A Volume-Of-Fluid Type Algorithm for Compressible Two-Phase Flows

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Abstract. We present a simple approach to the computation of a simplified two-phase flow model involving gases and liquids separated by interfaces in multiple space dimensions. In contrast to the many popular techniques which are mainly concerned with the incompressible flow, we consider a compressible version of the model equations without the effect of surface tension and viscosity. We use the γ-law and the Tait equation of state for approximating the material property of the gas and the liquid in a respective manner. The algorithm uses a volume-of-fluid formulation of the equations together with a stiffened gas equation of state that is derived to give an approximate model for the mixture of more than one phase of the fluids within grid cells. A standard high-resolution shock capturing method based on a wave-propagation view-point is employed to solve the proposed model. We show results of some preliminary calculations that illustrate the viability of the method to practical application without the occurrence of any spurious oscillation in the pressure near the interfaces. This includes results of a planar shock wave in water over a bubble of air.

1. Introduction

We are interested in a two-phase flow problem with interfaces that separate regions of two different fluid components consisting of gases and liquids. We consider a two-dimensional flow as an example, and use the compressible Euler equations to modeling the motion of the gases,

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho u\\ \rho v\\ \rho\mathcal{E}\end{pmatrix}+\frac{\partial}{\partial x}\begin{pmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ (\rho\mathcal{E}+p)u\end{pmatrix}+\frac{\partial}{\partial y}\begin{pmatrix}\rho v\\ \rho uv\\ \rho v^2+p\\ (\rho\mathcal{E}+p)v\end{pmatrix}=0. \qquad (1)$$

Here ρ is the density, u and v are the velocities in the x- and y-direction respectively, p is the pressure, and $\mathcal{E}$ is the total energy per unit mass. We assume that

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the equation of the state for the gas satisfies the γ-law, where γ is the ratio of specific heats ($\gamma > 1$). Then the internal energy is

$$e = \frac{1}{\gamma - 1}\frac{p}{\rho}, \tag{2}$$

and $\mathcal{E} = e + (u^2 + v^2)/2$. We note that the four components of Eqs. (1) express the conservation of mass, momenta in the x- and y-direction, and energy, respectively [5].

As it is often the case, we take the liquids to be *baratropic* that the pressure p is a function of the density ρ only, and in particular it fulfills the Tait equation of state of the form,

$$p(\rho) = \mathcal{A}\rho^{\gamma} - \mathcal{B}, \tag{3}$$

where $\mathcal{A}$ and $\mathcal{B}$ are material-dependent constants; these two parameters along with γ give a fundamental characterization of the fluid properties of interest and can be obtained from a fitting procedure of laboratory data [26]. Typical set of values are, for water, $\gamma = 7$, $\mathcal{A} = 3001$ atm, and $\mathcal{B} = 3000$ atm [5], and for human blood, $\gamma = 5.527$, $\mathcal{A} = 614.6$ MPa, and $\mathcal{B} = 614.6$ MPa [17], approximately. It is important to note that because of the mere dependency of the pressure p on the density ρ, the energy equation of the Euler Eqs. (1) plays no active role to the determination of this flow behavior, and hence can be neglected. For completeness, we write down the equations of motion for the liquid as follows,

$$\frac{\partial}{\partial t}\begin{pmatrix} \rho \\ \rho u \\ \rho v \end{pmatrix} + \frac{\partial}{\partial x}\begin{pmatrix} \rho u \\ \rho u^2 + p(\rho) \\ \rho u v \end{pmatrix} + \frac{\partial}{\partial y}\begin{pmatrix} \rho v \\ \rho u v \\ \rho v^2 + p(\rho) \end{pmatrix} = 0, \tag{4}$$

where the pressure p is governed by (3).

We want to use a state-of-the-art shock-capturing method on a uniform rectangular grid for the computation. For convenience, let us suppose that for each grid cell we have a volume-fraction function $\mathcal{Z}$ representing the type of fluid within the cell. For example, for the *liquid only* cells we may take $\mathcal{Z} = 1$, and therefore for the *gas only* cells we may set $\mathcal{Z} = 0$. In case there are some cells cut by the interfaces where $\mathcal{Z} \in (0, 1)$, we then have both of the gas and liquid components in the cells in which the liquid and the gas are occupied by the volume fractions $\mathcal{Z}$ and $1 - \mathcal{Z}$, respectively.

It is clear that, when $\mathcal{Z} = 0$ or $\mathcal{Z} = 1$, there is no problem in describing the motion of each of the gas and liquid flows individually, see Eqs. (1)–(4). The principle problem in the current application and also in the other multicomponent problems (cf. [1, 4, 7, 14, 15]) is however directed to the development of an efficient and yet accurate way that is capable of dealing with the fluid-mixture case when $\mathcal{Z} \in (0, 1)$. Motivated by the previous work by the author [20], the algorithm we employed uses a mixture model based on a volume-fraction (or called a volume-of-fluid) formulation of the equations that is devised to model the mixture of the two different equations of state (2) and (3) by the so-called stiffened gas equation of state (6) (see Section 2). Then from the energy equation of (1), we choose conditions that should be satisfied to ensure the pressure in equilibrium for these cells (see Section 3). Numerical results to be presented in Section 4 show that this is a viable approach for practical problems without any spurious oscillations in the pressure near the interfaces when we approximate the model equations in a consistent manner by a *fluctuation-and-signal* type of shock capturing method [11, 12, 19].

It is true that for real applications the effect of surface tension as well as viscosity are two important elements to the solutions of a two-phase flow problem under studied [18]. Among many of the approaches developed over the years to deal with these situations (cf. [10, 25]), the method based on the level set formulation [2, 22, 23] has shown to be quite effective for an incompressible version of the problem where the fluids are mostly in a low Mach number regime. Here in contrast to the work just mentioned, we consider a class of problems where the influence of compressibility of the fluids to the solutions is vital, but not the surface tension and viscosity. Examples of this kind cover a family of shock wave problems with interfaces [8, 9]. Our goal here is to establish a basic solution strategy for the problem (cf. [3, 6, 7, 24] for other approaches). Realization of this approach that couples with adaptive grid procedures such as front tracking and adaptive mesh refinement is in progress (cf. [21]). In a future work, we will take more physical factors into account, and also look at methods that are efficient for problems with low and high Mach number flow where the time step restriction is an important issue to be addressed.

This paper is organized as follows. In Section 2, we remark and discuss the equations of state that are used in our model two-phase flow problems with gases and liquids. In Section 3, we review the derivation of the model system based on a volume-of-fluid formulation of the equations. Numerical results for some sample problems are shown in Section 4.

2. Equations of State

It is known that in gases the specific entropy, denoted by $\mathcal{S}$, has great influence to the behavior of the pressure p, while in liquids the influence of its changes is negligible to the pressure [5, 26]. In fact, because of this little dependency of the pressure on the entropy and a consequence of the first law of thermodynamics, we may write the internal energy of a liquid as a *separable energy* of the form

$$e = e^{(1)}(\rho) + e^{(2)}(\mathcal{S}),$$

where with the Tait equation of state (3) we find

$$e^{(1)}(\rho) = \frac{1}{\gamma - 1}\left(\frac{p(\rho) + \gamma\mathcal{B}}{\rho}\right). \tag{5}$$

From this, it is easy to observe strong resemblance of the equation of state of a liquid to that of an ideal gas (2). With this in mind, it should be sensible to use a generalized version of Eq. (5), namely, the stiffened gas equation of state,

$$e = \frac{1}{\gamma - 1}\left(\frac{p + \gamma\mathcal{B}}{\rho}\right), \tag{6}$$

without the explicitly dependence on the density ρ to the pressure p to modeling mixtures of the components of gases and liquids within a grid cell. Note that a stiffened gas reduces to a γ-law gas when $\mathcal{B} = 0$, and to a *baratropic* gas of the form (3) when the pressure p is independent of the entropy $\mathcal{S}$. Oftentimes, the equation of state (6) has been used in other applications to model materials including compressible liquids and solids [16]. Here we find it is suitable for the current application, when combining (6) with a two-phase flow algorithm described in the next section, see results shown in Section 4 for numerical verification of this statement.

3. Volume-Of-Fluid Algorithm

We now discuss the basic idea of our approach to modeling cells that contain both of the gas and liquid phases. We use the Euler Eqs. (1) as a model system that describes the motion of the mixtures of conserved variables such as ρ, ρu, ρv, and $\rho\mathcal{E}$ in a gas-liquid coexistent grid cell. Then with the use of the equation of state (6) the pressure p in the equations (1) can be set by

$$p = (\gamma - 1)\left[\rho\mathcal{E} - \frac{(\rho u)^2 + (\rho v)^2}{2\rho}\right] - \gamma\mathcal{B}, \tag{7}$$

when the mixture of material-dependent parameters γ and $\mathcal{B}$ are defined and known a priori. It is important to note that in our approach the conditions for γ and $\mathcal{B}$ are chosen so that the pressure p in (7) retains in equilibrium for a gas-liquid mixture cell. The derivation of the evolution equations for γ and $\mathcal{B}$ in the current case follows directly from procedures developed in [20]. However, to make the paper self-contained, a brief overview of this approach is undertaken below.

We begin by considering a model two-phase flow problem that the pressure p and the velocity field (u, v) are constant in the domain, while the other variables such as the density ρ and the equation of state parameters: γ and $\mathcal{B}$, are having jumps across a gas-liquid interface. We write Eqs. (1) in the following non-conservative form,

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} + v\frac{\partial \rho}{\partial y} + \rho\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) &= 0,\\
\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{1}{\rho}\frac{\partial p}{\partial x} &= 0,\\
\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{1}{\rho}\frac{\partial p}{\partial y} &= 0,\\
\frac{\partial}{\partial t}(\rho e) + \frac{\partial}{\partial x}(\rho e u) + \frac{\partial}{\partial y}(\rho e v) + p\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) &= 0,
\end{aligned}$$

and obtain easily equations describing the motion of the gas-liquid interface as

$$\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial x} + v\frac{\partial \rho}{\partial y} = 0,$$
$$\frac{\partial}{\partial t}(\rho e) + u\frac{\partial}{\partial x}(\rho e) + v\frac{\partial}{\partial y}(\rho e) = 0. \tag{8}$$

To see how the pressure p would keep in equilibrium as it should be for this model problem, we insert the equation of state (6) into (8), and have

$$\frac{\partial}{\partial t}\left(\frac{p+\gamma\mathcal{B}}{\gamma-1}\right) + u\frac{\partial}{\partial x}\left(\frac{p+\gamma\mathcal{B}}{\gamma-1}\right) + v\frac{\partial}{\partial y}\left(\frac{p+\gamma\mathcal{B}}{\gamma-1}\right) = 0. \tag{9}$$

Then with the volume-fraction function $\mathcal{Z}$ defined previously in Section 1, the total internal energy ρe can be expressed as a function of the volume fraction by

$$\rho e = \frac{p+\gamma\mathcal{B}}{\gamma-1} = \mathcal{Z}\left(\frac{p^{(l)}+\gamma^{(l)}\mathcal{B}^{(l)}}{\gamma^{(l)}-1}\right) + (1-\mathcal{Z})\left(\frac{p^{(g)}}{\gamma^{(g)}-1}\right), \tag{10}$$

where the superscript "l" and "g" of the states p, γ, and $\mathcal{B}$ represent the values for the liquid and gas phases, respectively. When substituting (10) to (9), and after some algebraic manipulation, it is not difficult to show the satisfaction of the required pressure equilibrium, $p = p^{(l)} = p^{(g)}$, when the following evolution equation for the volume-fraction function is hold,

$$\frac{\partial \mathcal{Z}}{\partial t} + u\frac{\partial \mathcal{Z}}{\partial x} + v\frac{\partial \mathcal{Z}}{\partial y} = 0. \tag{11}$$

Note that in this instance, the mixture of γ and $\mathcal{B}$ are computed by

$$\gamma = 1 + 1\bigg/\left(\frac{\mathcal{Z}}{\gamma^{(l)}-1} + \frac{1-\mathcal{Z}}{\gamma^{(g)}-1}\right), \tag{12a}$$

and

$$\mathcal{B} = \left(\frac{\mathcal{Z}\gamma^{(l)}\mathcal{B}^{(l)}}{\gamma^{(l)}-1}\right)\bigg/\left(1 + \frac{\mathcal{Z}}{\gamma^{(l)}-1} + \frac{1-\mathcal{Z}}{\gamma^{(g)}-1}\right). \tag{12b}$$

In summary, the model equations we proposed to solve two-phase flow problems with gases and liquids consist of the following equations,

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \dfrac{\partial}{\partial x}(\rho u) + \dfrac{\partial}{\partial y}(\rho v) = 0 \\ \dfrac{\partial}{\partial t}(\rho u) + \dfrac{\partial}{\partial x}(\rho u^2 + p) + \dfrac{\partial}{\partial y}(\rho uv) = 0 \\ \dfrac{\partial}{\partial t}(\rho v) + \dfrac{\partial}{\partial x}(\rho uv) + \dfrac{\partial}{\partial y}(\rho v^2 + p) = 0 \\ \dfrac{\partial}{\partial t}(\rho\mathcal{E}) + \dfrac{\partial}{\partial x}\left[(\rho\mathcal{E}+p)u\right] + \dfrac{\partial}{\partial y}\left[(\rho\mathcal{E}+p)v\right] = 0 \qquad \text{if} \quad 0 \le \mathcal{Z} < 1 \\ \dfrac{\partial \mathcal{Z}}{\partial t} + u\dfrac{\partial \mathcal{Z}}{\partial x} + v\dfrac{\partial \mathcal{Z}}{\partial y} = 0, \end{cases} \tag{13}$$

where in case $\mathcal{Z} = 1$ the Tait equation of state (3) is used to compute the pressure p for a liquid, while Eq. (7) is employed when $0 \leq \mathcal{Z} < 1$ with γ and $\mathcal{B}$ defined by (12a) and (12b), respectively. We note that the model Eqs. (13) is not written in the full conservation form, but is rather a quasi-conservative system of equations. Numerical approximation based on the discretization of the model equations *via* the wave propagation approach [11, 12] has shown to be quite robust for a wide variety of problems of practical interests, see results presented in Section 4. The algorithmic details as well as many other numerical aspects of this approach may be found in the papers [20, 21].

4. Numerical Results

We now present two sample calculations to demonstrate the feasibility of the proposed approach described in Section 3 for practical applications (cf. [21] for more numerical results).

EXAMPLE 4.1. To begin, we consider a radially symmetric problem that the computed solutions can be compared with the one-dimensional results for numerical validation. We use the same setup as done by Davis [6] that inside a circular membrane of radius $r_0 = 0.2$ the fluid is air with density $\rho = 1.25$, pressure $p = 2.75$, and the adiabatic gas constant $\gamma = 1.4$, while outside the circular membrane the fluid is liquid with density $\rho = 1$ and the Tait equation of state (3) of parameter values: $\mathcal{A} = 1, \mathcal{B} = 1$, and $\gamma = 7$. Initially both of the air and the liquid are in a stationary position, but due to the pressure difference between the fluids, breaking of the membrane occurs instantaneously. For this problem, the resulting solution consists of an outward-going shock wave in liquid, an inward-going rarefaction wave in air, and a contact discontinuity lying in between that separates the air and the liquid.

In Fig. 1, we show numerical results for the density ρ as well as the pressure p at time $t = 0.07$. We use a 100×100 grid with the high resolution version of the wave propagation method (cf. [11, 12]) for the computation (the computational domain is a square with dimensions $[0, 0.5] \times [0, 0.5]$). From the contours of the plots, it is easy to see the wave pattern as just mentioned after the breaking of the membrane, where the dashed line in the pressure contours is the approximate location of the interface. From the scatter plots, we find good agreement of the results as compared with the "true" solution obtained from solving the one-dimensional multicomponent model with appropriate source terms for the radial symmetry using the high-resolution method [20] (with mesh side $h = 1/2000$). Noticeably, here the pressure near the interface behaves in a satisfactory manner without any spurious oscillations, and the shock wave and contact discontinuity appear to be very well located.

EXAMPLE 4.2. Our next example concerns a planar shock wave in water over a bubble of air. We take an initial condition that is similar to the one used by Grove and Menikoff [9] where anomalous reflection of a shock wave at a fluid

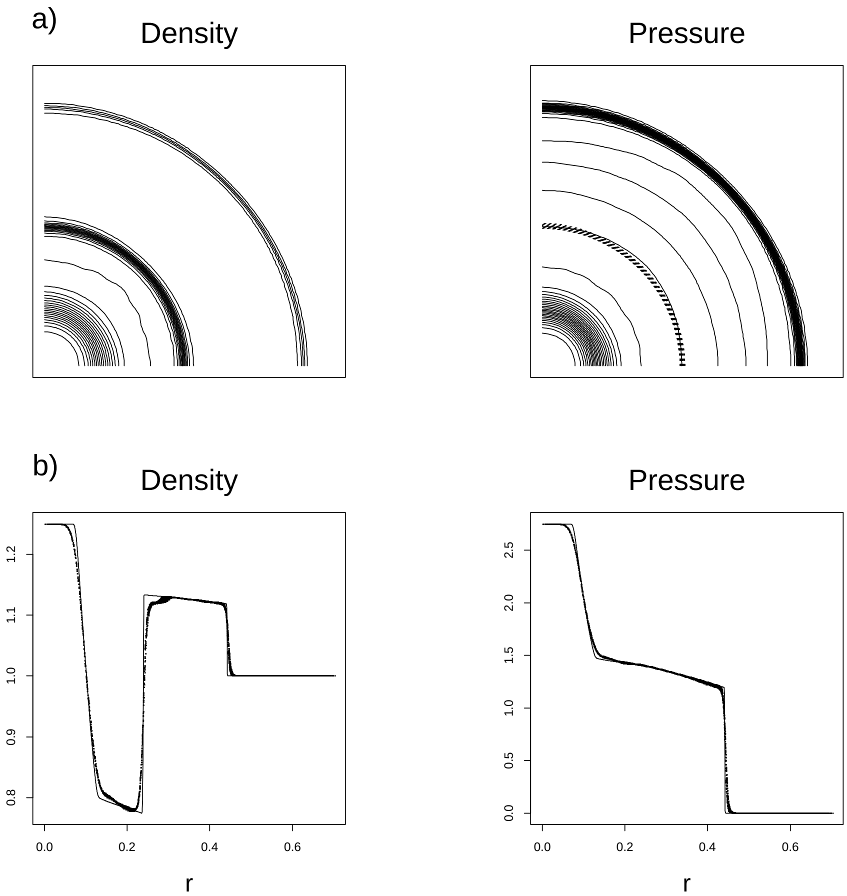

FIGURE 1. High resolution results for a radially symmetric problem at time $t = 0.07$. (a) Contours of the density ρ and the pressure p. (b) Scatter plots of the density ρ and the pressure p with locations measured as a distance from a point of the solution to the center $(0, 0)$. The solid line in the scatter plot is the "true" solution obtained from solving the one-dimensional multicomponent model with appropriate source terms for the radial symmetry using the high-resolution method. The dotted points are the two-dimensional result. The dashed line in the pressure contour is the approximate location of the interface.

interface is examined closely there. Here to test the proposed method, we consider a downward-moving Mach 1.587 shock wave in water with data in the

$$(\rho,\ u,\ v,\ p)_{\text{preshock}} = (1,\ 0,\ 0,\ 1),$$

and data in the post-shock state by

$$(\rho,\ u,\ v,\ p)_{\text{post-shock}} = (1.233,\ 0,\ -43.467,\ 10^4).$$

The parameters we used for the equation of state of the water are: $\mathcal{A} = 3001$ atm, $\mathcal{B} = 3000$ atm, and $\gamma = 7$. In addition to this, we assume that there is a stationary bubble of air of radius 0.2 located just below the shock with density $\rho = 0.0012$ (dimensional unit g/cc) and the adiabatic gas constant $\gamma = 1.4$ for the γ-law equation of state (2). We note that the ratio of acoustic impedances $(\rho c)_{water}/(\rho c)_{air} \approx 3535$ is large for the problem studied here, where c is the speed of the sound of the material of interests. In fact, this is a much more difficult test than those ones considered in EXAMPLE 4.1 and also in [20].

Fig. 2 shows preliminary results of this problem using the high resolution method with a 200×200 grid on a unit square domain. In the figure, reasonable resolution of the results are obtained by the method where the density ρ and the pressure p contours (in logarithmic scale) at three different times, $t = (1, 2, 3) \times 10^{-3}$, are present (cf. [9]). Some works are in progress to further validate the approach introduced here (cf. [21]). This includes results of a model water splash problem that due to gravity a water drop is fallen from the air to a water surface in below [18, 23].

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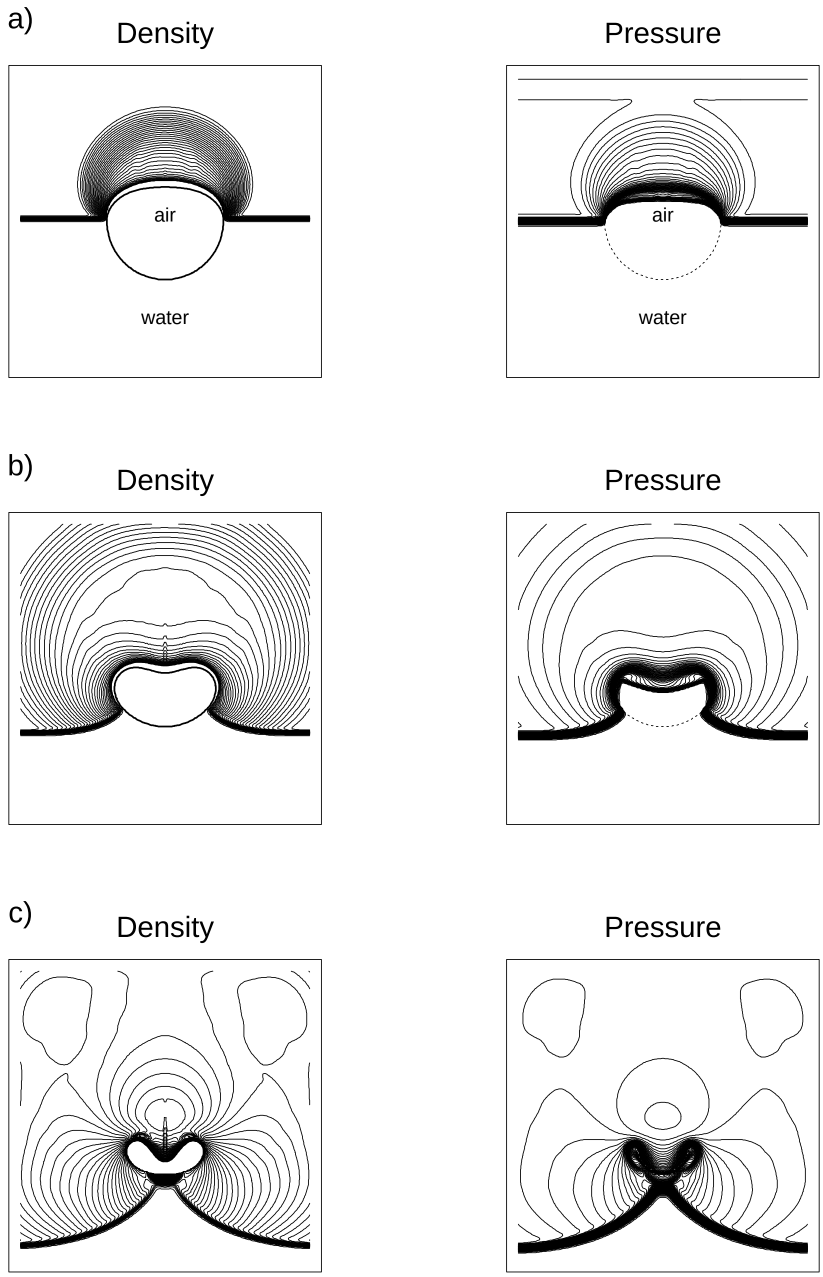

FIGURE 2. High resolution results for a planar Mach 1.587 shock wave in water over a bubble of air. Contours of the density ρ and the pressure p are shown (in logarithmic scale) at three different times. (a) at time $t = 0.001$ (b) at time $t = 0.002$. (c) at time $t = 0.003$. The dashed line in the pressure contour is the approximate location of the interface.