Numerical simulations of interactions between shock wave and gas-liquid-air interfaces

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Abstract. A gas-liquid-air model and problems of interactions between the shock wave and the interfaces during the expansion process are rather familiar in the study of liquid explosive dispersal and underwater explosion near air-water surface. It involves large density discontinuity and large pressure gradient at the same time which brings difficulties for the numerical simulations. In this paper, we use the level-set methods to capture the interface and the modified ghost fluid method (MGFM) to treat the interface conditions. Strong shock-interface interactions and influences of the disturbance on the two interfaces are investigated. The initial fragmentation of the liquid is studied based on the analyses of the fluid pressure distribution and the variation of the interface, combining the conditions of the cavitations occurrence in the liquids.

1. Introduction
The initial period of liquid explosive dispersal and under water explosion near air-water surface have similar characteristics. Both of these two kinds of problems involve complex physical phenomena which can be characterized by propagation of shock wave in multi-medium flow consisting of gas, liquid and air [1-3]. When the shock wave produced by explosion passes through the gas-liquid-air interfaces, strong refractive shock wave and rarefaction wave will be formed due to the large density discontinuity between gas and liquid. The large density discontinuity between gas and liquid and large pressure gradient corresponding to the shock wave coexist in these problems and make their numerical simulations very difficult.

In fact, for the aforementioned strong shock-interface interaction problems, two kinds of problems should be solved. One of them is to capture the moving material interface. The other is to treat the interface conditions of flow. Due to that interface problems involving external physics arise in various areas of science, a lot of methods to track the interface have been developed, such as front tracking, phase-field methods, the volume of fluid (VOF) approach and level set method [3-7]. Among of them, the level set method devised by Osher and Sethian has had major successes in this area as a simple and versatile method for computing and analyzing the motion of an interface in two or three dimensions. Mulder et al [8] firstly applied the level set method to two phase inviscid compressible flow but the method suffered from spurious pressure oscillations at the interface. This problem was overcome by the development of the ghost fluid method (GFM) which can couple the level set representation of

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discontinuities to finite difference calculations of compressible flows [9]. The main appealing features of the GFM are maintenance of a sharp interface without smearing and to make the interface “invisible” during computations and the computations are carried out as for a single-medium manner such that its extension to multi-dimensions becomes fairly straightforward. But the single-medium manner across the interface in the GFM may cause numerical inaccuracy when there is a strong shock wave interacting with the interface. To enhance its accuracy, Liu et al [10] developed a modified GFM (MGFM) with a predicted more reasonable ghost fluid status. The MGFM was further modified to apply to nearly cavitating flow and found to be quite robust and can provide relatively reasonable results [11]. However, as other popular high resolution schemes, the MGFM may also give inaccurate numerical results even over a very fine mesh when applied to gas flows with an initial high density ratio as well as a high pressure ratio [12].

In this paper, strong shock impacting on gas-liquid-air interfaces is investigated. Here the level-set methods are used to capture the moving material interfaces and the modified ghost fluid method (MGFM) to treat the interface conditions. In section 2, the formulation of gas-liquid-air problem is given. Its one dimension case is discussed in section 3. In section 4, 2D models corresponding to the initial period of liquid explosive dispersal and under water explosion near air-water surface are investigated respectively by numerical simulation and compared with experimental results. Some conclusions are given in section 5.

2. Mathematical formulations and numerical methods

2.1. Governing equations for the fluid

The governing equations for compressible fluid are the conservative form of the Euler equations. The Euler equations for 2-D compressible flows are written as

\[
\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} + \frac{\partial G(U)}{\partial y} = 0
\]

(2.1)

where \( F(U) = \left[ \rho u, \rho u^2 + p, \rho u v, (E + p)u \right]^T \), \( G(U) = \left[ \rho v, \rho u v, \rho v^2 + p, (E + p)v \right]^T \), \( U = \left[ \rho , \rho u , \rho v , E \right]^T \). Here, \( \rho \) is the density; \( u \) and \( v \) are the velocity components in the respective \( x \) and \( y \) directions; \( p \) is the pressure and \( E \) is the total energy per unit volume which is the sum of internal energy and kinetic energy. In this work, a second-order Total Variation Diminishing (TVD) scheme is applied to solve the Euler equations.

2.2. Equations of state (EOS)

In the present work, we are interested in the interaction with the strong shock wave and the interfaces with large density ratio. Two kinds of EOS are considered. The first one is the \( \gamma \) – law for perfect gases, which is written as

\[
p = (\gamma - 1) \rho e
\]

(2.2)

We let \( \gamma = 1.4 \) for all gases for simplicity. The second one is the Tait’s EOS for water, which is written as

\[
p = B \left( \frac{\rho}{\rho_0} \right)^N - B + A
\]

(2.3)

where \( N = 7.15, B = 3.31 \times 10^8 \text{Pa}, A = 10^5 \text{Pa} \).
2.3. Level set equation

In the level set approach, the interface is defined implicitly as an iso-surface of a smooth function \( \phi \), which is defined as signed distance function here. The transport of the interface can simply be described by

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

(2.4)

In this work, the fifth-order weighted essentially non-oscillatory (ENO) scheme is used to discretize the spatial derivatives with the third-order Runge-Kutta time discretization. In order to ensure that \( \phi \) remains a distance function, re-initialization is performed by solving a Hamilton-Jacobi equation

\[
\frac{\partial \phi}{\partial \tau} + S(|\nabla \phi| - 1) = 0
\]  

(2.5)

where \( S \) is a modified sign function (see [13] for details).

2.4. The MGFM algorithm

In a GFM-based algorithm, a given band of points as ghost cells is defined in the vicinity of the interface and the ghost fluid status is defined. Each medium with its ghost nodes is solved independently. By combining the solution for each medium according to the new interface location, the overall solution for the whole domain at the next time step is then obtained.

We applied MGFM method to treat the interface conditions. In this algorithm, equations below are solved for the status on the interface:

\[
\frac{p_I - p_L}{W_L} + (u_I - u_L) = 0
\]  

(2.6a)

\[
\frac{p_I - p_R}{W_L} - (u_I - u_R) = 0
\]  

(2.6b)

\[
W_L^2 = \rho_{IL} \rho_L \frac{p_I - p_L}{\rho_{IL} - \rho_L}  
\]  

(2.6c)

\[
W_R^2 = \rho_{IR} \rho_R \frac{p_I - p_R}{\rho_{IR} - \rho_R}  
\]  

(2.6d)

where subscripts ‘I’, ‘IL’, ‘IR’ refer to the interface, the left side of the interface and the right side of the interface, respectively (see [10] for details). For closure of (2.6a)-(2.6d), the relationship of density and pressure based on the energy jump condition, \( e_I - e_0 = \frac{1}{2}(p_I + p_0)(\frac{1}{\rho_I} - \frac{1}{\rho_0}) \), are applied.

The status \( (p_I, u_I, \rho_{IL}, \rho_{IR}) \) on the interface is obtained after solving the Riemann problem above via iteration and then assigned to the ghost nodes near the interface. Then the isobaric technique is applied to the proximate real fluid nodes to the interface to fix the real fluid density to suppress the possible “overheating” and also assign density for the ghost fluid.

3. One dimensional problem

Some shock tube-like problems are considered here. Let us consider a shock wave impacting on a gas-water interface from the left side and transporting in the water region and then transmitting to another gas medium, as shown in Figure 1. We are interested in the distribution of pressure and density behind the shock wave. Assuming that the pressure and velocity of each media to be uniform initially, the governing equation is the 1-D Euler equation and the initial condition is given as
\[ U_{x=0} = \begin{cases} U_1 & x < x_s \\ U_{10} & x_s < x < x_{gw} \\ U_{20} & x_{gw} < x < x_{wg} \\ U_{30} & x > x_{wg} \end{cases} \tag{3.1} \]

where \( U_{10}, U_{20}, U_{30} \) are the initial states in medium 1, 2 and 3 before the shock wave, and \( U_i \) is the status behind the incident shock and satisfies the Rankine-Hugoniot conditions.

Distribution of pressure and density under different strength of the incident shock and different initial density ratio will be discussed. The interface between left gas region and the water region (named F1) is initially located at \( x_{gw} = 0 \), where the interface between the water region and the right gas region (named F2) is initially located at \( x_{wg} = 0.5 \). The initial position of the incident shock front is the same as F1, that is, \( x_s = x_{gw} = 0 \). The calculations are done with CFL=0.5 and 501 uniform mesh points in a domain with dimensionless length 5.

Though the MGFM may give inaccurate numerical results even over a very fine mesh when applied to gas flows with an initial high density ratio as well as a high pressure ratio, it can provide helpful results here because that refer to [12], the calculation error mainly concentrates in the disability to provide the transmitted shock location accurately after it transfers a long distance while the value of the discontinuity is mostly correct. Therefore, analysis of the characteristic of the interaction between shock wave and the gas-liquid-air interfaces is still valuable.

The pressure and density profile for three different strength of incident shock under several time steps are shown in Figure 2 and Figure 3, where strength of the incident shock \( p_1/p_10 = 1000, 5000, 100000 \) are considered; other initial flow parameters are \( p_{10} = p_{20} = p_{30} = 10^5 \text{Pa} \), \( \rho_{10} = 0.001 \text{g/cm}^3 \), \( \rho_{20} = 1.0 \text{g/cm}^3 \), \( \rho_{30} = 0.001 \text{g/cm}^3 \). The short horizontal lines in Figure 2 indicate the location of the water region for different time steps. From Figure 2, the pressure behind the reflected shock wave is about 7.5 times higher than the incident shock pressure. The water regions are compressed and pushed forward. When the transmitted shock in the water region meets the water-air interface, a strong rarefaction wave is reflected and the pressure and density of the water drop greatly and approach to the initial states. Comparison among these figures shows that characteristics under different strength of incident shock are similar and the differences only lie in the values of the pressure and density.

Figure 4 shows the pressure and density distributions for incident shock strength \( p_1/p_10 = 5000 \) and \( \rho_{10}/\rho_{20} = 0.1 \). Other initial parameters are \( \rho_{20} = 1.0 \text{g/cm}^3 \), \( \rho_{30} = 0.001 \text{g/cm}^3 \), \( p_{10} = p_{20} = p_{30} = 10^5 \text{Pa} \). The high density of the upwind gas increases the velocity behind the shock and prevents the reflecting shock wave to propagate toward left side. Moreover, the refractive shock strength is only 4.4 times higher than the incident shock wave. Figure 5 shows the pressure and density distributions for incident shock strength \( p_1/p_10 = 5000 \) and \( \rho_{30}/\rho_{20} = 0.1 \). Other initial
parameters are $\rho_{10} = 0.001g/cm^3$, $\rho_{20} = 1.0g/cm^3$, $p_{10} = p_{20} = p_{30} = 10^5 Pa$. The distributions of pressure and density are similar with the cases shown in Figure 2 and 3 except that at the right water-gas interface, the transmitted shock wave is strengthened and the rarefaction wave is weakened greatly. Comparison between Figure 4 and 5 shows that the density of the left side gas influences the characteristics of the flow field more evidently than that of the right side gas.

Figure 2. Pressure profiles for different strength of incident shock. (a) Strength of incident shock: 1000. (b) Strength of incident shock: 5000. (c) Strength of incident shock: 100000
Figure 3. Density profiles for different strength of incident shock. (a) Strength of incident shock: 1000. (b) Strength of incident shock: 5000. (c) Strength of incident shock: 100000

Figure 4. Results of several time steps for $\rho_{10}/\rho_{20} = 0.1$. (a) Pressure profile. (b) Density profile.

Figure 5. Results of several time steps for $\rho_{30}/\rho_{20} = 0.1$. (a) Pressure profile. (b) Density profile.
4. Two dimensional problem

4.1. Liquid explosive dispersion
The interaction of shock wave and liquid during the liquid explosive dispersion is analyzed. The initiation of the detonator is represented by the high pressure gas in the centre of the water ring, which is the gas region in Figure 6(a). Water and the air are of the standard atmosphere pressure. The initial pressure of the explosion gas is 1000atm. The inner and outer radii of the water ring are 3cm and 8cm respectively (see Figure 6(a)).

![Figure 6. (a) A 2-D model for the initial period of a liquid explosive dispersion. (b) Experiment result obtained from a quasi-2-D liquid explosion dispersion](image)

Pressure profile and the contour of density for time \( t = 0.000044 \)s are shown in Figure 7. The colour of deep blue in the left figure indicates a region with very low pressure (about 22pa, which is the low point for the Tait’s EOS in effect) and the corresponding region in the figure of density contour is the outer region of the water. In this region, the pressure is lower than the saturation vapour pressure of water and the water in this region is hard to keep the continuous liquid state. This region is where cavitations are likely to happen. On the other hand, geometry of the water ring hasn’t been changed markedly yet at this time, so if there’s a solid shell outside the water ring, the shell should not have been broken yet. Thus, Figure 7 can equivalently show the status in a liquid explosion process just before the liquid jets out the crust, which means that as soon as the detonating occurs, the liquid’s characteristics have changed before the crust of the device of liquid explosive dispersion is broken. Cavitations and gasification may occur in the outer part of the liquid. Figure 6(b) is obtained from an experiment of liquid explosive dispersion 2ms after initiation of detonator and shows how the liquid jet out the thin crust [14]. It can be seen that the outer part of the water region is bright, where the property of water is obviously changed. We thought that cavitations or gasification has occurred in this region. This shows that the experimental results are consistent with the numerical results.

It should be pointed out that simulation broke down shortly after this time because the EOS for water doesn’t suit for the state of the region with very low pressure and a new EOS needs to be applied to this problem. However present simulation can point out the region where the pressure is low enough for the cavitations to occur.
Figure 7. Numerical results for the 2-D model in Figure 6(a). (a) Pressure distribution. (b) Density contour. (The scale for x and y is 10cm)

4.2. Underwater explosion near the water-air surface
Another case with interaction of shock wave and gas-liquid-air interfaces is underwater explosion problem near air-water surface. Ballhaus and Holt investigated an underwater spherical blast problem and proposed an analytical solution. Here the same underwater explosion problem near the water-air surface is investigated using MGFM method and compared with the analytical results in [2]. Moreover, influence of disturbance of water-air surface is discussed.

Figure 8 demonstrates the underwater explosion initial conditions (the initial position of the water surface and the gas sphere) with respect to undisturbed and disturbed water-air surface. The same parameters as that in [2] are used in the following analysis. The explosion centre is 1 meter below the water surface and at time t=0, the explosion produces a spherical shock wave that begins to propagate outward. The radius of the initial explosion gas sphere is 1/3 meter and initial pressure is 9000atm. Figure 9 shows the distributions of pressure and the density contours for time t=0.0010312s and
0.0011456s with respect to the undisturbed water-air surface. The shape and position of the water-air surface and the gas sphere is displayed in the density contour. In the figure of pressure profile, the color of deep blue indicates a region with very low pressure where cavitations are likely to happen. It can be seen that the low pressure region increases with the increasing of time. Figure 10 shows refractive wave series and the position of the water-air surface based on the analytical results in [2]. The region where pressure is lower than the initial value is labeled with dots. It shows that the low pressure region occurs firstly at the intersection of the refraction wave and the water-air surface. The region becomes larger with the increasing of time and new low pressure region generates in the middle of the water-air surface. This is consistent with the numerical results basically.

Figure 9. Distributions of pressure and the density contours for the undisturbed surface. (a) Pressure field at time \( t = 0.0010312s \). (b) Density contour at time \( t = 0.0010312s \). (c) Pressure field at time \( t = 0.0011456s \). (d) Density contour at time \( t = 0.0011456s \).
The distributions of pressure and the density contours for time $t=0.00057338s$ and $0.0011456s$ with respect to the disturbed water-air surface are shown in Figure 11. It can be found by comparison with Figure 10 that when the water-air surface are disturbed, low pressure regions occur at more early time and distribute in wider range. In addition, the flow field becomes more irregular. The results show that the disturbance of water-air surface can make the cavitations generate more easily and the flow become more complex.

Figure 11. Distributions of pressure and the density contours for the disturbed surface. (a) Pressure field at time $t=0.00057338s$. (b) Density contour at time $t=0.00057338s$. (c) Pressure field at time $t=0.0011456s$. (d) Density contour at time $t=0.0011456s$. 
5. Conclusions
Interactions of strong shock wave with gas-liquid-air interfaces are investigated in this paper. Here the level-set and MGFFM methods are used to capture the moving material interfaces and treat the interface conditions, respectively. Firstly distributions of pressure and density under different strength of the incident shock and different initial density ratio are discussed for one dimensional problem. The results show that characteristics under different strength of incident shock are similar and the differences only lie in the values of the pressure and density. Moreover the density of the left side gas influences the characteristics of the flow field more evidently than that of the right side gas. Secondly two typical 2D models corresponding to liquid explosive dispersal and underwater explosion near air-water surface are investigated respectively. Numerical results are in good agreement with corresponding experimental or analytical results. The two typical problems have similar characteristics. Both of them have low pressure region which may generate cavitations or gasification. In addition, the disturbance of water-air surface can make the flow become more complex. The future work is to introduce more reasonable model to treat the two phase flow problem caused by cavitations.

Acknowledgments
The work in this paper was supported by National Science Foundation Committee of China, No.10572149 and Allied Key-projects by China Academy of Engineering Physics and National Science Foundation Committee of China (NSAF), No.10676120.

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