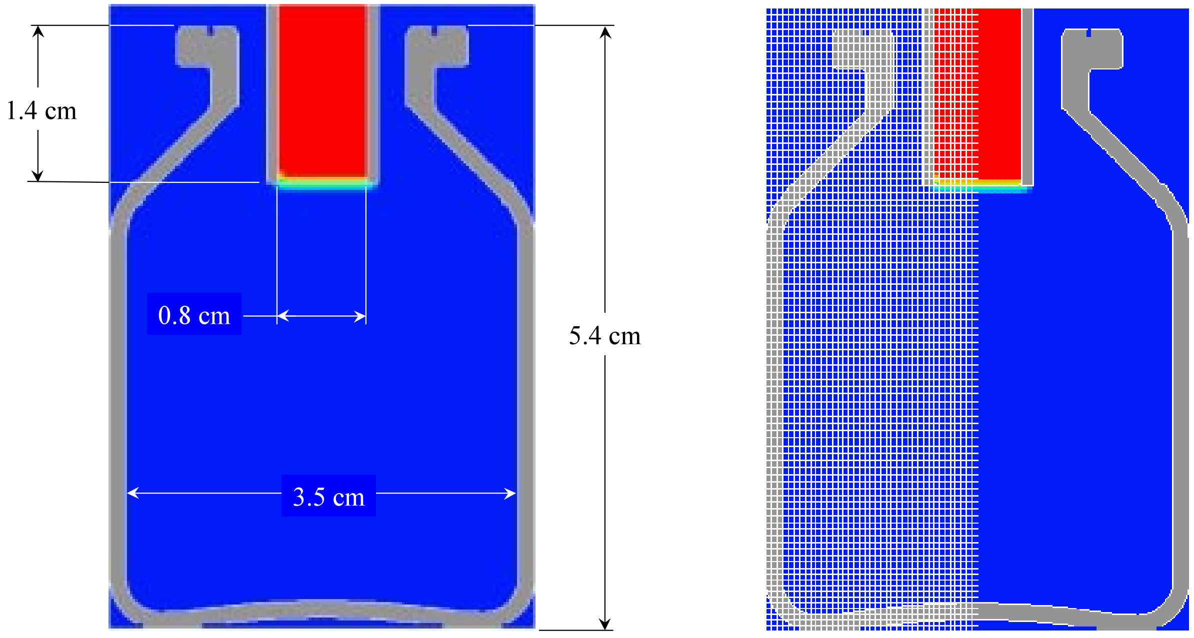
FIGURE 1
COMPUTATIONAL SCHEME FOR THE VOF METHOD

CASE STUDY 1 - OPTIMIZED FILLING OF A 30 ml VIAL

In the first case study the filling line and bottle geometry already exist. In this situation a 30 ml vial is being filled with a liquid having properties similar to water (specific gravity of 1.0, viscosity of 1.0 cP, and surface tension of 72 dynes/cm). Due to increased demand the speed of the filling line must be increased by 20%, reducing the time actually spent in filling the vial from 1.2 seconds to 1.0 second. The difficulty in doing this is that the fluid will foam if filling is too violent. This will cause the liquid to overflow the vial, resulting in deviation from label claims on volume and reduction in cleanliness of the filling line.

The geometry of the 30 ml vial is shown in Figure 2. This figure also includes a plot showing the computational grid used in the simulation. The grid is 40 (radial) x 90 (axial) cells in size. The plot shows the grid covering only the left half of the vial. This is because the filling is analyzed as a 2-dimensional axisymmetric problem. This approach is acceptable so long as the filling nozzle enters the vial square and concentric with the vertical walls.

The first attempt at increasing throughput is to simply rescale the existing filling profile by 20%. This is shown in Figure 3. The fill rate is ramped from 0 to 33.3 ml/s over the first 0.1 sec, held at this rate for 0.8 sec and then ramped back to 0 over the last 0.1 sec (Note that this and later profiles are idealized for the purpose of modeling. Actual profiles would smooth the transitions to eliminate sudden changes in acceleration, i.e. “jerk.”). In this case the filling is accomplished from the top, with the filling nozzle only slightly inserted into the vial. The results of this approach are shown in Figure 4 at several times throughout the fill. This figure immediately indicates that there will be problems with this fill profile. This can be seen in the large splash which occurs at 0.225 seconds. Fluid is driven up the wall of the vial to a height of 2.7 cm. The fluid sheet on the wall cannot support itself for long and crashes into the pool of fluid at the bottom of the vial. This splash and collapse entrains large amounts of air and will lead to foaming. In addition, the collapse



a. Dimensions **b. Computational Grid**

FIGURE 2
MODEL OF 30 ml VIAL

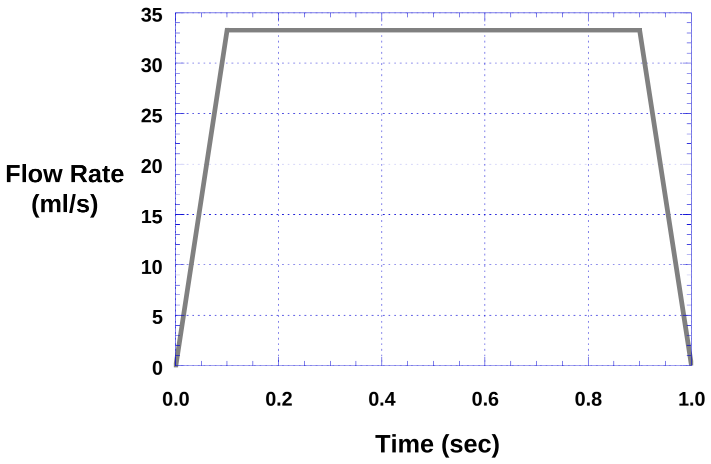


FIGURE 3
VIAL FILLING PROFILE #1

disturbs the free surface of the fluid in the pool and this surface remains uneven through 0.45 seconds. However, by the end of the hold period at 0.9 seconds the liquid-air interface is smooth and undisturbed. This suggests that the fill rate is not inherently too fast but rather that the method of introducing the liquid at the beginning of the fill needs work.

A straightforward way to modify the filling of the vial to provide a gentler initial fill is to use a diving nozzle. Filling Profile #2 shown in Figure 5 uses the same flow rate profile as in Figure 3 but starts with the nozzle 1 cm above the bottom of the vial and withdraws the nozzle using a profile which keeps the tip of the nozzle just above the mean free surface of the liquid. The results of this modification are shown in Figure 6. The results show that Profile #2 reduces the height of the initial splash to by more than 50%, to approximately

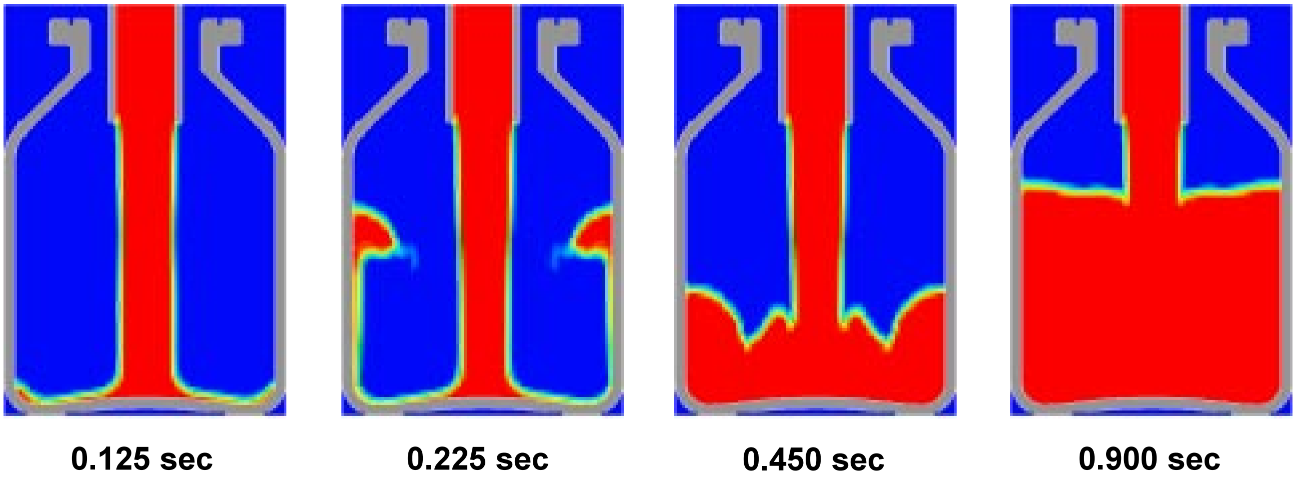

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FIGURE 4
RESULTS FOR VIAL FILLING PROFILE #1

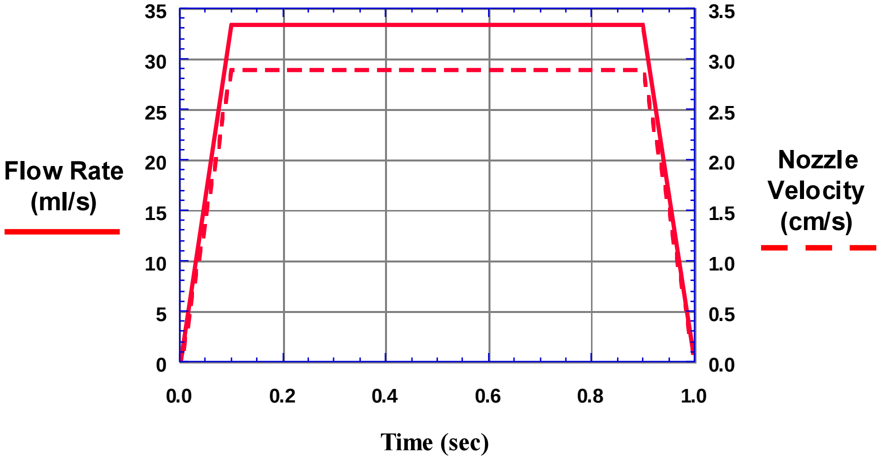

FIGURE 5
VIAL FILLING PROFILE #2

1 cm. This reduces the violence of the collapse substantially and the later filling is much more uniform, as can be seen at 0.45 seconds.

At first inspection it does not appear reasonable that the use of a diving stem should decrease the violence of the initial splash as significantly as a comparison of Figures 4 and 6 indicates. After all, the velocity at which liquid exits the nozzle is identical in these two cases, reaching 66.2 cm/s at 0.1 seconds. However, the effect of gravitational acceleration is significant, even over the 3.75 cm of drop seen in Figure 4. To see this the impact velocity of the fluid stream which leaves the nozzle a velocity V_o at a distance L above the bottom of the vial will be calculated. The velocity V at impact is given by

$$V = V_o\,(1 + 2\,L\,g/V_o^2)^{1/2}\,, \tag{1}$$

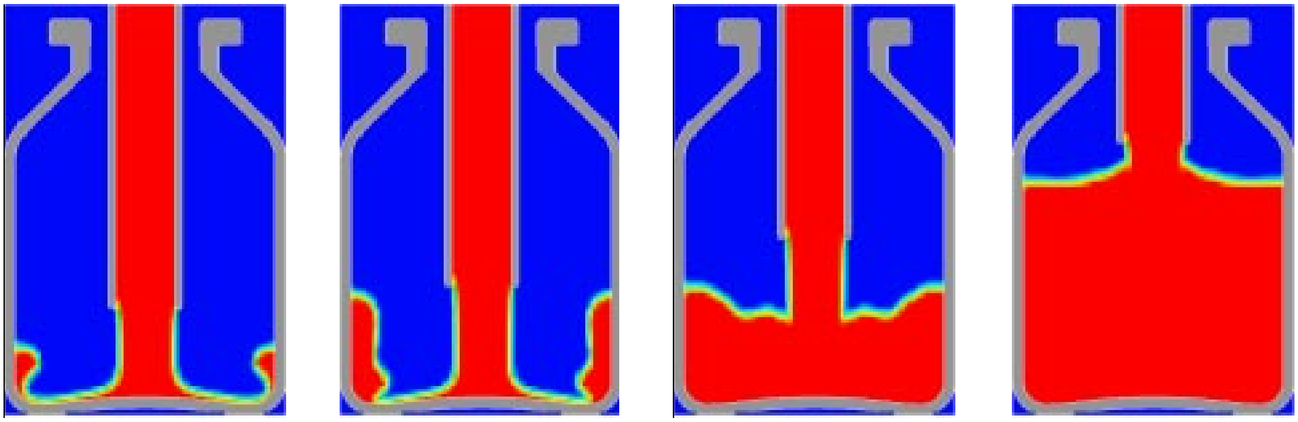

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FIGURE 6
RESULTS FOR VIAL FILLING PROFILE #2

where g is the gravitational acceleration. If L=3.75 cm and L=1.0 cm for Profiles #1 and #2, respectively, are substituted into equation (1) we find that the impact velocities are 108.4 cm/s for Profile #1 and 79.7 cm/s for Profile #2. Therefore, using a diving stem decreases the impact velocity by 27%. Also, since kinetic energy is proportional to the square of the velocity, this change decreases the energy input to the flow by 46%. Given this comparison it is easy to see why the use of the diving stem significantly improves filling using Profile #2.

The results of Profile #2 are a significant improvement over Profile #1. However, there remains a large splash at the start of the fill which is likely to cause foaming. In order to improve the filling further, profile shaping will be required. As a first step we start with the observation that the initial fill should be slowed to eliminate the splash, while the later fill appears stable and thus might be sped up without generating significant foam. The most direct way of accomplishing these two changes is to ramp the fill gradually from 0 ml/s up to a peak fill rate at the end of the fill. Such a profile is shown in Figure 7. Here the fill rate is ramped up to 60 ml/s at 0.9 seconds and then returned to 0 over the next 0.1 seconds. As in Profile #2, the nozzle dives to within 1 cm of the bottom of the vial and is withdrawn so as to keep the tip above the liquid-air interface. The results are shown in Figure 8. This figure shows that the initial fill occurs quite smoothly, with almost no splashing. Smooth filling continues through 0.45 seconds. However, by the end of the ramp at 0.9 seconds the high velocity of the nozzle jet has blown a depression into the surface of the liquid pool. We refer to this phenomena as “blowout.” Blowout is caused by high momentum fluid impacting a relatively deep pool of fluid. This is a very disruptive phenomena as it results in air being drawn along with the liquid jet and forced into the pool of liquid; this generates significant levels of foam. Based on the results obtained with Profile #3 an upper limit can be established on the fill rate. The fill rate can be greater than the 33.3 ml/s used in Profile #2 but must be substantially less than 60 ml/s.

The results of Profile #3 indicate that the initial splash can be eliminated. The remaining problem is how to fill slowly enough at the start of the cycle to eliminate the splash while not using up so much of the fill time as to require a very fast flow rate at the end of the cycle. A potential solution to the problem is shown in Figure 9. This fill profile uses two plateaus. The first plateau is at a rate of 20 ml/s. Flow is ramped up to this level over the first 0.1 seconds and is held at 20 ml/s for 0.2 seconds. This first plateau accomplishes three things. First, the ramp up to this plateau accelerates the fluid at 200 ml/s^2, as opposed to the 333 ml/s^2 used in Profile #2. This reduces the rate of energy increase in the system and allows any initial splash to dissipate. Second, the ramp terminates at a lower velocity level, 20 ml/s versus 33.3 ml/s in Profile #2. This limits the initial peak energy input rate at 64% less than in Profile #2. Finally, the 0.2 second hold at the reduced flow rate allows the flow to stabilize while a cushion of fluid is built up in the bottom of the vial. After the first plateau the profile ramps from 20 to 40 ml/s over the next 0.1 sec. The 40 ml/s plateau is held for 0.5 seconds before the ramp down to 0.

The results of Profile #4 are shown in Figure 10. The results show a small amount of splashing at 0.225 sec, more than was seen in Profile #3 but much less than in Profile #2. As the fill continues fluid is driven a short distance up the wall at 0.45 seconds but by 0.9 seconds filling is smooth. The situation at 0.45 seconds is a mild case of blowout. However, this blowout has very little energy and will probably not result in significant foaming. It does indicate that the 40 ml/s peak fill rate is probably as high as we can go with this vial. In general Profile #4 shows the best overall flow stability. Minor modifications can still be made. For instance, the 20 ml/s plateau might be shortened from 0.2 to 0.15 seconds to allow the peak fill rate to be reduced from 40 ml/s. To within such small changes, however, Profile #4 is our choice for an optimized filling profile.

A number of additional steps can be taken to improve the fill without changing the fill rate profile. The simplest of these is to increase the diameter of the filling nozzle. There are, however, practical limits to how

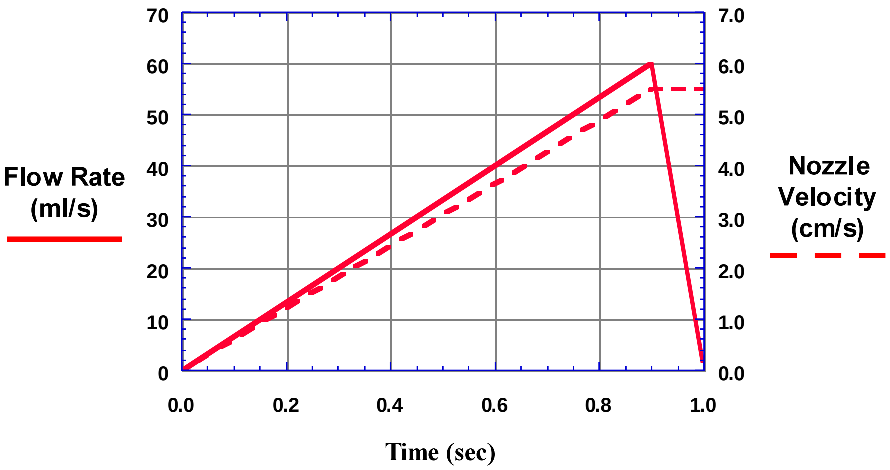

FIGURE 7
VIAL FILLING PROFILE #3

much the diameter may be increased. The most obvious of these limits is the I.D. of the bottle finish, since clearance must be left for escape of air and easy insertion of the nozzle. The other important limit is the stability of the fluid in the nozzle. The maximum nozzle diameter for which surface tension will hold a stable meniscus at the tip of the nozzle is given by

$$D_{max} = 4.81\,(\sigma/\rho g)^{1/2}, \tag{2}$$

where ρ is the density of the fluid and σ is its surface tension (Michael (1981)). In practice the actual diameter must be less than this theoretical maximum to guard against vibration dropping the column of fluid

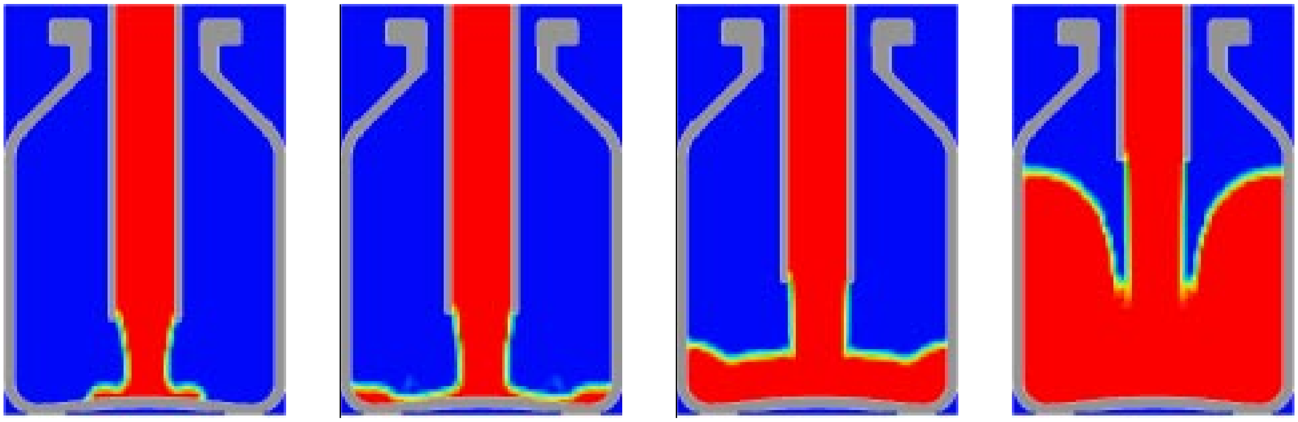

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FIGURE 8
RESULTS FOR VIAL FILLING PROFILE #3

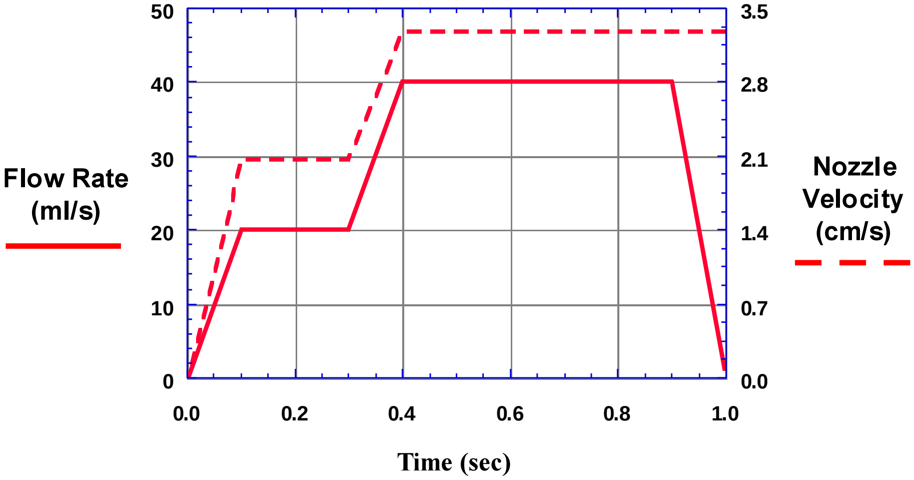

FIGURE 9
VIAL FILLING PROFILE #4

being held in the nozzle.

A second simple method of improving the stability of filling is to allow the tip of the nozzle to become immersed in the pool of fluid in the vial. This technique is unacceptable in many applications since it tends to leave a drip of fluid on the outside of the nozzle which can become dislodged before the nozzle is inserted into the next vial. However, where practical this method should be considered due to the dramatic increase in stable fill rate which it allows. As an example we have modified Fill Profile #4 to allow the tip of the nozzle to become immersed; the modified profile is shown in Figure 11. Comparing Figures 9 and 11 it can be seen that the fill rate profile is unchanged, while the nozzle withdrawal profile is modified to delay the start of withdrawal until after the nozzle tip is immersed. The results of this new profile are shown in Figure

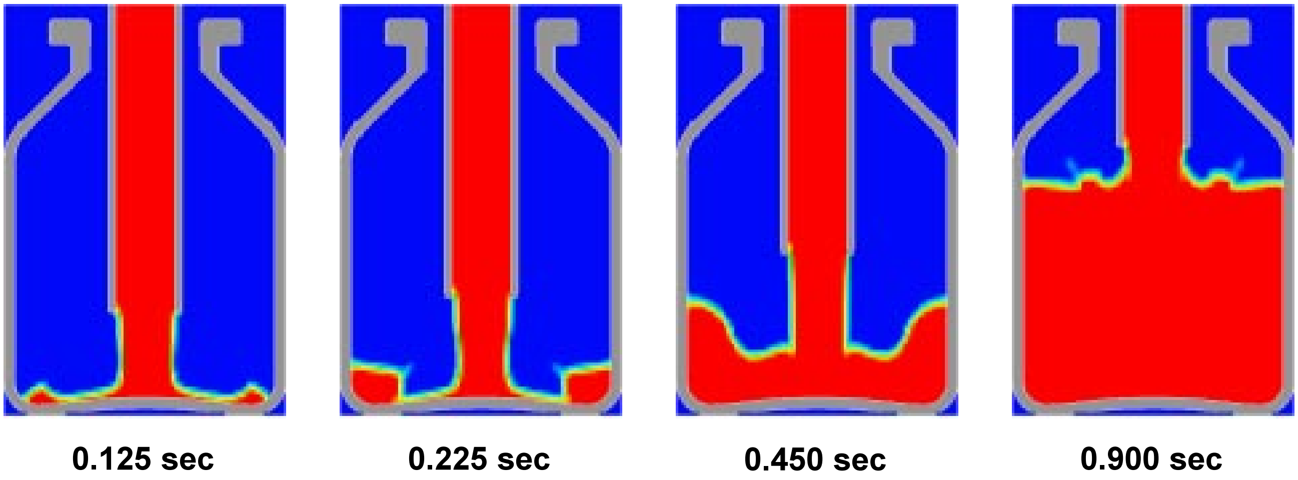
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FIGURE 10
RESULTS FOR VIAL FILLING PROFILE #4

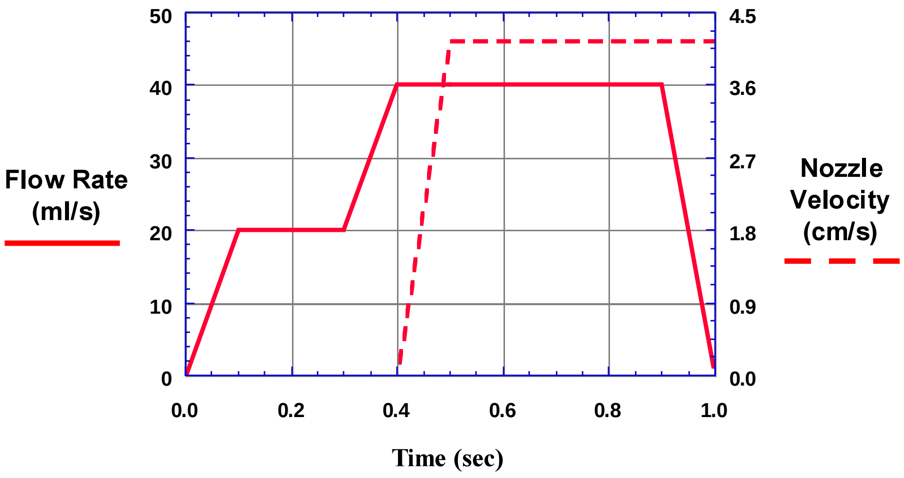
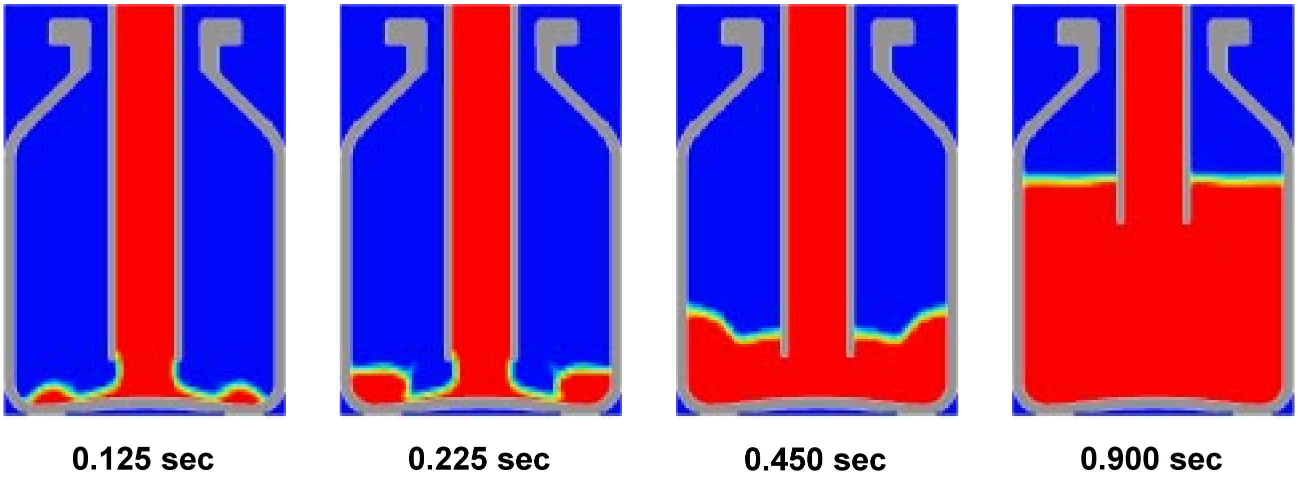


FIGURE 11
VIAL FILLING PROFILE #5

12. Comparing Figure 12 with Figure 10 indicates no change at 0.125 or 0.225 seconds. This is expected since the nozzle tip has not become immersed by 0.225 seconds. However, the liquid-air interface at 0.45 and 0.9 seconds is much smoother with Profile #5 than was seen with Profile #4. This suggests that the initial fill through 0.3 seconds might be slowed to inhibit splashing further, while the later fill rate could be increased, taking advantage of the stabilizing influence of the immersed tip.



0.125 sec **0.225 sec** **0.450 sec** **0.900 sec**

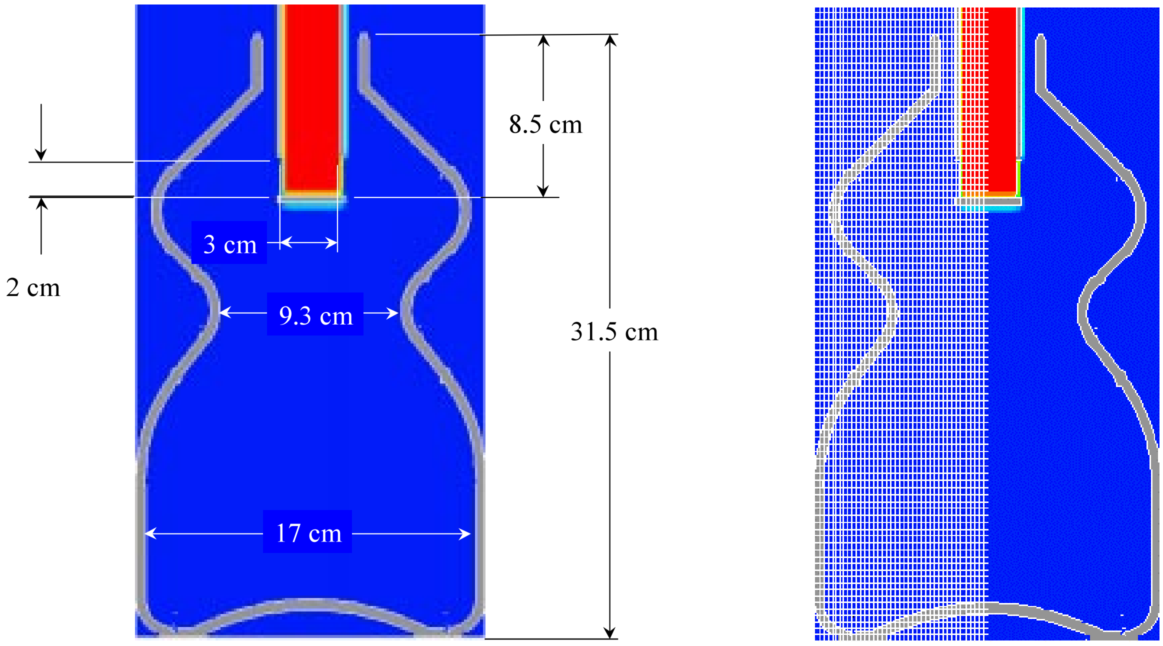
FIGURE 12
RESULTS FOR VIAL FILLING PROFILE #5

CASE STUDY 2 - FILLING EVALUATION OF A 4-LITER BOTTLE

The second case study illustrates the use of CFD modeling to evaluate a bottle design for filling. The proposed bottle design is shown in Figure 13a. This is a 4 liter pinch-waisted bottle. Filling is to be done using a side-ported filling nozzle having a total open area of 18.8 cm^2. The bottle is to be filled with a liquid detergent having a specific gravity of 1.0, a viscosity of 1000 cP, and a surface tension of 45 dynes/cm. The total filling time has not been established, though filling in under 3 seconds is desirable. The goal is to find a filling time and profile which allow the bottle to be filled from the top by draining a sheet of fluid down the sides of the bottle. Establishment of this sheet is the reason for the use of a side-ported nozzle.

The grid for the CFD model is shown in Figure 13b. The grid has 40 cells in the radial direction and 90 cells in the axial direction. The model is two-dimensional, axisymmetric. The use of an axisymmetric model is acceptable if the side-ported nozzle takes the form of a disk which opens axially from the nozzle tip as shown in Figure 13. However, most side-ported nozzles are actually configured to have 2, 3, or 4 holes angled radially outward from the axis. This allows air to escape from the bottle through the spaces between the liquid jets An axisymmetric model would not be able to capture the effects of these discrete holes. However, even when using a nozzle with discrete holes, once the fluid hits the side of the bottle it will spread out into a sheet, reducing the downstream flow to near axisymmetry.

The evaluation of the bottle takes the form of proposing a filling profile, running the CFD simulation, and examining the results to determine whether a successful fill is obtained. In this case success is establishment of a fluid film running done the sides of the bottle. The first proposed profile is shown in Figure 14. This is a simple ramp-and-hold profile lasting 3.0 seconds. The fill rate is ramped from 0 to 1379 ml/s over the first 0.1 seconds, held at this fill rate for 2.8 seconds and then ramped back to 0. The results are shown in Figure 15. These plots show two important features. First the flow does not form a sheet on the walls of the lower



a. Dimensions

b. Computational Grid

FIGURE 13
MODEL OF 4 LITER BOTTLE

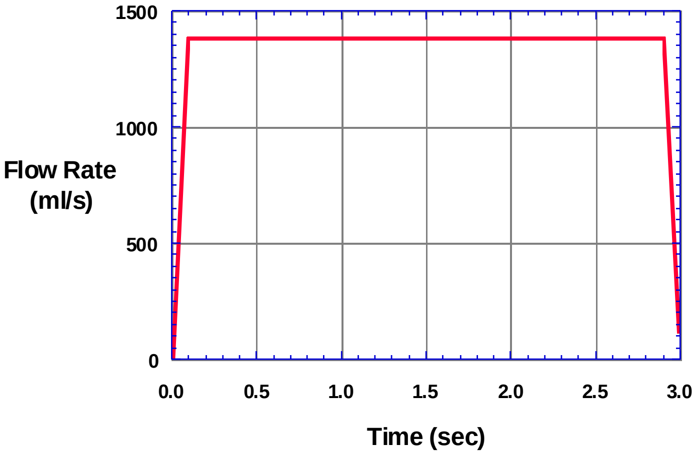


FIGURE 14
BOTTLE FILLING PROFILE #1

chamber of the bottle. Second when the sheet of fluid which falls from the bottle waist hits the pushup a large splash occurs. By 1.2 seconds this splash has dissipated but the impact of the falling sheet continues to disturb the air-liquid interface. A feature which can be inferred from the plots is that as filling continues the air trapped between the falling sheet and the bottle wall will be compressed. At some time during the course of filling the pressure will become high enough to disrupt the sheet of fluid, temporarily blowing a hole in the sheet. This will occur chaotically and will result in foaming. This is the reason we want the fluid to hug the wall as it fills the lower portion of the bottle.

The failure of Profile #1 to meet the goal may be due to a badly shaped bottle, too rapid filling, or a combination of these. In order to eliminate the possibility that too rapid filling is the cause, we will test a

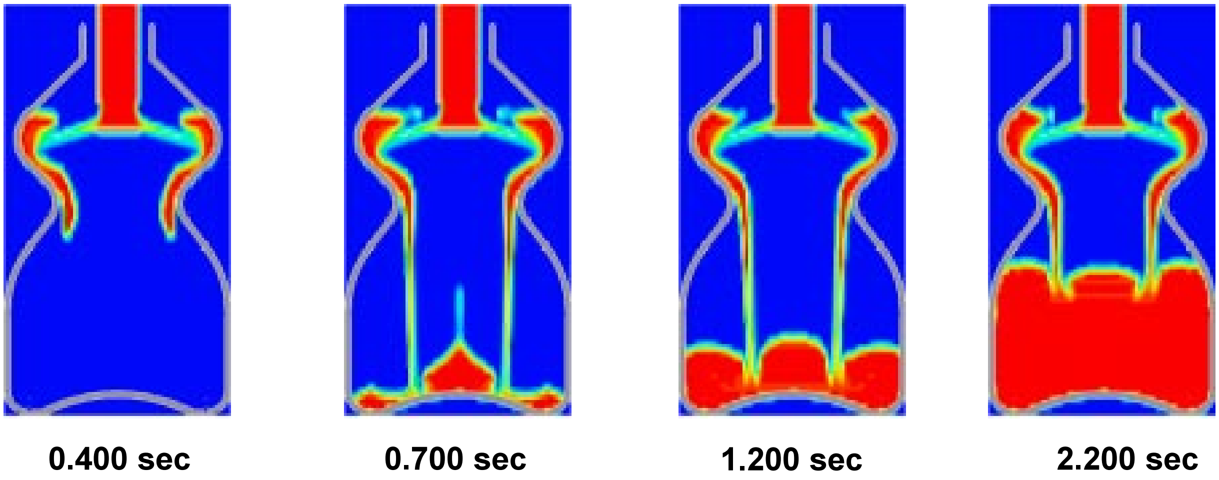


FIGURE 15
RESULTS FOR BOTTLE FILLING PROFILE #1

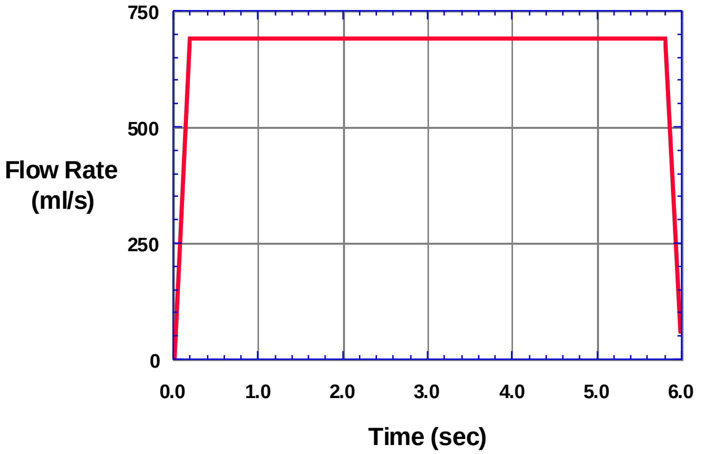


FIGURE 16
BOTTLE FILLING PROFILE #2

much slower fill. Figure 16 shows a second filling profile. This profile is obtained by scaling Profile #1 by a factor of 2. Therefore, the peak filling rate is 690 ml/s and the fill duration is 6 seconds. This is clearly far beyond our goal of filling in under 3 seconds and would be economically unacceptable. Therefore, this simulation serves as an upper bound check on the effect of bottle geometry. The results are shown in Figure 17. This figure shows that halving the fill rate does not slow the fluid to the point where it can remain attached to the wall. While the liquid does impact at a lower velocity, thus splashing less, the overall goal of filling by draining a film down the bottle walls has not been accomplished. Given that Profile #2 provides a very slow fill, it can be concluded that the proposed bottle shape has too severe a pinch to allow this filling strategy to be used. Increasing the waist diameter may allow top filling using a side-ported nozzle. If the bottle geometry cannot be changed, then profiled filling using a diving stem nozzle should be considered.

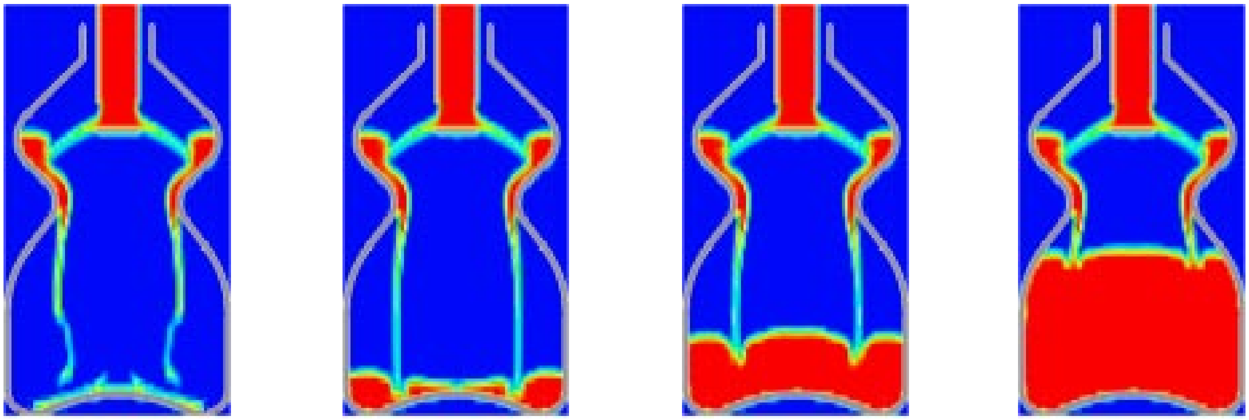


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FIGURE 17
RESULTS FOR BOTTLE FILLING PROFILE #2

CONCLUSION

The use of computational fluid dynamics simulation for the evaluation of filling problems has been demonstrated in two case studies. Both of these cases have used axisymmetic models. Such models are relatively simple to set up and can be run in only a few hours on a high-end personal computer. More complex simulations are possible, including three-dimensional modeling, non-Newtonian fluid properties, and the tracking of bubbles in the fluid, though such simulations will require more time and computational resources. The simulations provide substantial information to guide selection of filling profiles or evaluation of bottle shapes. However, this information is of a qualitative nature and must be interpreted by a user familiar with both filling operations and CFD modeling.

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