Simulation of bubble dynamics by a compressible Volume Of Fluid method

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Introduction

When a cavitating bubble collapses near a solid surface, a jet penetrates inside the bubble, finally perforating the bubble to impact on the solid surface. In this two-phase flow problem the gas inside the bubble is considered to be compressible and to behave like an ideal gas. The liquid surrounding the bubble is assumed incompressible. The effect of gravity and surface tension is neglected in the model. The numerical simulation of the bubble dynamics is challenging due to the high density ratio at the bubble-liquid interface combined with the high pressure and temperature gradients at the interface. Moreover, the numerical method has to track a sharp interface and be able to simulate the bubble breakup resulting from the jet perforation. The objective of the current paper was to develop a numerical method to simulate the compressible bubble dynamics. The numerical model is based on the previous work of Wemmenhove et al. [1]. The Navier-Stokes equations are solved in the whole domain to predict the flow conditions inside and outside the bubble. The Volume OF Fluid approach (VOF) is incorporated to capture the bubble-liquid interface. The advantages of the VOF algorithm are the conservation of a sharp interface and of the gas phase mass inside the bubble. VOF is also shown to allow the simulation of the break-up of the bubble-liquid interface.

Numerical method

The Navier-Stokes equations expressing, respectively, the mass, momentum and energy balance for the entire flow field are:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \tag{1}
\]

\[
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u u) = -\nabla p + \nabla \cdot (\mu \nabla u) \tag{2}
\]

\[
\frac{\partial (\rho e)}{\partial t} + (\rho e + p) \nabla \cdot u = \nabla \cdot (k \nabla T) \tag{3}
\]

where \( u, p, e \) and \( T \) are, respectively, the velocity vector, the pressure, the internal energy and the temperature. The density in the liquid phase, \( \rho_l \), is constant and the density in the gas phase, \( \rho_g \), is defined by the ideal gas law.

In the VOF method, the interface is determined by the volume fraction of the liquid phase, \( \alpha_l \). The flow regions containing pure liquid are identified by \( \alpha_l=1 \) and the flow regions containing pure gas phase are identified by \( \alpha_l=0 \). Interfacial cells are such as \( 0 < \alpha_l < 1 \). The material properties \( (\rho, \mu, k) \) in Eq. (1-3) are defined, for example for the density, as: \( \rho = \alpha_l \rho_l + (1 - \alpha_l) \rho_g \). The liquid being incompressible, the advection of the interface is:

\[
\frac{\partial}{\partial t} (\alpha_l) + \nabla \cdot (u \alpha_l) = 0 \tag{4}
\]

It is to note that the internal energy in Eq.(3) is averaged according to the mass fraction of the phases:

\[
e = \frac{c_v \alpha_l \rho_l T + c_v (1 - \alpha_l) \rho_g T}{\rho}
\]
As the density depending on the liquid volume fraction is in the temporal terms in Eqs. (1-3), Eqs. (1-3) and Eq. (4) are coupled. It should be noted that this would not be the case for an incompressible flow. However using Eq. (4) inside Eqs. (1-3) allows to write Eqs. (1-3) as:

\[
\frac{(1-\alpha)}{\rho} \left[ \frac{\partial \rho}{\partial t} + u \cdot \nabla \rho \right] + \nabla \cdot \mathbf{u} = 0
\]

(5)

\[
\frac{\partial u}{\partial t} + u \cdot \nabla u = \frac{1}{\rho} \nabla p + \frac{1}{\rho} \nabla \cdot \left( \mu \nabla u \right)
\]

(6)

\[
\frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{u} T) \left[ c_{\text{v}} \rho \alpha + c_{\text{v}} (1-\alpha) \right] + \rho \nabla \cdot \mathbf{u} - c_{\text{v}} T \rho \nabla \cdot \mathbf{u} = \nabla \cdot \left( k \nabla T \right)
\]

(7)

It allows solving Eq. (4) sequentially, i.e. after Eqs. (5-7).

To discretize Eqs. (5-7), the flow domain is subdivided into a finite number of control volumes. The variables \( \rho, u, T \) and \( \alpha \) are stored in the control volume centre while the velocities \( u \) are stored in the control volume face (staggered arrangement). The temporal terms in Eqs. (5-7) are discretized by the Euler Explicit Scheme. An upwind differencing scheme is used to discretize the convective fluxes at the cell face. A central differencing scheme is used to discretize the diffusive fluxes at the cell face. The density required at the cell face in Eq. (6) is cell-weighted averaging.

The compressible governing equations (5-7) are solved by a pressure-based solver. The procedure to solve the governing equations is based on the SIMPLE algorithm.

This procedure is as follows:
- A predictor value \( T^* \) is determined from (7) using velocity, density and pressure values at the previous iteration. The predictor value \( T^* \) is used as an update for the temperature, \( T^{n+1} = T^* \).
- A predictor value \( u^* \) is determined from (6) using pressure and density values at the previous iteration.
- The velocity and pressure corrections are determined from the SIMPLE algorithm for compressible flows [2]. The pressure and the velocity are updated.
- The equation of state is used to update the density, \( \rho^{n+1} = \frac{p^{n+1}}{RT^{n+1}} \).
- A next iteration step begins if no convergence is achieved.

When Eqs (5-7) are solved, the Volume Of Fluid (VOF) algorithm developed by Hirt and Nichols [3] is used to advect the interface (Eq. (4)).

**Results**

To validate the model and simulation code, the dynamics of a bubble in an infinite liquid is simulated. The bubble of 1 mm is initially at rest and the pressure and the temperature in the entire domain are, respectively, 1 bar and 300 K. At the initial time, the pressure in the liquid at infinity is fixed at 5 bar. Due to this pressure, the bubble collapses and its motion is only radial. This radial motion is simulated and compared to the analytical Rayleigh model [4]. The gas inside the bubble is assumed adiabatic. The mesh is composed of 1000 uniform cells in the initial compressible phase and of 97 non-uniform cells in the incompressible phase. The ratio between two cells in the incompressible phase is 1.1.

The bubble radius as a function of time is shown in Figure 1. The numerical and Rayleigh models are seen to predict a similar bubble radius and in particular the same minimum bubble radius. The pressure inside the bubble as a function of time is shown at Figure 2. The pressure predicted by the numerical model is seen to correspond to the one predicted by the Rayleigh model. The numerical model is able to solve the high pressure gradient at the bubble-liquid interface.

The grid independency of the numerical results was verified and the key factor was found to be the number of cells in the compressible phase. Increasing this number decreases the gas phase mass loss inside the bubble, necessary for the results to become grid independent.
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**Reference**


