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Numerical simulation of compressible two-phase flow using a diffuse interface method

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ABSTRACT

In this article, a high-resolution diffuse interface method is investigated for simulation of compressible two-phase gas–gas and gas–liquid flows, both in the presence of shock wave and in flows with strong rarefaction waves similar to cavitations. A Godunov method and HLLC Riemann solver is used for discretization of the Kapila five-equation model and a modified Schmidt equation of state (EOS) is used to simulate the cavitation regions. This method is applied successfully to some one- and two-dimensional compressible two-phase flows with interface conditions that contain shock wave and cavitations. The numerical results obtained in this attempt exhibit very good agreement with experimental results, as well as previous numerical results presented by other researchers based on other numerical methods. In particular, the algorithm can capture the complex flow features of transient shocks, such as the material discontinuities and interfacial instabilities, without any oscillation and additional diffusion. Numerical examples show that the results of the method presented here compare well with other sophisticated modeling methods like adaptive mesh refinement (AMR) and local mesh refinement (LMR) for one- and two-dimensional problems.

1. Introduction

Numerical simulation of multiphase or multi-component flow is a challenging subject with many applications in industry and in modeling natural phenomena. For example, multiphase or multi-component flows are significant in the physics of explosion, astrophysics, supersonic combustion systems, the detonation of high energy material and shock wave treatment of cancer in the medical industry. The models and numerical simulations presented in recent literature present different levels of accuracy and complexity. In general, these types of methods can be separated into two categories by how each considers the interfaces:

1. Sharp interface method (SIM)
2. Diffuse interface method (DIM)

In the sharp interface methods, a special effort is made to find the right location of the interface and to treat the interface explicitly. This method includes: general types of Lagrangian methods (Shopov et al., 1990); Euler methods, including the level set and VOF approaches (Pilliod and Puckett, 2004; Sethian, 1996; Osher and Fedkiw, 2001; Hu et al., 2009) combined Euler–Lagrangian methods, including front tracking and front tracking with ghost fluid approaches (Unverdi and Tryggvason, 1992; Terashima and Tryggvason, 2009, 2010), ALE[1] methods (Doneal et al., 2004; Anbarlooei and Mazaheri, 2009) and MMIT[2] methods (Quan and Schmidt, 2007). The main weaknesses of these methods are high complexity, high computational cost, long CPU time and failure in interface prediction when the phenomena has no beginning or initial state for the interface (Saurel and Le Metayer, 2001). It should be emphasized that the ability to dynamically create interfaces that are not present initially is very important for flows with cavitations. For complicated interface conditions, the above-mentioned methods exhibit numerical diffusion and high numerical inaccuracy. Additionally, it is difficult to develop them to higher spatial cases (2D or 3D). Recently Chang and Liou (2007) have developed a stratified flow model that is capable of modeling compressible gas–liquid flows. However, the implementation of their method is highly complex.

In the second group of numerical methods, DIM, the interface is modeled as a numerically diffused zone (area), which is similar to capturing a discontinuity in gas dynamics (Saurel and Le Metayer, 2001). In fact, it can be mentioned that this type of diffused interface is a kind of artificial diffusion that is created by numerical calculations. These methods are divided into two general categories: those based on the Euler equations and those based on multiphase equations. The works based on the Euler equations include (Johnsen

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[1] Arbitrary Lagrangian–Eulerian.
[2] Moving mesh interface tracking.

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and Colonius, 2006; Kawai and Terashima, 2010; Shyue, 1998, 2010). These methods are restricted to applications in simple physical models with simple state equations. These methods are inaccurate in estimating the internal energy and temperature at the interface. The other category of models is based on multiphase equations (Abgrall, 1996). The most complete model is the seven-equation model introduced by Saurel and Abgrall (1999). This model contains two velocities and two pressures and is efficient for problems where the difference of phasic velocities is important. Application of this model can present challenges due to non-conservative terms in the momentum, energy and volume fraction advection equations. In this basis many effort has been spent for modeling with this model (Munkejord, 2010; Tokareva and Toro, 2010; Dumbser and Toro, 2010). Another convenient model for simulation is the single-velocity six-equation model. This model is obtained by assuming the velocity relaxation time to be zero and was first introduced by Kapila et al. (2001). This model shows good capability in simulating two-phase flow with an interface when validated by Saurel et al. (2009). Another model that is suitable for multiphase flow simulation is the reduced five-equation model, also known as the Kapila model (Kapila et al., 2001; Murrone and Guillard, 2005). There are two main problems in using this model. First, the mixture sound velocity at the interface has non-monotonic behavior. Second, the volume fraction equation has a non-conservative term (Saurel et al., 2009). This model consists of two mass conservation equations, one momentum conservation equation, one energy conservation equation in the conservative form and one volume fraction advection equation in the non-conservative form. Recently, efforts to propose a suitable numerical method for the five-equation model have increased (Kreeft et al., 2010; Qamar and Ahmed, 2009; Kokh and Lagoutière, 2010). Murrone et al. (2005) applied the reduced five-equation model for two-phase flow simulation. In their two-dimensional test cases, the velocities were low, and the shock wave interaction with the interface of the two-phase flow was not considered. Kreeft and et al. (2010) presented a new version of the five-equation Kapila model. Their model was well behaved for two-dimensional compressible gas–gas flows. However, the model behavior for a two-dimensional gas–liquid interface was not demonstrated. Deledicque and Papalexandris (2007) suggested a conservative approximation for the five-equation model. This method is suitable for modeling of two-pressure solid–gas models or two phases with big differences in the material properties. This model has limited application and can only be used for two-phase solid–gas flow. Saurel et al. used the five-equation model in several recent studies (Petitpas et al., 2007, 2009; Saurel et al., 2007). In these studies, a new method and a new theory are added to the model based on shock wave relationships. In fact, their method is based on the development of a relaxation-projection method for the Euler equations. The projection method is an indirect method for differentiation of the advection equation. This method is more efficient than previous methods, but it is more difficult to implement and extend to unstructured grids. The main objective of the present work is to accurately simulate two-phase gas–gas and gas–liquid interfacial problems, as well as cavitation flow problems, with less computational cost by using reduced five-equation models. In this study, the HLLC Riemann solver is used for numerical simulation of compressible two-phase flow. To circumvent the inherent difficulties in solving the five-equation models outlined earlier, the following four steps were taken:

- Using appropriate sound velocity with less non-monotonic behavior, the wood sound relation is not applicable.
- A suitable discretization of the advection equation.
- Preventing negative pressure during numerical calculation of cavitation zones due to strong rarefaction waves reflecting from free surfaces by adapting a suitable cavitation equation of state.
- Numerical simulation of the governing equations using the Godunov numerical method and the HLLC solver.

In this article, the mathematical properties of the five-equation model and the Schmidt cavitation model are presented in Section 2. The numerical method is explained in detail in Section 3. The development of the model from the one- to two-dimensional case with second-order accuracy is presented in Sections 4 and 5. Finally, model verification and simulation results in one and two dimensions are presented in Section 6 and concluding remarks are presented in Section 7.

2. Kapila two-fluid flow model

The single speed, equal pressure, five-equation model is also known as the reduced five-equation, or Kapila, model. This model is the reduced model of Baer and Nunziato (1986). The multi-space governing equations of this model, with the exclusion of heat and mass transfer, are as follows:

$$\frac{\partial \alpha}{\partial t} + \vec{u} \cdot \vec{\nabla}\alpha = 0 \tag{1a}$$

$$\frac{\partial(\alpha_1\rho_1)}{\partial t} + \nabla \cdot (\rho_1\alpha_1\vec{u}) = 0 \tag{1b}$$

$$\frac{\partial(\alpha_2\rho_2)}{\partial t} + \nabla \cdot (\rho_2\alpha_2\vec{u}) = 0 \tag{1c}$$

$$\frac{\partial(\rho\vec{u})}{\partial t} + \nabla \cdot (\rho\vec{u} \otimes \vec{u}) + \vec{\nabla}P = 0 \tag{1d}$$

$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot ((\rho E + P)\vec{u}) = 0 \tag{1e}$$

where $\alpha, \rho, \vec{u}, P, E, e$ are the volume fraction, density, velocity vector, pressure, total energy and internal energy, respectively. The density is obtained from

$$\rho = (\alpha_1\rho_1 + \alpha_2\rho_2) \tag{2}$$

The two-phase mixture internal energy is calculated from

$$e = Y_1 \cdot e_1(\rho_1, P) + Y_2 \cdot e_2(\rho_2, P) \tag{3}$$

where

$$Y_K = \frac{(\alpha\rho)_k}{\rho} \tag{4}$$

where the subscript $k = 1, 2$ representing gas or liquid phase, respectively. In the present work, the stiffened-gas equation of state (SGS) is used. In the equal-pressure condition, the internal energy of phase, $e_k = e_k(\rho_k, P)$, is calculated using the following equation:

$$\forall k, \quad \rho_k e_k = \frac{P + \gamma_k \cdot P_{\infty,k}}{\gamma_k - 1} \tag{5}$$

where γ_k and $P_{\infty,k}$ are constant parameters of stiffend gas equation of state and are different for each fluid. The following equation for pressure is used to close the set of equations:

$$P(\rho, e, \alpha_k) = \frac{\rho e - \sum_k \frac{\alpha_k\gamma_k P_{\infty,K}}{\gamma_k - 1}}{\sum_k \frac{\alpha_k}{\gamma_k - 1}} \tag{6}$$

For this model the mixture sound velocity is defined as

$$c = \sqrt{\frac{\gamma \cdot (P + P_\infty)}{\rho}}$$

$$\frac{1}{\gamma - 1} = \sum_k \frac{\alpha_k}{\gamma_k - 1}$$

$$\frac{\gamma . P_\infty}{\gamma - 1} = \sum_k \frac{\alpha_k\gamma_k P_{k\infty}}{\gamma_k - 1} \tag{7}$$