Numerical investigation of collapse of a bubble near the rigid boundary with specific microstructure

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Abstract. The dynamics of a vapour bubble close to a rigid boundary with the micrometer-scale microstructure is numerically simulated based on the Volume of Fluid (VOF) method. The simulated results show that the bubble close to the groove boundary exhibits distinctly different behaviour as the non-dimensional stand-off parameter \( \gamma \) is changed. Deformation of the part around the bubble-wall contact positions of bubble is constrained due to the effect of adsorption on the wall. The evolution of shape of the bubble close to the groove boundary is significantly different for different \( \gamma \). Moreover, the maximum jet velocity, the collapse pressure, and the peak pressure on the groove wall are affected by \( \gamma \). Cavitation erosion of the groove wall is mainly determined by action of shock wave in the three cases considered.

1. Introduction
The bubble dynamics near to the different boundaries is a classical problem, which has received extensive attention from researchers [1]. Rayleigh firstly established the bubble dynamics equation for a spherical bubble, namely Rayleigh equation [2], in which liquid viscosity and liquid compressibility was neglected. Rayleigh equation predicts that a local high pressure will be generated during the collapse phase of a spherical symmetrical bubble. However, quite a few experiments and numerical results demonstrate that bubbles near a boundary behave a non-spherical collapse characteristic [3] [4]. The existence of boundary and different boundary condition have a significant effect on bubble shape evolution, jet generation, collapse pressure and jet velocity [1]. The boundaries can be classified into the rigid wall, the elastic wall and the free surface in terms of the boundary physical properties or into the plain boundary and non-plain boundary in terms of the boundary profile. It should be noted that exploration on interaction of the bubbles with the boundaries having special profile deserves special attention, which can provide a good insight into ultrasonic cleaning, cavitation erosion and medical application of cavitation. However, few experimental and theoretical works focusing on this issue has been reported. In this paper, the effect of boundary with specific microstructure on collapse of bubble was numerically investigated by the homogeneous multiphase model and volume of fluid (VOF) method.

2. Numerical method
The physical description of the problem discussed in this paper is the dynamics of a spherical vapor bubble close to a rigid boundary with the micrometer-scale groove structure. It is assumed that only
vapor, not other gas such as non-condensable gas, is contained in the single bubble. The vapor inside
the bubble is compressible and assumed to behave like an ideal gas. The liquid surrounding the bubble
(e.g. water) is considered as an incompressible newtonian fluid. The fluid flow state is laminar. The
viscosity of water and vapor is considered in simulation. The effect of gravity is neglected. Moreover,
mass transfer between vapor and water is not taken into account in the paper.

2.1. Governing equations

The volume of fluid (VOF) method based on homogeneous flow theory was adopted to simulate collapse
of the cavitation bubble close to the rigid boundary with micrometre-scale groove structure. In the model,
the flow is assumed as a homogenous mixture fluid consisting of liquid and vapor, neglecting inter-
phase relative motion. The two components share the same physical velocity and pressure.

The mass, momentum, and energy equations for the mixture flow are

\[ \frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \bar{v}) = 0 \] (1)

\[ \frac{\partial \rho_m \bar{v}}{\partial t} + \nabla \cdot (\rho_m \bar{v} \bar{v}) = -\nabla p + \nabla \cdot \left[ \mu_m (\nabla \bar{v} + (\nabla \bar{v})^T) - \frac{2}{3} \mu_m \nabla \cdot \bar{v} I \right] + \bar{F}_m \] (2)

\[ \frac{\partial \rho_m E \bar{v}}{\partial t} + \nabla \cdot \left[ \bar{v} (\rho_m E + p) \right] = \nabla \cdot (k \nabla T) \] (3)

where \( p \) is pressure, \( \bar{v} \) is velocity vector, \( \rho_m \) and \( \mu_m \) denotes the density and dynamic viscosity of the
mixture, respectively, \( E \) is total energy, \( T \) is temperature and \( k \) are thermal conductivity. In equation (2),
\( I \) represent the identity matrix.

The surface tension effect of bubble-water interface is included with the continuum surface force
(CSF) model [5], which appends the surface tension term \( F_\sigma \) to the source term of the momentum
equation (2) as a volume force.

\[ \bar{F}_\sigma = \sigma \frac{\rho_m k \nabla \alpha_l}{0.5(\rho_g + \rho_l)} \] (4)

where \( \sigma \) is the surface tension, \( \kappa \) is the curvature of the interface, and \( \alpha_l \) is the volume fraction of the
liquid phase in every cell.

The transportation equation of the volume fraction of liquid phase \( \alpha_l \) is is given by

\[ \frac{\partial \alpha_l}{\partial t} + \nabla \cdot (\alpha_l \bar{v}) = 0 \] (5)

As \( \alpha_l=1 \) or 0 for a grid cell at some time, it means that the grid cell is filled with pure liquid phase or
pure gas phase. As \( 0<\alpha_l<1 \), it represents that the interface between the two phase is located in this grid
cell [6-7].

The density and the dynamic viscosity of the mixture are defined as

\[ \rho_m = \alpha_l \rho_l + (1-\alpha_l) \rho_g \] (6)

\[ \mu_m = \alpha_l \mu_l + (1-\alpha_l) \mu_g \] (7)
where the subscripts l and g correspond to liquid and vapor, respectively. The value of the liquid density is constant. Considering the compressibility of vapor, the density in the gas phase, $\rho_g$, is calculated by the ideal gas state equation.

$$\rho_g = \frac{M_m}{R_g T} \frac{p}{\gamma}$$

where $R_g$ and $M_m$ represent the universal gas constant and the gas molar mass, respectively.

2.2. Computational domain and Mesh generation
The experimental observation shows that collapse of a bubble in proximity to a boundary has the axial symmetry property [8]. Therefore, a 2D axisymmetric model is applied in the numerical simulation. The geometry of the computational model and the boundary condition is shown in figure 1. A distributed rectangular groove with depth $d$ of 0.2mm and width $w$ of 0.2mm is arranged on the rigid boundary. The interval $s$ of every groove unit is designed to be 0.2mm. The most significant geometrical parameter affecting the bubble dynamics, is the non-dimensional stand-off parameter, defined as the ratio of the distance of the initial bubble center from the solid surface $h$ to the maximum bubble radius $r_{\text{max}}$, which is denoted by $\gamma$.

![Figure 1. Computational model](image)

The left boundary is set as axisymmetric boundary and the bottom boundary is set as wall with no-slip boundary condition in the 2D rectangular domain. Both of the right and left boundaries are chosen as pressure outlet with the value being equal to 101kPa. To decrease the effect of pressure boundary condition on the computational result, the distance between any two opposite boundaries is designed to be 50 times as the initial size of bubble. The zone surrounding the bubble (I zone) of interest is densely meshed in order to capture the details of the dynamics for bubble collapse. The structured quadrilateral meshes are generated by using ICEM CFD in order to ensure simulation accuracy and computational precision. The minimum cell size in I zone is about $5\times5\mu m^2$. The total mesh number of all computational models in this paper is more than 160 thousand.

2.3. Discretization scheme and Solution algorithm
The finite volume method is adopted to discretize the governing equations. Because bubble collapse is transit, the PISO algorithm is employed for the pressure-velocity coupling in unsteady computation. The
temporal term is discretized with the first-order implicit scheme. The gradient term is discretized with the least squares cell-based scheme. The liquid volume fraction at a cell interface is computed using Geo-Reconstruct scheme. The density term, the momentum term and the energy term are discretized by using the second-order upwind scheme, respectively. The pressure term is calculated by the body-force-weighted scheme. The fixed time step method is used in the calculation with the time step of 1ns.

3. Results and Discussion
A great number of experimental and numerical results show that the non-dimensional stand-off parameter $\gamma$ is a significant parameter closely related to the impulse pressure on the wall, jet velocity and bubble shape evolution [9]. Three non-dimensional stand-off parameter $\gamma$ of 1, 2 and 3 are selected in the numerical simulation. Only the initial bubble radius of 0.1mm is considered because the initial radius of cavitation bubble has a negligible influence on the jet velocity and the impact pressure on the wall [9].

Figure 2 depicts evolution of the bubble shape during collapse for $\gamma=1$. The vapor bubble contacts with the groove wall at three positions for the initial state in this case (figure 2(a)). Firstly, the bubble continuously contracts due to pressure difference between the inside and outside of the vapor bubble meanwhile the bubble-wall contact area increases (Figure 2(a)). Deformation of the lower part of bubble is inhibited. The upper bubble-liquid interface quickly moves downward and tends to be flat, which has an unchanged transverse size due to the effect of adsorption on the walls. As $t=9.0\mu s$, the whole upper bubble-liquid interface is nearly flat. The pressure gradient becomes significant above the bubble during this initial period (figure 3(a)). No high-pressure zone appears above the bubble in this case, which is different from collapse of the bubble near to the plain boundary [10]. Subsequently, liquid starts to penetrate inside the bubble forming a jet (figure 2(b)). At $t=16.6\mu s$, the liquid jet directly impacts the bottom wall after it passes through the bottom of bubble with the velocity of 17m/s (figure 3(b)). The jet velocity is rather low, which attributes to the small pressure difference between above and below the bubble. The peak impact pressure on the bottom wall induced by jet reaches 2.88MPa (figure 3(c)). After the jet reaches the bottom wall of groove, it moves along the bottom wall, which leads to detachment of the bubble from the bottom wall. The bubble splits into a free toroidal bubble ‘A’ and an attached bubble ‘B’ to the side wall of groove (figure 2(d) and (e)). Subsequently, both of the bubbles ‘A’ and ‘B’ collapse successively (figure 2(f)). A high collapse pressure of 645MPa occurs at the bubble ‘B’ center. The collapse of the attached bubble ‘B’ forms a shock wave. The bottom wall is subjected to an impact pressure of 564MPa (figure 3(d)). Therefore, it is concluded that cavitation erosion of the groove wall in this case should be controlled by the shock-wave action.

![Figure 2. Evolution of the bubble shape for $\gamma=1$.](image-url)
As the stand-off parameter $\gamma$ is increased to be 2, the vapor bubble contacts with the side wall and the liquid below the bubble is closed in the groove at the initial time. Figure 4 depicts evolution of the bubble shape during collapse for $\gamma=2$. Firstly, the upper part of bubble deforms downward significantly meanwhile the transversal size of bubble is unchanged due to the effect of adsorption on the side wall (figure 4(a)). At $t=9.5\mu s$, a high-pressure zone appears above the bubble and the top of bubble-liquid interface is completely flat (figure 5(a)). Then the liquid jet passes through the bubble with the velocity of 77.4m/s at $t=10.84\mu s$ (figure 5(b)). Subsequently, the bubble splits into several toroidal bubbles ‘A’~‘D’ and an attached bubble ‘E’ to the side wall. The bubbles ‘A’ and ‘B’ near the axisymmetric axis move towards the bottom wall under action of the jet (figure 4(e) and (f)). At $t=15.032\mu s$, both of the bubbles ‘A’ and ‘B’ collapse in proximity to the bottom wall, producing the collapse pressure of 154MPa, which causes the impact pressure of 130MPa on the bottom wall (figure 5(c)). The bubbles ‘C’ and ‘D’ behave the characteristics of oscillation (figure 4(f)~(i)). As the bubble ‘C’ starts to rebound after its volume is compressed to the minimum at $t=16.472\mu s$, the pressure at the bubble center is 20MPa (figure 5(d)). The attached bubble ‘E’ continuously contracts and finally detaches from the side wall caused by the jet along the side wall (figure 4(i)).
Figure 4. Evolution of the bubble shape for $\gamma=2$.

Figure 5. Pressure field (on the left-half part) and velocity field (on the right-half part) around collapsing bubble at different time for $\gamma=2$. The black solid line is the bubble-liquid interface.
As the stand-off parameter $\gamma$ is further increased to be 3, the whole bubble is above the groove at the initial time. Figure 6 presents evolution of the bubble profile during collapse. The bubble center approaches the bottom wall as the bubble contracts. At $t=10.15\mu s$, the bubble-liquid interface is completely flat at the top and a high-pressure zone of 0.7MPa appears above the bubble (figure 7(a)). Then a liquid jet forms and the bubble takes on a heart-like shape. A toroidal bubble occurs when the jet passes through the bottom of bubble with the maximum jet velocity of 111m/s at $t=10.93\mu s$ (figure 7(b)). Finally, the toroidal bubble collapses at $t=11.148\mu s$, which generates the collapse pressure of 218MPa, meanwhile the groove wall is subjected to the impulse pressure of 60MPa (figure 7(c)). After the jet moves about 0.235mm along the symmetric axis, the core jet reaches the bottom wall at $t=20.9\mu s$. However, the jet velocity decays to be 35.4m/s, which results in the weak impact pressure of 0.5MPa on the bottom wall (figure 7(d)). It is indicated that cavitation erosion of the groove wall in this case is mainly resulted from action of the shock wave.

Comparing the maximum jet velocity for different $\gamma$ shown in figure 8(a), it is indicated that the maximum jet velocity increases as the stand-off parameter $\gamma$ rises. It is mainly because the pressure difference between above and below the bubble grows with $\gamma$ during development of the jet as shown in figure 8, which directly determines the acceleration of jet. Figure 8(b) presents variation of the collapse pressure and the peak pressure on the bottom wall of groove with $\gamma$. It is shown that the peak pressure on the bottom wall decreases with raising $\gamma$. Moreover, the peak pressure on the bottom wall of groove is close to the collapse pressure for $\gamma=1$ and 2, respectively. The reason is that collapse center of bubble is near to the bottom wall in the two cases under action of the shock wave. However, the peak pressure on the bottom wall is far smaller than the collapse pressure for $\gamma=3$. It is because the shock wave rapidly decays with the increase of propagation distance and the bottom wall is relatively far to the collapse center in the case of $\gamma=3$.

Figure 6. Evolution of the bubble profile during collapse for $\gamma=3$. 

(a) $t=10.15\mu s$  
(b) $t=10.93\mu s$
Figure 7. Pressure field (on the left-half part) and velocity field (on the right-half part) around collapsing bubble at different time for $\gamma=3$. The black solid line is the bubble-liquid interface.

Figure 8. (a) The maximum jet velocity and the pressure difference between above and below the bubble, and (b) the peak pressure on the bottom wall and the collapse pressure for different $\gamma$.

4. Conclusion
The volume of fluid method based on a two-phase flow consisting of an incompressible liquid and a compressible gas is used to simulate the dynamics of a vapor bubble close to a boundary with the micrometer-scale groove structure. Deformation of the bubble in the groove is significantly limited because the bubble is adsorbed to the wall as it contacts with the groove. The evolution of shape of the bubble for different $\gamma$ exhibits its distinct characteristics. The maximum jet velocity increases with $\gamma$. Cavitation erosion of the groove wall is dominantly caused by action of the shock wave in the three cases considered. The impulse pressure on the groove wall decreases with the increase of $\gamma$.

Acknowledgments
This work was financially supported by Natural Science Foundation of Liaoning Province of China (2015020136 and 201602090) and Liaoning Province Education Committee (L2015068).

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