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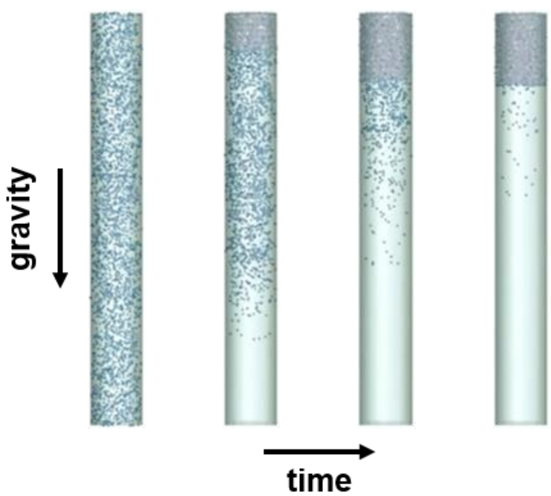
subject: Evaluation of the Barracuda Software Package for Simulating Bubble Motion in Vibrating Liquid-Filled Containers

**Graphical Abstract**




**Executive Summary**

The commercial software package Barracuda, developed by CPFD Software for simulating particle-laden fluid flows, is evaluated as a means to simulate the motion of bubbles in vibrating liquid-filled containers. Demonstration simulations of bubbles rising due to buoyancy forces in a cylinder filled with silicone oil and angled at 0, 30, 45, and 60 degrees from the vertical were performed by CPFD Software. The results of these simulations are discussed, and the capabilities of Barracuda for simulating bubble motion are assessed. It was determined that at present Barracuda does not meet the needs of the desired application. Further developments that would enable its use for this application are highlighted.

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## Introduction

Understanding and predicting the motion of gas bubbles in vibrating containers partially filled with liquid continues to be of interest. This problem has been the subject of recent experimental (O'Hern et al., 2012), theoretical (Romero et al., 2014; Romero et al., 2016; Torczynski et al., 2019), and computational investigations (Ferraro and Torczynski, 2020; McMullen and Torczynski, 2021). Nonetheless, the ability to perform simulations that accurately and efficiently predict the bubble motion in vibrated liquid-filled containers is still lacking.

The computational particle fluid dynamics (CPFD) method (O'Rourke et al., 2009) is attractive for simulating multiphase flows in which one phase consists of discrete particles. This method is an extension of multiphase particle-in-cell methods (Snider, 2001), in which an Eulerian description for the continuous phase is strongly coupled to a Lagrangian description for the discrete phase. Some of the relevant advantages of the CPFD method include the abilities to simulate an arbitrary particle size distribution, model volume fractions from fully dilute to close-packed, and perform simulations with large numbers of particles. Therefore, we investigate here the feasibility of using the CPFD method to simulate bubble motion in vibrating liquid-filled containers using the commercial code Barracuda, developed by CPFD Software.

## Simulation Details

Here, we provide the details of the demonstration simulations performed by CPFD Software, beginning with the system description. Simulations of bubbles rising in a cylindrical vessel due to buoyancy forces were performed for four different angles between the cylinder axis and the vertical: 0, 30, 45, and 60 degrees. The cylinder has diameter 12.7 mm and height 101.6 mm and is filled with 20-cSt silicone oil ($\mu_l = 0.019$ Pa s, $\rho_l = 950$ kg m$^{-3}$). 2620 incompressible air bubbles ($\rho_g = 1.184$ kg m$^{-3}$) with diameters ranging from 0.5 mm to 1.75 mm are distributed randomly throughout the cylinder, occupying 10% of the total volume. The temperature and reference pressure of the system are 300 K and 101.325 kPa, respectively.

Next, we discuss the relevant numerical details. The duration of all simulations is 10 s with a time step of 0.02 s. Barracuda uses a uniform Cartesian grid and a cut-cell method to create the mesh, resulting in the cylinder being discretized into 3087 cells. The close-packed volume fraction of the bubbles is 0.6, which is the highest attainable by Barracuda for incompressible flows. Drag on the bubbles is calculated using the Wen-Yu/Ergun model (Ergun, 1952; Wen and Yu, 1966).

The following parameters describe how the bubbles behave during collisions. The maximum momentum redirection from collision, which dictates the degree of random scatter in a bubble's post-collision velocity vector, is 0.2. The normal-to-wall and tangent-to wall momentum retention determine the percentage of a bubble's momentum that is retained after a collision with a solid surface in the normal and tangent directions, respectively; here, both are 0.85. Diffuse bounce controls the range of scatter angles of a bubble after a collision with a solid surface; i.e., a diffuse bounce of 0 corresponds to specular reflection. The value of diffuse bounce for the present simulations is 5. We note that all of these are the default values of the parameters in Barracuda and that determination of the most appropriate values for air bubbles is beyond the scope of this memo.

All parameter values discussed in this section are summarized in Table 1.

**Simulation Results**

In this section, we discuss the simulation results. Figures 1-4 show time series from the 0, 30, 45, and 60 deg simulations, respectively, which were extracted from a video provided by CPFD Software. Overall, the simulations result in bubble-rise behavior that appears to be qualitatively reasonable. As can be seen in Figure 1, bubbles gradually rise into the headspace, and the Boycott effect (Boycott, 1920) is observed for the 30, 45, and 60 deg cases: gravity-driven particle transport takes place at a much higher rate when tubes are tilted from the vertical. Furthermore, while details of the computational platform used to run these simulations were not provided by CPFD Software, they stated that the run times were less than a minute and did not require GPU acceleration, indicating that they are not computationally expensive.

However, the simulations exhibit unphysical behavior in several ways. In the 0 deg simulation, the fraction of the cylinder height occupied by the bubbles at the end of the simulation is approximately 0.176, whereas a close-packed volume fraction would result in the bubbles occupying 0.167 of the cylinder height. This is possibly the result of the bubbles being relatively large in comparison with the cell sizes. For example, the volume of a 1 mm diameter bubble is approximately 1/8 the average cell volume. Since the cell volumes are used to determine the volume fraction, this results in a coarse discretization of the range of volume fractions below the close-packed value of 0.6. Additionally, bubbles flow up into the headspace much like how sand grains flow down a dune, as if they have an angle of repose. CPFD Software informed us that this could be due to the low value of the maximum momentum redirection used. Finally, some bubbles can be seen “sticking” to the cylinder wall and rising slowly up it; see, e.g., the bottom three images in Figure 2. A possible explanation for this is that the default values of the wall interaction parameters used for these simulations are suited for solid particles but not for bubbles. For example, a higher value of the momentum retention parameters would result in less “sticking.”

**Limitations of Barracuda**

Here, we enumerate several limitations of Barracuda that are relevant to the application of simulating bubble motion in vibrating containers. First, the maximum close-packed value 0.6 is quite low for bubbly flows; a value of 0.9-1.0 would be more realistic. Second, Barracuda does not simulate cohesive forces between bubbles or allow for coalescence. This means that no way exists for two or more smaller bubbles to merge into a single larger bubble, which is frequently observed in experiments. Third, solving additional user-defined partial differential equations (PDEs) on the mesh is not supported. For a vibrated container, a Helmholtz equation must be solved to compute the rectified bubble force. Alternatively, rectified motion can be simulated with compressible bubbles in conjunction with an oscillating gravity field. However, neither user-defined PDEs nor compressible bubbles are currently supported in Barracuda. Finally, added mass is not included in the bubble equation of motion. We note that several of these limitations, including the maximum close-packed volume fraction and added-mass effects, have been identified by CPFD Software as the focus of future development work and thus that some of these limitations may be removed in the next few years.

**Conclusions**

In order to demonstrate the capabilities of the Barracuda software package, CPFD Software performed several simulations of bubbles rising in a cylindrical vessel filled with silicone oil oriented at different angles from the vertical. While these simulations show qualitatively reasonable bubble-rise behavior, we have, through further discussion with CPFD Software, identified limitations of Barracuda that preclude its use for simulating bubble motion in vibrating liquid-filled containers. CPFD Software has identified several of these limitations as the subject of further development, so Barracuda may become a viable option for this application at some point in the future.

Table 1. Simulation parameters

| **Parameter** | **Value** |
|---|---|
| Cylinder diameter | 12.7 mm |
| Cylinder height | 101.6 mm |
| Cylinder angle from vertical | 0, 45, 60 deg |
| Liquid viscosity, $\mu_l$ | 0.019 Pa s |
| Liquid density, $\rho_l$ | 950 kg m$^{-3}$ |
| Gas density, $\rho_g$ | 1.184 kg m$^{-3}$ |
| Number of bubbles | 2620 |
| Bubble diameter | 0.5-1.75 mm |
| Total gas volume fraction | 0.1 |
| Temperature | 300 K |
| Reference pressure | 101.325 kPa |
| Simulation duration (physical time) | 10 s |
| Time step | 0.02 s |
| Number of computational cells | 3087 |
| Close-packed volume fraction | 0.6 |
| Maximum momentum redirection from collision | 0.2 |
| Normal-to-wall momentum retention | 0.85 |
| Tangent-to-wall momentum retention | 0.85 |
| Diffuse bounce | 5 |

Figure 1. Time series from 0 deg simulation. Times from left to right are 0 s to 9.0 s in increments of 1.0 s.

Figure 2. Time series from 30 deg simulation. Times from left to right and top to bottom are 0 s to 2.5 s in increments of 0.5 s.

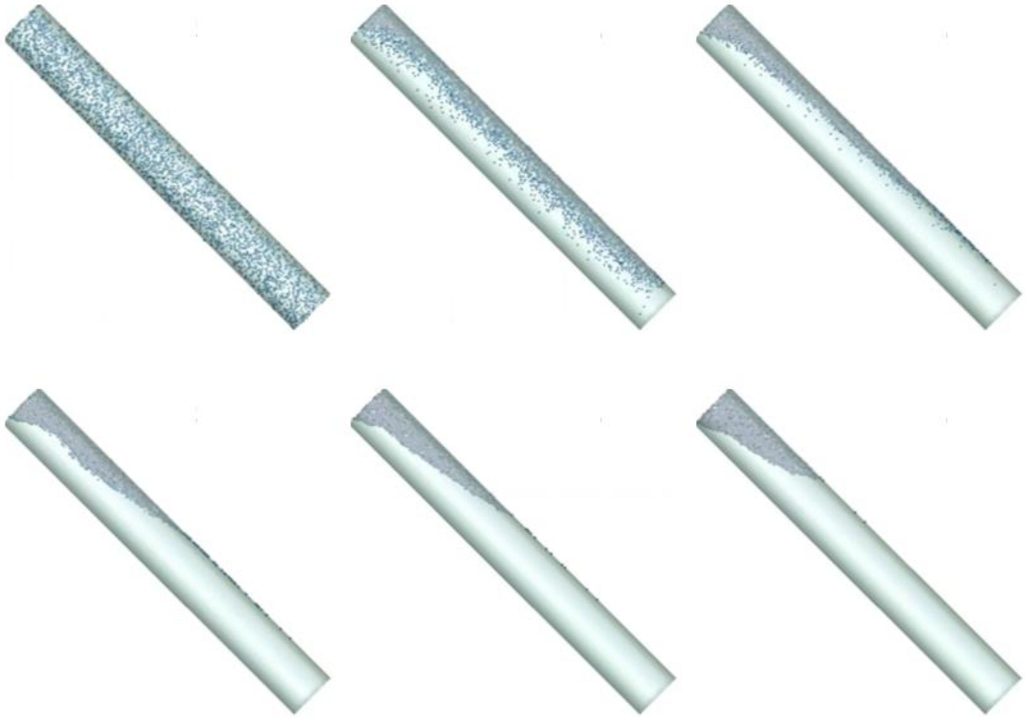

Figure 3. Time series from 45 deg simulation. Times from left to right and top to bottom are 0 s to 2.5 s in increments of 0.5 s.

Figure 4. Time series from 60 deg simulation. Times from left to right and top to bottom are 0 s to 2.5 s in increments of 0.5 s.

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**Administration**

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