Development of Numerical Simulation Method for Compressible Gas-Liquid Two-Phase Flows

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Abstract. A numerical simulation method of compressible gas-liquid two-phase flow is developed for analyses of a cavitation bubble. Thermodynamic state of both phases is described with stiffened gas equation of state. Interface of two phases is captured by Level-Set method. As internal energy jump between two phases is critical for the stability of computation, total energy equation is modified so that inviscid flux of energy is smoothly connected across the interface. Detail of governing equations as well as their discretization is described followed by the result of one-dimensional simple example computation.

1. Introduction
A strong pressure waves emitted from a collapsing cavitation bubble is very important issue in many engineering fields. However the numerical analysis of a collapsing bubble has some difficulties, e.g. moving interface between two phases exists, density ratio of two phases is large, compressibility of both phases must be considered to capture pressure waves (consequently energy equation / thermodynamics relation is inevitably required). There are a few researches in the literature. For example, Takahira et al. [1] developed improved ghost fluid method and Ochiai et al. [2] applied homogenization model used in cavitating flow simulations. Both of them successfully simulated bubble deformation and collapse. The former is based on two-fluid model and latter one-fluid model. In this research, two-fluid model is adopted because the interface should be clearly defined to capture the collapse of a bubble. Instead of (improved) ghost fluid method, which has rather complicated algorithm, the Level-Set method [3] is applied to capture interface and then the numerical algorithm is expected to be simpler and suitable for large-scale parallel computing, which should be required for detailed analysis of bubble collapse or bubble fission. The present author has tried to simulate two-dimensional / axisymmetric bubble collapse problems [4] which showed numerical instability in the case of practical density / pressure ratio of two phases. Detailed examination suggested that instability is not caused by the large density difference but by the internal energy difference given by the stiffened gas equation of state, also used in [1]. Hence the energy equation is modified in the present algorithm to overcome the numerical instability. In the next section, the detail of the present algorithm is described, followed by the result of simple one-dimensional problems to discuss its validity.

2. Governing equations and numerical method
Let the volume fraction of liquid be $\psi$. $\psi$ takes the value of 0 or 1 in almost whole region and the value between 0 and 1 in the vicinity of the interface. In such region, assuming that velocity and
Pressure are the same in both phases, the following governing equations are derived in one-dimensional inviscid flow.

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0
\]

\[
\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = 0
\]

\[
\frac{\partial e}{\partial t} + \frac{\partial (e + pu)}{\partial x} = 0
\]

(1)

where

\[
\rho = \rho_L \psi + \rho_G (1 - \psi)
\]

\[
e = \rho_L \varepsilon_L \psi + \rho_G \varepsilon_G (1 - \psi) + \frac{1}{2} \rho u^2
\]

\[
p = (\gamma_L - 1) \rho_L \varepsilon_L - \psi \Pi_L = (\gamma_G - 1) \rho_G \varepsilon_G
\]

The subscripts \(L\) and \(G\) denote liquid phase and gas phase, respectively. Thermodynamic relation is given by stiffened gas equation of state and

\[
\gamma_L = 2.8, \quad \Pi_L = 8.5 \times 10^8 \text{ Pa}, \quad \gamma_G = 1.4 \ [5].
\]

As the atmospheric pressure has the order of \(10^5\) Pa, large difference of internal energy in two phases exists obviously. Once \(\psi\) is obtained, pressure is calculated from eq. (2).

The volume fraction of liquid \(\psi\) is expressed with the so-called Level-Set function \(\phi\), which indicates the signed distance from the interface as

\[
\psi = 0.5 + H(\phi).
\]

(3)

\(H\) is called the Heaviside function and expressed with the half width of the smoothed interface \(\alpha\) as

\[
H = \begin{cases} 
0.5, & \phi > \alpha \\
-0.5, & \phi < \alpha \\
\frac{1}{2} \left( \frac{\phi}{\alpha} + \frac{\pi \phi}{\alpha} \right), & \text{otherwise}
\end{cases}
\]

(4)

\(\alpha\) is typically 2.5 times of the grid spacing. \(\phi\) is advected by the fluid velocity and requires the re-initialization process after (each) advection step to maintain the function of distance from the interface. These are

\[
\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = 0
\]

\[
\frac{\partial \phi}{\partial \tau} = S(\phi) \left( 1 - \frac{\partial \phi}{\partial x} \right) \quad \text{or} \quad \frac{\partial \phi}{\partial \tau} + \tilde{W}_S \frac{\partial \phi}{\partial x} = S(\phi), \quad S(\phi) = \frac{\phi}{\sqrt{\phi^2 + \delta^2}}, \quad \tilde{W}_S = S(\phi) \frac{\partial \phi}{\partial x} \left( \frac{\partial \phi}{\partial x} \right).
\]

(5)

Here \(\tau\) in the lower equation is a virtual time and the equation is iteratively solved to obtain the steady state solution which recovers the signed distance.

Equations (1) – (5) give the complete set of governing equations. As all of the equations are advection ones, upwind schemes are suitable and Harten-Yee’s upwind TVD scheme [6] is adopted here. The Roe’s average is simply applied to calculate the interface values and the minimod limiter is used to obtain the second order accuracy. The speed of sound appearing in their scheme is described as

\[
c = \sqrt{\gamma_m p + \frac{\gamma_m - 1}{\gamma_L - 1} \gamma_L \psi \Pi_L}, \quad \gamma_m = \left( \frac{\psi}{\gamma_L - 1} + \frac{\gamma_L - 1}{\gamma_G - 1} \right)^{-1} + 1.
\]

(6)

As described in the introduction, the computation tends to be unstable near the interface. Here the energy equation is modified as
Formally this modification smoothly connects the internal energy of liquid phase and that of gas phase across the interface to avoid numerical instability. Note that equation (6) is still valid even though the above modification seems also modifying the characteristic speed of sound. The right-hand side of eq. (7) can be re-written using the following mass conservation equation of liquid under the assumption without phase change at the interface,
\[
\frac{\partial (\rho_L \psi)}{\partial t} + \frac{\partial (\rho_L u \psi)}{\partial x} = 0,
\]
and finally one obtains
\[
\frac{\gamma_L \Pi_L}{\gamma_L - 1} \left[ \frac{\partial \psi}{\partial t} + \frac{\partial (\psi u)}{\partial x} \right] = \frac{\gamma_L \Pi_L}{\gamma_L - 1} \frac{1}{\rho_L} \frac{D \rho_L}{D t}.
\]
When the liquid density change is negligible (compared with the order of $\Pi_L$), the right-hand side of eq. (7) is found to be small.

Table 1. Computational conditions.

|                | Liquid       | Gas         |
|----------------|--------------|-------------|
| density        | 1100 kg/m³  | 1.2 kg/m³  |
| pressure       | 2 atm        | 1 atm       |
| temperature    | 15°C         | 15°C        |
| no. of grid points | 20         | 50         |
| time step      | 4.41 μs      |             |

Figure 1. Compression process: (a) density, (b) pressure, (c) $H(\phi)$.

3. Numerical results

Results of one-dimensional two-phase flows are presented. The left side is liquid and the right side is gas. Liquid length is 2.5mm and gas length is 1.0mm. Pressure is fixed at the left boundary and the
symmetric condition is posed on the right boundary. Detailed conditions are tabulated in Table 1. To stabilize the computation, the right-hand side of eq. (7) is set to be zero near the interface.

Figure 1 shows density, pressure and Heaviside function changes during the compression process while Figure 2 shows those during the expansion process. The results of several time steps are plotted. The interface is clearly captured as shown in Fig. 1 (a), (c) and Fig. 2 (a), (c) (density and \( H(\phi) \) are independently computed in the present method). Initial pressure discontinuity rapidly disappears as the pressure wave travels toward the liquid side with the liquid speed of sound. After that, liquid pressure gradually increases or decreases along with the compression or the expansion of the gas phase. The entire process is successfully and stably simulated with a small numerical oscillation of pressure observed in Fig. 2 (b). The case of larger pressure ratio of 10 (10 atm to 1 atm) is also examined. The numerical solution is again successfully obtained even though there is larger oscillation observed in pressure.

4. Conclusions
A new numerical method for compressible two-phase flow was proposed. Extension from the existing single-phase compressible flow code is straightforward. For the future works, the present method is extended to multi-dimensions and applied to bubble collapse or bubble fission problems.

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